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Monograph No. 3

Vibrational and Electronic Energy Levels of Polyatomic Transient Molecules

Marilyn E. Jacox

*National Institute of Standards and Technology
Gaithersburg, Maryland 20899-0001*


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Jean W. Gallagher, Editor

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Foreword

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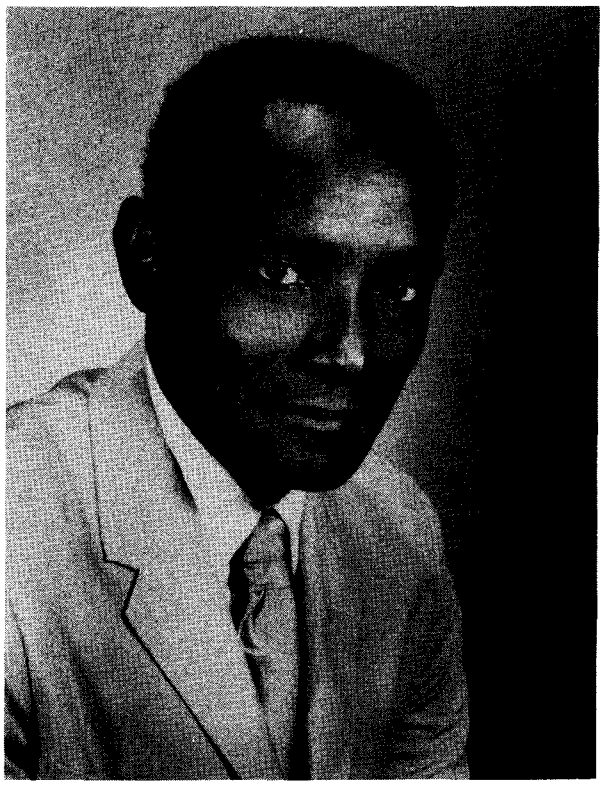
The regular issues of the *Journal of Physical and Chemical Reference Data* are published bimonthly and contain compilations and critical data reviews of moderate length. Longer works, volumes of collected tables, and other material unsuited to a periodical format have previously been published as *Supplements to the Journal.* In 1989 the generic title of these works was changed to *Monograph,* reflecting their character as independent publications. This volume, "Vibrational and Electronic Energy Levels of Polyatomic Transient Molecules" by Marilyn E. Jacox, is presented as *Monograph No. 3* of the *Journal of Physical and Chemical Reference Data.*

Jean W. Gallagher, Editor
Journal of Physical and Chemical and Reference Data



Dolphus E. Milligan

This monograph is dedicated to the memory of the late Dr. Dolphus E. Milligan, whose insight and perseverance contributed greatly to the development of the matrix isolation technique for obtaining vibrational and electronic spectra of free radicals and molecular ions.

Vibrational and Electronic Energy Levels of Polyatomic Transient Molecules

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A critical evaluation and summary of the experimentally determined vibrational fundamentals and electronic band origins of more than 1550 neutral and ionic transient molecules possessing from three to sixteen atoms is presented. Data are included for species containing the heavy elements. Although the emphasis is on species with lifetimes too short for study using conventional sampling techniques, there has been selective extension of the compilation to somewhat less reactive species such as OClO, HNCO, H_2O_2, *cis*- and *trans*-HONO, and $HONO_2$ which have presented spectral evaluation problems and which are important in a wide variety of environmental and industrial chemical systems. Radiative lifetimes and the principal rotational constants are included. Observations in the gas phase, in molecular beams, and in rare-gas and nitrogen matrices are evaluated. The types of measurement surveyed include conventional and laser-based absorption and emission techniques, laser absorption with mass analysis, and photoelectron spectroscopy.

Key words: electronic energy levels; emission spectra; experimental data; free radicals; gas phase; infrared spectra; laser-excited fluorescence; matrix isolation; molecular ions; photoelectron spectroscopy; polyatomic molecules; radiative lifetimes; Raman spectra; rotational constants; transient molecules; ultraviolet absorption; vibrational energy levels.

[a] Technology Administration, U.S. Department of Commerce.

Contents

1. Introduction

Most chemical processes—including not only laboratory and industrial chemical syntheses but also those which occur in flames, propellant systems, the initiation of energetic materials, atmospheric pollution, chemical vapor deposition, and plasma processing—consist of a complicated sequence of interrelated reactions in which neutral and charged molecular fragments play essential roles. Although these fragments are present in only very small concentration, they are highly chemically reactive. If a specific molecular fragment is removed from the system, as by introducing a scavenger molecule, the reactions in which that fragment participates stop. Other parts of the overall process continue, resulting in very significant changes in product distribution and yield.

In the early studies of complex chemical processes, it was necessary to postulate mechanisms involving such transient intermediates, present in concentrations too small for direct detection. Conventional end product analysis has provided much valuable information regarding the validity of the proposed mechanisms, but generally does not yield a complete description of the system. Consequently, the improvement of industrial chemical processes often is achieved by semiempirical experimentation. The determination of the detailed chemical mechanism would, in turn, permit the development of rational strategies for removing undesired products and enhancing the yield of the desired species.

In recent years, there has been great progress in the development of techniques suitable for monitoring chemical reaction intermediates. Molecular spectroscopy is especially well suited to this task. Optical detection can be used not only for gas-phase measurements, but also for studies of processes which occur on surfaces or in the condensed phase. Furthermore, it affords the important advantage of permitting remote sensing. A wide variety of recently developed laser-based spectroscopic detection schemes are not only highly sensitive but also space and time specific. Although the development of spectroscopy-based diagnostics for chemical reaction systems is in its infancy, already the laboratory application of sophisticated sampling and observation techniques has yielded a wealth of vibrational and electronic spectral data for reaction intermediates.

For many years, the most important source of vibrational and electronic energy level data for small polyatomic reaction intermediates was the compilation of spectroscopic data for small polyatomic molecules (3–12 atoms) given by Herzberg.[1] To meet the need for an updated, critically evaluated compilation of the ground-state vibrational energy levels of small polyatomic reaction intermediates, the first publication in this series,[2] which provided data for approximately 480 transient molecules possessing from three to sixteen atoms, appeared in 1984. A second compilation,[3] concerned with the electronic energy levels of approximately 500 transient molecules possessing from three to six atoms, was published in 1988. Vibrational fundamentals in the ground and excited electronic states and radiative lifetimes were included. To aid in spectral identification, the principal rotational constants were also given to three decimal places. For many of the approximately 150 species common to the two sets of tables, significant revisions of the ground-state vibrational energy levels occurred in the four-year period between the two compilations. In late 1990, a supplement to the two earlier compilations was published.[4] This supplement presented new data for approximately 500 molecules, with selective extension to species which contain heavy atoms and to electronic energy levels of important species with more than six atoms. In order to avoid redundancy, where a molecule had been considered in one of the earlier compilations only the more recent material was included. The master index, which facilitated access to the earlier material, included approximately 1200 molecules. These tables have provided the basis for a software database for personal computers (Vibrational and Electronic Energy Levels of Small Polyatomic Transient Molecules, National Institute of Standards and Technology Standard Reference Database 26), designed to supplement the published compilations by providing a capability for rapid searches by molecule or wavenumber. The 1992 upgrade of this database included information on 1334 molecules.

The rapid growth in the scientific literature concerned with the spectroscopic study of transient molecules and with their detection in chemical reaction systems continues. In addition, there has been great progress in the spectroscopic characterization of small metal clusters and of the transient species produced by the reaction of metal atoms with small molecules. With the need for a scientific base to support new technologies such as those of plasma processing and chemical vapor deposition, studies of reaction intermediates which contain the heavier elements have also multiplied rapidly. This volume attempts to provide a comprehensive, critically evaluated summary of currently available data on the vibrational and electronic energy levels of small polyatomic transient molecules, in order to support further research.

2. Scope of Review

This review provides a critical evaluation of the vibrational and electronic spectral data available through early 1993 for more than 1550 small polyatomic transient molecules. This number represents a considerable increase over the total number of species present in the master index of the 1990 publication in this series.[4] Despite the considerable growth in the literature, perusal of the tables in this volume will reveal many gaps in our knowledge of the energy levels of the species represented, and many new and potentially important transient molecules remain to be discovered.

Data have been selectively included for some molecules which are important in environmental and industrial chemical reaction systems but which can be studied only with difficulty using conventional sampling techniques because of the ease with which they

decompose, rearrange, or polymerize. Among these species are HOF, HOCl, OClO, HNCO, HCNO, H_2O_2, H_2S_2, O_2F_2, FN_3, *cis*- and *trans*-HONO, and $HONO_2$. In view of the growing importance of reaction intermediates which contain atoms of the heavier elements, such species are also included. The coverage of electronic spectral data for transient molecules with from seven to sixteen atoms has been greatly expanded, and a section reporting both vibrational and electronic spectral data for molecules related to benzene has been created.

3. Types of Measurement

Studies in the gas phase offer the potential for the most precise, detailed measurements. Because of the high chemical reactivity of transient molecules, it is difficult to obtain gas-phase survey infrared spectra of them. The well known advantages of Fourier transform infrared measurements, coupled with sophisticated digital data handling procedures, have permitted the acquisition of gas-phase survey spectra for a few transient molecules.

Although vibrational frequencies of ground-state molecular ions have frequently been estimated from structure in Rydberg transitions of the parent neutral species, such data are not included in this compilation, since many of these transitions have residual valence character, resulting in significant variations in vibrational frequencies from one Rydberg state to another.

As in the earlier compilations, spectral data obtained in rare gas and small covalent molecule matrices are included. The application of matrix isolation sampling for the stabilization and spectroscopic study of uncharged reaction intermediates has recently been reviewed.[5] Because nitrogen and the rare gases are transparent through the entire infrared spectral region, matrix isolation measurements provide a potentially valuable survey tool. In these matrices, infrared absorptions are typically sharp, with half band widths between 0.1 and 1 cm^{-1}. Rotational structure is, with few exceptions, quenched. Multiple trapping sites occur, often resulting in the appearance of several absorption maxima—usually one or two of which predominate—over a range of a few cm^{-1}.

Matrix shifts for molecules trapped in solid neon or argon often are quite small. A comparison[6] of the positions of the ground-state vibrational fundamentals of over two hundred diatomic molecules observed in the gas phase and in nitrogen and rare-gas matrices has shown that, typically, the smallest matrix shift occurs for neon matrix observations, with successively greater matrix shifts for the heavier rare gases and for nitrogen. Except for very weakly bonded molecules and for the alkali metal and Group IIIa halides, matrix shifts of most diatomic molecules isolated in solid argon are smaller than 2%. The generalization that matrix interactions are minimal for neon and that they increase as the mass of the rare gas is increased and become even more important for nitrogen and other small molecule matrices is supported both by experimental observations on larger molecules and by recent *ab initio* calculations[7] for the weakly bonded CaH_2 and CaF_2 molecules complexed with the rare gases and with nitrogen. Fig. 1 compares the observed matrix shifts for the ground-state fundamental vibrations of both neutral and charged transient molecules trapped in solid neon and argon. For both matrices, the maximum in the distribution lies near 0.0%, and most of the matrix deviations from the gas-phase values amount to less than 1%. In an argon matrix, shifts greater than 1% occur for only about 10% of the frequencies available for comparison. For molecular ions, neon is the matrix of choice. Polarization and charge-transfer interactions become successively more important for the heavier rare gases. Charge delocalization sometimes also occurs for ionic species trapped in the rare gases.[8,9] The anomalously large matrix shift for ν_3 of $ClHCl^-$ may be attributed to this phenomenon. Until very recently, the matrix shift data for molecular ions was heavily weighted by data for the halogen-substituted benzene cations. New data for smaller cation species trapped in solid neon are consistent with the matrix shift generalization given above. Very few comparisons are possible for molecular anions. A number of these species have been generated in rare-gas (usually argon) matrices by charge transfer between a precursor molecule and an alkali metal atom. Recent studies of such species as CO_2^- and SO_2^- generated instead by photoionization and/or Penning ionization and trapped in solid neon indicate that shifts on the order of 50 cm^{-1} may be attributed to the relatively strong interaction of the anion with the nearby alkali metal cation. On the other hand, when the uncharged molecule has a relatively large electron affinity, as is true for C_2 and for NO_2, charge transfer occurs at a relatively great separation, and a substantial fraction of the anion population may be trapped in sites in which interaction with the alkali metal cation is minimal.

Many other matrix materials have also been employed for spectroscopic studies. However, complications due to reaction or to relatively strong interaction (e.g., hydrogen bonding) of the transient molecule with the matrix frequently occur. Therefore, observations in such media as solid hydrocarbons and aqueous solutions and studies of condensed reaction products without an inert carrier have been excluded.

Because of the prevalence of electronic emission spectra and the sensitivity, rapid time response, and cumulative detection capability of the photographic plate in the visible and ultraviolet spectral regions, the study of the electronic spectra of gas-phase reaction intermediates has a comparatively long history. Flash photolysis has permitted the preparation of relatively high concentrations of transient species. Many electronic band systems of gas-phase transient molecules have been discovered through flash photolysis studies. More recently, a wide variety of laser-based techniques have also been used for electronic spectral observations, often with exceptionally high detection sensitivity. The spatial configuration of the laser beam makes it an extremely powerful tool for studies of the energy levels of molecules in molecular beams and gives it great promise for application in the

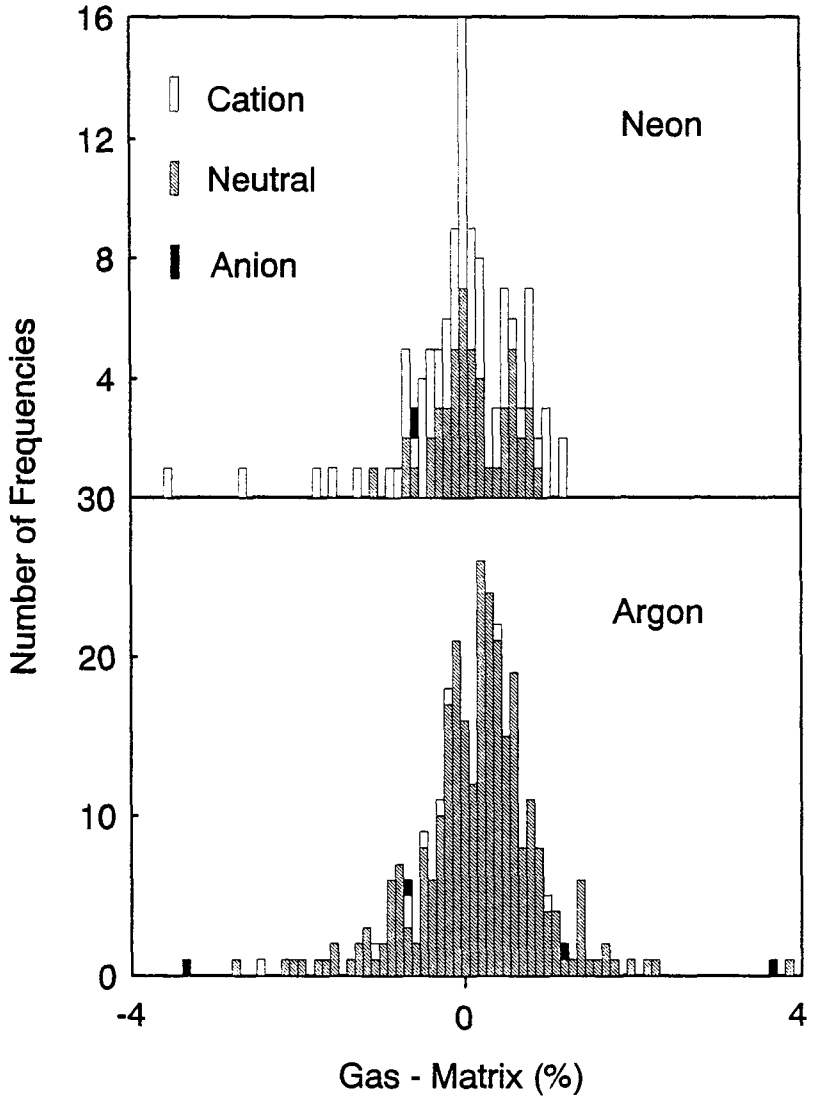

FIG. 1. Ground-state vibrations of transient molecules.

development of probes for chemical reaction intermediates in the environment, the laboratory, and the industrial plant. Laser studies may be broadly classified according to whether the interaction of the molecule with the laser beam(s) is followed by photon or mass detection. Photon-based observations are amenable to remote sensing applications. Because pulsed lasers offer an exceptionally wide range of time specificity, they are very useful for determining radiative lifetimes and rates of elementary chemical reactions.

Much valuable information on the energy levels of molecular cations has been obtained from photoelectron spectroscopy. Selective coverage of the voluminous literature on photoelectron spectroscopic measurements is employed in these tables. The number of stable molecules which possess more than six atoms for which photoelectron spectra have been reported is too great to permit the inclusion of low-to-moderate resolution photoelectron spectral data for molecular cations with more than six atoms. Those who need such data for larger molecules may find the reviews by Turner et al.,[10] Rabalais,[11] and Kimura et al.[12] helpful. An effort has been made to choose the best data available for each molecule. Several criteria are important in determining whether a given reference should be included. The first criterion is resolution. In the few instances in which high resolution photoelectron data are available, these are heavily weighted. Where direct spectroscopic observation is possible, the results of such measurements generally are of considerably higher precision than are photoelectron data, which are then omitted from the tables. A second criterion is the availability of adiabatic ionization potentials. In order to obtain information on the positions of electronic transitions from photoelectron spectral data, it is necessary to subtract the first ionization potential from the energy of the photoelectron band. Where there is

little change in the molecular geometry in the transition, the difference between the vertical ionization potentials gives a reasonable approximation to the position of the electronic transition. However, this is not the general case. Therefore, priority is given to papers which include adiabatic ionization potentials.

For most photoelectron spectroscopic transitions, structure has not been resolved. Many of these states are dissociative. Further information on the dissociation products can be obtained from values of the appearance potentials for various products in photoionization studies on the parent molecule. Such studies are beyond the scope of this review. The tables of ionization and appearance potentials by Lias and co-workers[13,14] constitute a valuable source of information on the appearance potentials of photofragments.

The range of tunability of visible and ultraviolet lasers, like that of infrared lasers, is limited. Therefore, a preliminary survey using conventional gas-phase and/or matrix-isolation spectroscopic studies is often desirable. A comparison of the positions of the electronic band origins of diatomic molecules in the gas phase and in rare-gas and nitrogen matrices has been published.[15] As in the determination of ground-state vibrational energy levels, neon is the matrix material of choice, with a sharp maximum at 0.0% in the distribution of matrix deviations for valence transitions of covalently bonded molecules. In argon-matrix observations, most such band origins are shifted by less than 2% from the gas-phase values. At the somewhat higher temperatures often used for electronic spectral observations in matrices of the heavier rare gases or of nitrogen, relatively broad phonon bands become prominent. The blue shift of the phonon maximum from the zero-phonon line in absorption measurements, and the red shift in emission measurements, typically amount to approximately 1 to 1.5%. Rydberg transitions of molecules in matrices often are greatly broadened and experience much larger shifts. Further details of the behavior of electronic transitions of matrix-isolated molecules have previously been discussed.[3,5,15]

Contrary to earlier expectation, the radiative lifetime of a relatively large molecule isolated in a rare-gas matrix is frequently related to the radiative lifetime in the gas phase by a simple refractive index correction.[16] In a neon matrix, such a correction typically decreases the radiative lifetime by about 15%. For such molecules, often intramolecular mechanisms for nonradiative energy transfer are available both in the gas phase and in the matrix. On the other hand, the density of excited states is much lower for small molecules, and matrix shifts may alter perturbation interactions between strongly coupled electronic states, providing a path for nonradiative deactivation. In this circumstance, fluorescence which is prominent in the gas phase may even be completely quenched in the matrix.

4. Guide to the Compilation

The goal of this compilation is to provide a comprehensive, critically evaluated compilation of vibrational and electronic spectroscopic data for small polyatomic transient molecules. The literature has been surveyed through March 1993; only limited addition of more recent data has been possible. Unfortunately, it is not possible to include data for stable molecules, with a few exceptions such as OClO and $HONO_2$. However, the spectra of many of these species are relatively well established, and sources of data such as the tables of Herzberg[1] and Shimanouchi[17] remain extremely useful. In obtaining spectral identifications with the help of the present compilation, it is crucial that the possible contribution of absorptions or emissions by a stable molecule also be considered.

Considerable effort has been expended to provide a critical evaluation of the data. However, for many species the available data are meager. The identities of some species have been proposed on the basis of chemical evidence. While such evidence may be quite compelling, it is not definitive. Many examples could be cited in which a spectrum was later reassigned to characteristic impurities in the sample. Where chemical evidence has provided a reasonable basis for the assignment of vibrational or electronic bands to a transient molecule, data have been included in this compilation, in the hope that further testing of the assignment will be facilitated.

While every effort has been made to make these tables as complete as possible, for various reasons omissions do occur. There remains some selectivity in the coverage of electronic spectral data for larger molecules. It is planned to support this database, with further selective extension, by the preparation of periodic supplements. Data from the earlier tables have sometimes been omitted from this monograph because more recent data dictate a reassignment or because there has been a subsequent refinement. An important example of this latter situation is the replacement of low resolution photoelectron spectral data by spectroscopic studies with appreciably higher resolution and greater precision. Candidate molecules or energy levels may also have been inadvertently omitted. Suggestions of additions or needed revisions to the data to be included in subsequent extensions of this database are welcome, as are inquiries regarding new data added after the publication cutoff data for this compilation.

Molecular formulas are used in this compilation. In order to permit a compact index, an attempt has been made to provide as much structural information as possible in a minimal amount of space. This restriction is especially severe for larger molecules. The following formula abbreviations have been used:

br bridged

cyc cyclic. If parentheses follow, only the atoms enclosed in them are included in the ring.

c cis

t trans

Where several isotopic peaks are resolved, data are given for the most abundant isotopic species (e.g., ^{7}Li, ^{11}B, ^{35}Cl, ^{79}Br).

As in the earlier compilations, the tables are grouped by the number of atoms in the molecule and, secondarily, by the number of hydrogen atoms present. Molecules within a given section of the tables are arranged in the order of increasing number of valence electrons. For species with the same number of valence electrons, molecules with a simple chain of three heavy atoms are listed in the order, first, of the number of valence electrons in the central atom of the chain and, second, of the row which this atom occupies in the Periodic Table. For larger molecules, the sequence is somewhat arbitrary, but criteria of increasing molecular size and grouping in the Periodic Table (e.g., the order N, P, O, S) are used. Halogen-substituted species are placed immediately after the related hydrides. Data for molecules related to benzene are presented in a separate section. As in the earlier tables, data are included for both the normal and the fully deuterium-substituted molecule. However, only the hydrogen-containing species is listed in the index.

The heading for each electronic state gives its symmetry, the point group to which the molecule belongs in that electronic state, and, where available, references to the determination of a quantitative molecular structure. For C_{2v} molecules, there is potential ambiguity in the definition of the molecular symmetry axes. The convention in which the x axis is chosen perpendicular to the plane of the molecule, recommended by the Joint Commission for Spectroscopy of IAU and IUPAP,[18] has been adopted. Often this has required the interchange of published assignments of energy levels with B_1 and B_2 symmetry.

Most authors of papers on photoelectron spectroscopy have proposed assignments for the various photoelectron bands, using arguments based on molecular orbital theory and often on semiempirical or *ab initio* calculations. These assignments have been included in the present tables. Where several conflicting assignments have been given in the literature, an attempt has been made to choose the most satisfactory one. Generally, the assignments of photoelectron spectra have been made with the presumption that the point group to which the molecular cation belongs is the same in all of its excited states. Structural data for these excited states are extremely rare. Therefore, the molecular point group which has been adopted in the analysis of the photoelectron spectrum is given in these tables. In practice, it is likely that there is some variation in excited-state molecular symmetries. Thus, a bent molecular ion may become linear in some of its excited states. For highly symmetric species, Jahn-Teller distortion may reduce the molecular symmetry.

The energy of the electronic transition follows the state designation and symmetry information. Where possible, T_0, the energy separation between the electronic energy level of interest and the ground electronic, vibrational, and rotational states of the molecule, is given. However, where only low resolution data or photoelectron data are available, often only band maxima have been given in the literature. With photoelectron data, T_0 is derived by subtracting the value of the first ionization potential from that of the higher ionization potential which corresponds to the state of interest. When data for the first adiabatic ionization potential are available, the footnote phrase "from vertical ionization potential" implies that the first adiabatic ionization potential is known but that the higher ionization potential is measured to the peak maximum; the phrase "from vertical ionization potentials" implies that the energy difference between the higher and the first absorption maximum was used. If the first photoelectron transition has a gradual onset, a better value of the first ionization potential may have been obtained from photoionization data or from the extrapolation of Rydberg series in the spectrum of the parent molecule. Supplementary sources of data for the first ionization potential are cited in the tables. However, if the difference between the first adiabatic ionization potential obtained in the photoelectron spectrum and that obtained in other measurements amounts to only 10 or 20 meV, the photoelectron spectroscopic value is used, because of the advantage of a consistent set of measurements. Where threshold energies differ by one quantum in a vibrational progression, a best value for the ionization potential is chosen which coincides with the most probable position of the vibrationally unexcited transition. Because of inherent uncertainties in the determination of higher ionization potentials in many photoelectron spectral measurements, photoelectron peaks above about 18 eV are often omitted. Except where otherwise indicated, the units of all quantities in these tables are cm^{-1}. Error estimates are those of the authors of the original literature. The numbers in parentheses give these estimated errors in relation to the last digits of the electronic or vibrational frequency (e.g., $1234.567(89) \equiv 1234.567 \pm 0.089$). Where the error includes a decimal point, the decimal point is retained inside the parentheses. When the uncertainty is not explicitly indicated, the value is given to the estimated number of significant figures. As in the tables of Herzberg,[1] T_0 values are given to the center of multiplet structure. For doublet states, the two components differ by $\pm A$ (the spin-orbit splitting constant), and the energy difference is measured from the average of the two bands, whereas for triplet states the three components fall at 0, $\pm A$ with respect to the position from which the band energy is measured. This convention is also followed here unless specific states are given. However, in matrix isolation absorption and laser excitation studies only the lowest component is accessible.

Except for transitions with relatively small values of A, this is also likely to be true for studies using cooled molecular beams. Often these latter studies give T_0 values for the lowest energy component with a precision better than that to which A is known.

The wavelength range (nm) in which various electronic transitions have been observed is also tabulated. This range is a composite of the values typical of absorption and emission observations. Laser-excited fluorescence studies often include both excitation and resolved emission measurements. Since the position of the band origin is given, ambiguity should not arise. For information on the range in which the band system is observed for a given type of measurement, see the original literature cited for that measurement technique.

The format of the vibrational tables is similar to that used in the earlier compilations. The vibrational numbering convention is that used by Herzberg.[1] Within a given symmetry species, vibrations are numbered starting with the highest frequency. The same convention is followed for deuterated species. Therefore, a given type of vibration may be numbered differently for the deuterated than for the unsubstituted molecule. For triatomic molecules, the bending vibration is always designated as ν_2. For aromatic molecules, an alternate vibrational numbering scheme developed by Wilson[19] has often been used in the literature. Where both the Herzberg and the Wilson numbering schemes have been used for the published data, the Herzberg numbering is adopted, and the Wilson numbering is sometimes shown in parentheses. For a few species, only the Wilson numbering has been used. To avoid confusion, this is retained in the present tables, and the use of the Wilson numbering is indicated in a footnote. Where possible, the values of $\Delta G(1/2)$, the separation between the $v = 0$ and $v = 1$ levels for the vibration of interest, have been used. The expression of uncertainties is similar to that described for electronic band origins. Where vibrational frequencies have been determined with a precision greater than two decimal places, the tabulated values have been rounded off. If a bending fundamental is split by Renner-Teller interaction, the position of the unperturbed fundamental is given. Where specific components of such a split fundamental have been studied, they may also be listed, with the transition designated in a footnote. For a more complete treatment of the Renner effect and definitions of the parameters included in many of these footnotes, see the discussion by Herzberg[1] and the references cited for the molecule of interest. A few of the species in these tables possess out-of-plane vibrations which have resolved inversion splitting structure. For these, the specific component for which the vibrational frequency is reported is designated in a footnote. Relative intensities of vibrational bands are dependent on the technique used for the measurement. When possible, the relative intensities of *ground-state infrared absorptions* are included. It is not feasible to give the corresponding relative intensities for other types of observation. Relative intensity abbreviations include:

vw	very weak
w	weak
m	medium
s	strong
vs	very strong
sh	shoulder
br	broad

Where radiative lifetimes have been measured, they are cited following the vibrational energy level table for the appropriate electronic state. τ_0, the radiative lifetime of the vibrationless transition, is given whenever possible. If the lifetime is accessible only for excited vibrational states, the subscripts give the vibrational quantum numbers of the observed band.

When spin-orbit splitting occurs and the splitting constant, A, is known, it is included in the compilation.

Finally, as an aid in the recognition of vibrational bands and electronic band systems observed with comparatively high resolution, the principal rotational constants are summarized. Where possible, the values associated with the vibrationless transition (A_0, B_0, C_0) are given. Occasionally these values have not been determined, and the subscript gives the vibrational quantum numbers appropriate to the band for which the rotational constants have been measured. These constants are truncated at three decimal places. Often a far more detailed set of molecular constants, with much greater precision, has been derived from the analysis of high resolution spectra. Microwave spectroscopy is an important source of detailed, highly precise rotational data for molecules in their ground states. The references to the experimental literature which are included in the compilation should facilitate the location of such high resolution data.

5. Abbreviations

Many sophisticated laser techniques—frequently employing two or more laser beams—have been used for studies of transient molecules. The laser is frequently used both in the preparation of the transient molecule and in the detection scheme. For example, ions may be generated by multiphoton ionization and detected by absorption of radiation from a probe laser. Often the developers of such techniques have designated them by complicated acronyms. In these tables, an attempt has been made to avoid relatively lengthy and unfamiliar acronyms by designating only the generic type of detection, using the abbreviations defined below. (Velocity modulation, designated as a separate detection technique in the first of this series of data evaluations,[2] is widely used and is considered to be a measurement tool rather than a type of observation. The type of laser used for the absorption measurement in an infrared detection scheme employing velocity modulation is instead specified in these tables.)

AB	near infrared-visible-ultraviolet absorption
CC	color-center laser
DL	diode laser absorption
DPI	depletion photoionization
ED	electron diffraction
EF	electron-excited fluorescence
EM	near infrared-visible-ultraviolet emission
ESR	electron spin resonance
HFD	high frequency deflection
IB	ion beam
ID	ion drift, ion depletion (see specific reference)
IR	infrared absorption (conventional or Fourier transform)
LD	laser difference frequency
LF	laser-excited fluorescence (excitation and resolved emission)
LMR	laser magnetic resonance
LS	laser Stark spectroscopy
MO	molecular orbital calculations
MODR	microwave-optical double resonance
MPI	multiphoton ionization
MW	microwave and millimeter wave
ND	neutron diffraction
PD	electron photodetachment
PE	photoelectron spectroscopy
PEFCO	photoelectron-photon coincidence
T-PEFCO	threshold photoelectron-photon coincidence
PEPICO	photoelectron-photoion coincidence
PF	photofragment spectroscopy
PI	photoionization
PIFCO	photoion-photon coincidence
PIR	photoionization resonance
Ra	Raman
SEP	stimulated emission pumping
TPE	threshold photoelectron spectroscopy, including ZEKE detection
UV	near infrared-visible-ultraviolet absorption and emission

6. Tables

6.1. H_3^+, H_3, and Triatomic Dihydrides

H_3^+

$\tilde{X}$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Ring breathing	3178.3[a]	gas	IR, PI LD	11,13,14 20
e'	2	Deformation	2521.31[a]	gas	LD,IR	1,4,16

$B_0 = 43.571(5)$; $C_0 = 20.62$ LD[1,4]DL[4]IR[11]

H_2D^+

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Ring breathing	2992.51	gas	LD	3,6,12
	2	Deformation	2205.87	gas	LD,DL	7
b_2	3	Deformation	2335.45	gas	LD,DL	7

A_0 = 43.438(2); B_0 = 29.134; C_0 = 16.601 LD,MW[6,7,12]

D_2H^+

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Ring breathing	2736.98	gas	LD	5,12,15
	2	Deformation	1968.17	gas	DL	9,15
b_2	3	Deformation	2078.43	gas	DL	9,15

A_0 = 36.199; B_0 = 21.869; C_0 = 13.070 LD[5,12,15]DL[9,15]

D_3^+

$\tilde{X}$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Ring breathing	2303[b]	gas	MO	8
e'	2	Deformation	1834.67	gas	IB,DL	2,10

B_0 = 21.824; C_0 = 10.510 DL[10]

[a] Hot bands arising from ν_1 and ν_2 of H_3^+ have been observed,[17,20] as have been the first[18] and second[19] overtones of ν_2.

[b] Ab initio calculation[8] of gas-phase band center. All other calculated band centers for the fundamentals of H_3^+ and its deuterium-substituted counterparts agree within 5 cm^{-1} with the observed band centers.

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H_3

Higher Rydberg states have been detected using photoionization and field ionization. The ionization limit observed for vibrationally and rotationally unexcited H_3 from its $2p\ ^2A_2''$ state is 29562.6(5).[12,15,16] Ion depletion studies have also yielded frequencies for the ring breathing vibration of a number of these higher Rydberg states.[23] Near the lowest ionization threshold, predissociation has been found to be induced by very weak electric fields.[25] Rotational and vibrational interactions, autoionization, and predissociation in the *np* Rydberg manifold have been studied.[27]

$3d\ ^2A_1'$ D_{3h} Structure: EM[8]

T_0[a] = 18511 gas EM[8]PF[26] $3d$–$2p^2A_2''$ 568–615 nm
EM[8] $3d$–$3p2E'$ 3891–4456 cm^{-1}
B_0 = 42.99; C_0 = 22.73 EM[8]

$3d\ ^2E''$ D_{3h} Structure: EM[8]

T_0[a] = 18409 gas EM[8]PF[14,26] $3d$–$2p^2A_2''$ 568–615 nm
EM[8] $3d$–$3p^2E'$ 3891–4456 cm^{-1}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Ring breathing	3168[b]	gas	PI	19,23
e'	2	Deformation	2518	gas	EM,PF	22

B_0 = 42.99; C_0 = 22.735 EM[8]

$3d\ ^2E'$ D_{3h} Structure: EM[8]

T_0[a] = 18037 gas EM[8] $3d$–$2p^2A_2''$ 568–615 nm
EM[8] $3d$–$3p^2E'$ 3891–4456 cm^{-1}
B_0 = 42.99; C_0 = 22.735 EM[8]

$3p\ ^2A_2''$ D_{3h} Structure: EM[3]

T_0[a] = 17789 gas EM[2,3,8] $3p^2A_2''$–$2s^2A_1'$ 556–574 nm
τ = 37(4) ns gas EM[10]
B_0 = 47.45; C_0 = 23.495 EM[8]

$3s\ ^2A_1'$ D_{3h} Structure: EM[6]

T_0[a] = 17600 gas EM[3]PF[13,14] $3s^2A_1'$–$2p^2A_2''$ 592–615 nm
EM[6] $3s^2A_1'$–$3p^2E'$ 3178–3847 cm^{-1}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Ring breathing	3212.1(3)[b]	gas	PI	19,23
e'	2	Deformation	2588(2)	gas	EM,PF	22

B_0 = 44.19; C_0 = 22.676 EM[6]

$3p\ ^2E'$ D_{3h} Structure: EM[6]

T_0[a] = 13961 gas EM[2,4] $3p^2E'$–$2s^2A_1'$ 708–736 nm
EM[6] $3s^2A_1'$–$3p^2E'$ 3178–3847 cm^{-1}
EM[8] $3d$–$3p^2E'$ 3891–4456 cm^{-1}
τ = 1.1(+0.2,−1.0) ns gas EM[21]
B_0 = 42.15; C_0 = 21.505 EM[6]

$2p\ ^2A_2''$ D_{3h} Structure: EM[6]

T_0[a] = 993 gas EM[3,6] $3s^2A_1'$–$2p^2A_2''$ 592–615 nm
EM[8] $3d$–$2p^2A_2''$ 568–615 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Ring breathing	3255.38(3)	gas	PI	17-19
e'	2	Deformation	2618.34(3)	gas	PI	18

B_0 = 44.58; C_0 = 22.288 EM[6]
τ_{00} = 640(+300,−100) ns; τ_{10} = 740(+300,−100) ns gas PI[24]PF[26]

$2s\ ^2A_1'$[c] D_{3h} Structure: EM[3]

gas EM[2,3] $3p^2A_2''$–$2s^2A_1'$ 556–574 nm
gas EM[4] $3p^2E'$–$2s^2A_1'$ 708–736 nm
B_0 = 46.82; C_0 = 23.41 EM[3]

H_2D

$3s\ ^2A_1$ C_{2v}
$\tau \cong 4$ ns gas EM[20]

$3p\ ^2B_1$ C_{2v}
τ = 29(3) ns gas EM[20]

$3p\ ^2A_1, {}^2B_2$ C_{2v}
τ = 2.5(+0.3,−0.7) ns gas EM[21]

D_2H

3s $^2A_1$ C_{2v}
$\tau \cong 5$ ns gas EM[20]

3p $^2B_1$ C_{2v} Structure: EM[9]
T_0[a] = 17834.4 gas EM[9] $3p^2B_1$–$2s^2A_1$ 560 nm
τ_1 = 31.5(3.2) ns; $\tau_2 \cong 8.9$ ns gas EM[20]

3p $^2A_1$, $^2B_2$ C_{2v}
τ = 5.0(7) ns gas EM[21]

2s $^2A_1$ C_{2v} Structure: EM[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a_1	1	Ring breathing	2950(20)	gas	EM	20

D_3

The ionization limit of D_3 with respect to the vibrationless level of its $2p\ ^2A_2''$ state has been found to be 29602.[21]

3d $^2A_1'$ D_{3h} Structure: EM[8]
T_0[a] = 18530 gas EM[8] $3d$–$2p^2A_2''$ 569–601 nm
EM[8] $3d$–$3p^2E'$ 3772–4517 cm^{-1}
τ = 12(1) ns gas EM[9,20]
B_0 = 21.72(2); C_0 = 10.91(2) EM[8]

3d $^2E''$ D_{3h} Structure: EM[8]
T_0 = 18433 gas EM[8] $3d$–$2p^2A_2''$ 569–601 nm
EM[8] $3d$–$3p^2E'$ 3772–4517 cm^{-1}
τ = 12(1) ns gas EM[9,20]
B_0 = 21.72(2); C_0 = 10.91(2) EM[8]

3d $^2E'$ D_{3h} Structure: EM[8]
T_0[a] = 18098 gas EM[8] $3d$–$2p^2A_2''$ 569–601 nm
EM[8] $3d$–$3p^2E'$ 3772–4517 cm^{-1}
τ = 12(1) ns gas EM[9,20]
B_0 = 21.72(2); C_0 = 10.91(2) EM[8]

3p $^2A_2''$ D_{3h} Structure: EM[3]
T_0[a] = 17872 gas EM[2,3,8]LF[7] $3p^2A_2''$–$2s^2A_1'$ 553–569 nm
τ_0 = 29(1) ns gas EM[9]
B_0 = 22.73(6); C_0 = 10.68(2) EM[8]

3s $^2A_1'$ D_{3h} Structure: EM[6]
T_0[a] = 17642 gas EM[3] $3s^2A_1'$–$2p^2A_2''$ 592–614 nm
EM[6] $3s^2A_1'$–$3p^2E'$ 3382–3768 cm^{-1}
$\tau \cong 10$ ns gas EM[20]
B_0 = 21.98; C_0 = 12.41 EM[6]

3p $^2E'$ D_{3h} Structure: EM[6]
T_0[a] = 14091 gas EM[2,4,21]LF[7] $3p^2E'$–$2s^2A_1'$ 700–765 nm
EM[6] $3s^2A_1'$–$3p^2E'$ 3382–3768 cm^{-1}
EM[8] $3d$–$3p^2E'$ 3772–4517 cm^{-1}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Ring breathing	2145T	gas	EM	21
e'	2	Deformation	1750T	gas	EM	4,21

τ = 17.5(2.0) ns gas EM[9,21]
B_0 = 21.15; C_0 = 10.59 EM[6]

2p $^2A_2''$ D_{3h} Structure: EM[6]
T_0[a] = 1052 gas EM[3,6]LF[7] $3s^2A_1'$–$2p^2A_2''$ 592–614 nm
EM[8] $3d$–$2p^2A_2''$ 569–601 nm
B_0 = 22.112; C_0 = 11.056 EM[6]

2s $^2A_1'$[c] D_{3h} Structure: EM[3]
gas EM[2,3]LF[7] $3p^2A_2''$–$2s^2A_1'$ 553–569 nm
EM[4,21] $3p^2E'$–$2s^2A_1'$ 700–765 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a_1'	1	Ring breathing	2457(10)	gas	EM	4,20,21
e'	2	Deformation	1890T	gas	EM	21

B_0 = 23.09; C_0 = 11.544(6) EM[3,21]

[a] Measured with respect to lowest bound state, $2s\ ^2A_1'$. Structure observed[1] in the dissociation spectrum of H_2 has been reinterpreted[5] as arising from the predissociation of H_3 ($2s\ ^2A_1'$) into H + H_2. Unstructured emission observed[11] between 190 and 280 nm, with a maximum near 230 nm, upon charge transfer between K and H_3^+ or D_3^+ has been attributed to transitions originating in bound Rydberg states of H_3 or D_3 and terminating in the dissociative ground-state continuum. Photofragment spectroscopy[14] has placed the $2p\ ^2A_2''$ state 5.563(20) eV above the ground-state H + H_2 dissociation limit.

[b] Observed for N = 1 rotational level.

[c] Predissociated by vibronic interaction with the $2p\ ^2E'$ repulsive ground state; linewidth is approximately 15 cm^{-1} for H_3 and 6 cm^{-1} for D_3.[2]

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MgH_2

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	430	Kr	IR	1
			417	Xe	IR	1
Σ_u^+	3	Asym. stretch	1558	Kr	IR	1
			1569	Xe	IR	1
			1544			

MgD_2

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	309	Kr	IR	1
			300	Xe	IR	1
Σ_u^+	3	Asym. stretch	1153	Kr	IR	1
			1160	Xe	IR	1
			1144			

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CaH_2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CaH_2 s-stretch	1267.0w	Kr	IR	1
			1239.8	Xe	IR	1
b_2	3	CaH_2 a-stretch	1192.0s	Kr	IR	1
			1163.8	Xe	IR	1

CaD_2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CaD_2 s-stretch	899.1	Kr	IR	1
			885.2	Xe	IR	1
b_2	3	CaD_2 a-stretch	866.8	Kr	IR	1
			847.8	Xe	IR	1

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TiH_2

$\tilde{X}$ C_{2v} Structure: IR^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	TiH s-stretch	1483.2	Ar	IR	1
			1477.9m	Kr	IR	1
			1473.1m			
	2	Bend	496.1	Kr	IR	1
b_2	3	TiH a-stretch	1435.5	Ar	IR	1
			1416.5vs	Kr	IR	1
			1412.1vs			

TiD_2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	TiD s-stretch	1071.0	Ar	IR	1
			1058.7m	Kr	IR	1
			1055.4m			
	2	Bend	376.5	Kr	IR	1
b_2	3	TiD a-stretch	1041.1	Ar	IR	1
			1028.1vs	Kr	IR	1
			1024.5vs			

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VH_2

$\tilde{X}$ C_{2v} Structure: IR^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	VH s-stretch	1532.4	Ar	IR	1
			1545.2m	Kr	IR	1
	2	Bend	529	Kr	IR	1
b_2	3	VH a-stretch	1508.3	Ar	IR	1
			1490.7vs	Kr	IR	1

VD_2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	VD s-stretch	1123.6	Ar	IR	1
			1111.5m	Kr	IR	1
	2	Bend	386	Kr	IR	1
b_2	3	VD a-stretch	1092.0	Ar	IR	1
			1079.5vs	Kr	IR	1

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CrH_2

$\tilde{X}$ C_{2v} Structure: IR[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CrH s-stretch	1651.3	Ar	IR	2
			1640.0	Kr	IR	2
b_2	3	CrH a-stretch	1614.9[a]	Ar	IR	2
			1606.4	Kr	IR	2

CrD_2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CrD s-stretch	1189.1w	Ar	IR	2
			1180.5s	Kr	IR	2
b_2	3	CrD a-stretch	1167.2wm[a]	Ar	IR	2
			1160.7vs	Kr	IR	2

[a] Ref. 1 gives 1591 and 1145 for CrH_2 and CrD_2, respectively, in an argon matrix. These frequencies are in the spectral regions of krypton-matrix absorptions observed by Ref. 2 in the presence of excess H_2 or D_2.

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MnH_2

In a xenon matrix, an absorption maximum is observed at 318 nm. Irradiation at this wavelength results in dissociation of MnH_2 into $Mn + H_2$.[2]

$\tilde{X}$ $^6A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	375	Xe	IR	2
			366			
b_2	3	Asym. stretch	1594.0	Ar	IR	1
			1591	Xe	IR	2
			1565			

MnD_2

$\tilde{X}$ $^6A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	276	Xe	IR	2
			266			
b_2	3	Asym. stretch	1155.6	Ar	IR	1
			1154	Xe	IR	2
			1137			

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[1]R. J. Van Zee, T. C. DeVore, J. L. Wilkerson, and W. Weltner, Jr., J. Chem. Phys. **69**, 1869 (1978).
[2]G. A. Ozin and J. G. McCaffrey, J. Am. Chem. Soc. **106**, 807 (1984).

FeH_2

In an argon, krypton, or xenon matrix, three broad absorptions appear[1] between 400 and 450 nm. Irradiation at 440 nm results in photodecomposition, producing $Fe + H_2$.[1,2]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	Bend	335	Ar	IR	2
			322	Kr	IR	1
			323	Xe	IR	1
	3	FeH a-stretch	1661	Ar	IR	2
			1647	Kr	IR	1,2
			1636	Xe	IR	1,2

FeD_2

In krypton and xenon matrices, three broad absorptions appear[1] between 400 and 450 nm, each slightly shifted from their FeH_2 counterparts. Irradiation at 440 nm results in the formation of $Fe + D_2$.[1,2]

$T_0 = 9530(180)$ gas PE[3]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	Bend	235	Ar	IR	2
			232	Xe	IR	1
	3	FeD a-stretch	1205	Ar	IR	2
			1195	Kr	IR	2
			1188	Xe	IR	1

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[1]G. A. Ozin and J. G. McCaffrey, J. Phys. Chem. **88**, 645 (1984).
[2]R. L. Rubinovitz and E. R. Nixon, J. Phys. Chem. **90**, 1940 (1986).
[3]A. E. S. Miller, C. S. Feigerle, and W. C. Lineberger, J. Chem. Phys. **84**, 4127 (1986).

CoH_2

Photodissociation into $Co + H_2$ was observed[2] on irradiation at 22000.

$T_0 \cong 2600$ gas PE[1]

$T_0 = 535(90)$ gas PE[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	Bend	380	Ar	IR	2
	3	CoH a-stretch	1685	Ar	IR	2
			1647	Kr	IR	2

CoD_2

$T_0 \cong 2600$ gas PE[1]

$T_0 = 440(60)$ gas PE[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	3	CoD a-stretch	1223	Ar	IR	2
			1215	Kr	IR	2

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[1]A. E. S. Miller, C. S. Feigerle, and W. C. Lineberger, J. Chem. Phys. **84**, 4127 (1986).
[2]R. L. Rubinovitz, T. A. Cellucci, and E. R. Nixon, Spectrochim. Acta **43A**, 647 (1987).

NiH_2

$T_0 \cong 1600$ gas PE[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Sym. stretch	2200T	gas	PE	1

NiD_2

$T_0 \cong 1600$ gas PE[1]

References

[1]A. E. S. Miller, C. S. Feigerle, and W. C. Lineberger, J. Chem. Phys. **84**, 4127 (1986).

ZnH_2

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	630.9	Ar	IR	1
			625.3	Kr	IR	1
Σ_u^+	3	ZnH_2 a-stretch	1870.8	Ar	IR	1
			1861.0	Kr	IR	1

ZnD_2

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	ZnD_2 a-stretch	1357.9	Ar	IR	1
			1350.9	Kr	IR	1

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[1]Z. L. Xiao, R. H. Hauge, and J. L. Margrave, High Temp. Sci. **31**, 59 (1991).

MoH_2

$\tilde{X}$ C_{2v} Structure: IR[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	MoH s-stretch	1752.7wm	Ar	IR	1
			1743.1s	Kr	IR	1
b_2	3	MoH a-stretch	1727.4m	Ar	IR	1
			1709.3vs	Kr	IR	1

MoD_2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	MoD s-stretch	1257.8m	Ar	IR	1
			1250.6s	Kr	IR	1
b_2	3	MoD a-stretch	1234.0ms	Ar	IR	1
			1227.2vs	Kr	IR	1

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[1]Z. L. Xiao, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **96**, 636 (1992).

HgH_2

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	773.0	Ar	IR	1
			771.1			
			769.7			
			769.2	Kr	IR	1
			772.5	H_2	IR	1
Σ_u^+	3	Asym. stretch	1895.8	Ar	IR	1
			1895.4			
			1893.1	Kr	IR	1
			1891.2			
			1889.2			
			1902.7	H_2	IR	1

HgD_2

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	555.2	Ar	IR	1
			553.3			
			555.8	D_2	IR	1
			553.3			
Σ_u^+	3	Asym. stretch	1365.4	Ar	IR	1
			1363.6			
			1362.8			
			1368.5	D_2	IR	1

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[1]N. Legay-Sommaire and F. Legay, Chem. Phys. Lett. **207**, 123 (1993).

MnH_2^-

Threshold for electron detachment from ground-state MnH_2^- = 3580(130) gas PE[1]

MnD_2^-

Threshold for electron detachment from ground-state MnD_2^- = 3750(115) gas PE[1]

References

[1]A. E. S. Miller, C. S. Feigerle, and W. C. Lineberger, J. Chem. Phys. **84**, 4127 (1986).

FeH_2^-

Threshold for electron detachment from ground-state FeH_2^- = 8460(115) gas PE[1]

FeD_2^-

Threshold for electron detachment from ground-state FeD_2 = 8375(105) gas PE[1]

References

[1]A. E. S. Miller, C. S. Feigerle, and W. C. Lineberger, J. Chem. Phys. **84**, 4127 (1986).

CoH_2^-

Threshold for electron detachment from ground-state CoH_2^- = 11700(115) gas PE[1]

CoD_2^-

Threshold for electron detachment from ground-state CoD_2^- = 11820(105) gas PE[1]

References

[1]A. E. S. Miller, C. S. Feigerle, and W. C. Lineberger, J. Chem. Phys. **84**, 4127 (1986).

NiH_2^-

Threshold for electron detachment from ground-state NiH_2^- = 15600(65) gas PE[1]

NiD_2^-

Threshold for electron detachment from ground-state NiD_2^- = 15540(60) gas PE[1]

References

[1]A. E. S. Miller, C. S. Feigerle, and W. C. Lineberger, J. Chem. Phys. **84**, 4127 (1986).

BH_2

$\tilde{A}\ ^2B_1(\Pi_u)$ [a] $D_{\infty h}$

T_0 = 4194.1 gas AB[1] $\tilde{A}$–$\tilde{X}$ 640–870 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	953.6	gas	AB	1

B_0 = 6.13 AB[1]

$\tilde{X}\ ^2A_1$ [a] C_{2v} Structure: AB[1]

A_0 = 41.649; B_0 = 7.241; C_0 = 6.001 AB[1]

BD_2

$\tilde{A}\ ^2B_1(\Pi_u)$ [a] $D_{\infty h}$

$B_0 \cong$ 3.2 AB[1]

$\tilde{X}\ ^2A_1$ [a] C_{2v}

A_0 = 24.1[b]; B_0 = 3.64; C_0 = 3.04 AB[1]

[a] The $\tilde{A}\ ^2B_1$ and $\tilde{X}\ ^2A_1$ states are perturbed by strong Renner-Teller interaction. While molecular orbital arguments indicate that the $\tilde{A}$ state should be linear, lower members of the bending progression could not be observed, and there may be a small barrier to linearity in the $\tilde{A}$ state.

[b] Assumed value.

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[1]G. Herzberg and J. W. C. Johns, Proc. Roy. Soc. (London) **A298**, 142 (1967).

AlH_2

$\tilde{A}\ ^2B_1(\Pi)$ $D_{\infty h}$ Structure: AB[1]

T_0 < 15200 gas AB[1] $\tilde{A}$–$\tilde{X}$ 658.4 nm

Other bands were also observed, but their analysis has not been reported. There is evidence for a predissociation limit at 15450.

B_0 = 3.57 AB[1]

$\tilde{X}\ ^2A_1$ C_{2v} Structure: AB[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	AlH s-stretch	1766vw	Kr	IR	2
	2	Bend	760m	Kr	IR	2
b_2	3	AlH a-stretch	1799w	Kr	IR	2

A_0 = 13.6; B_0 = 4.4; C_0 = 3.3 AB[1]

AlD_2

$\tilde{X}\ ^2A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	AlD s-stretch	1275vw	Kr	IR	2
	2	Bend	560m	Kr	IR	2
b_2	3	AlD a-stretch	1320w	Kr	IR	2

References

[1]G. Herzberg, *Molecular Spectra and Molecular Structure. III. Electronic Spectra and Electronic Structure of Polyatomic Molecules,* pp. 490–491, 583 (Van Nostrand, Princeton, NJ, 1966).
[2]J. M. Parnis and G. A. Ozin, J. Phys. Chem. **93**, 1215 (1989).

GaH_2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1727.9wm	Ar	IR	1
			1730.8	Kr	IR	1
b_2	3	Asym. stretch	1799.1s	Ar	IR	1
			1796.4	Kr	IR	1

GaD_2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1245.1	Ar	IR	1
			1244.2wm	Kr	IR	1
b_2	3	Asym. stretch	1303.4	Ar	IR	1
			1302.4s	Kr	IR	1

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CH_2^+

$\tilde{X}\ ^2A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	CH a-stretch	3131.37	gas	LD	1

$\frac{1}{2}(B + C)_0 = 7.381$ LD[1]

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[1]M. Rösslein, C. M. Gabrys, M.-F. Jagod, and T. Oka, J. Mol. Spectrosc. **153**, 738 (1992).

SiH_2^+

$\tilde{A}\ ^2B_1(II)$

gas PF[1] $\tilde{A}-\tilde{X}$ 567–659 nm

Predissociation into $Si^+ + H_2$ and into $SiH^+ + H$ was observed.
$B = 3.956(1)$ PF[1]

$\tilde{X}\ ^2A_1$ C_{2v}
$B = 5.094(2)$; $C = 3.772(4)$ PF[1]

References

[1]M. C. Curtis, P. A. Jackson, P. J. Sarre, and C. J. Whitham, Mol. Phys. **56**, 485 (1985).

CH_2

4p C_{2v}
$T_0 = 74254$ gas MPI[37]

$\tilde{D}$
$T_0 = 71592$ gas AB[1]MPI[36] $\tilde{D}-\tilde{X}$ 139.7 nm

$\tilde{C}$
$T_0 = 70917$ gas AB[1]MPI[36] $\tilde{C}-\tilde{X}$ 141.0 nm

$3d\ ^3A_2$ C_{2v} Structure: AB[7]
$T_0 = 70634$ gas AB[1]MPI[36] $3d^3A_2-\tilde{X}$ 141.5 nm
Diffuse. First member of Rydberg series converging to 83851. Higher members observed (AB[2]) at 76553, 79241, and 80688.
$B_0 = 6.89$[a] AB[1]

3p C_{2v}
$T_0 = 64126$ gas MPI[37]

$\tilde{c}\ ^1A_1$
gas AB[3] $\tilde{c}-\tilde{a}$ 330–362 nm

$\tilde{b}\ ^1B_1$[b] C_{2v} Structure: AB[3,29]
$T_0 = 10255(20)$ gas AB[1,3,27]LMR[21]LF[33,38,40] $\tilde{b}-\tilde{a}$ 490–920 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	570T	gas	AB	3

$\tau(0,14,0) = 4.6(1)$ μs LF[9,39]
$\tau(0,16,0) = 1.3(3)$ μs LF[11]
3.8(3) μs LF[39]
$B_0 = 7.74$ AB[1]
Barrier to linearity = 1617[29]

$\tilde{a}\ ^1A_1$[b] C_{2v} Structure: AB[3,29,31]
$T_0 = 3147(5)$ gas AB[1,3,27,28]LMR[21,26,30]PE[23,24]LF[32,38,40]SEP[32,34]
$\tilde{b}-\tilde{a}$ 490–920 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH s-stretch	2806.01(7)	gas	LF,LD	10,20,31
					IR	40
	2	Bend	1352.6	gas	AB,LF	3,27,28,40
b_2	3	CH a-stretch	2864.97(2)	gas	LD,IR	20,31

$\tau \cong 18$ s[c]
$A_0 = 20.118(2)$; $B_0 = 11.205(2)$; $C_0 = 7.069(2)$ AB[3,27,28]
Barrier to linearity = 9870 SEP[34]

$\tilde{X}\ ^3B_1$ C_{2v} Structure: ESR[4–6]AB[7]LMR[15,17]IR[17,26]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	963.10	gas	LMR	12,16
					DL	19,25
b_2	3	CH_2 a-stretch	3190(5)[d]	gas	IR	31

$A_0 = 73.811$; $B_0 = 8.450$; $C_0 = 7.184$ IR[25]
Barrier to linearity = 1931(30) [26]

CD_2

4p C_{2v}

T_0 = 74228 gas MPI[37]

$\tilde{D}$

T_0 = 70947 gas AB[1]MPI[36] $\tilde{D}-\tilde{X}$ 140.95 nm

$\tilde{C}$

T_0 = 71510 gas AB[1]MPI[36] $\tilde{C}-\tilde{X}$ 139.8 nm

3d $^3A_2$ C_{2v} Structure: AB[7]

T_0 = 70591.7 gas AB[1]MPI[36] $3d^3A_2-\tilde{X}$ 141.6 nm

B_0 = 3.595 AB[1]

3p C_{2v}

T_0 = 64082 gas MPI[37]

$\tilde{b}$ $^1B_1$ [b] C_{2v}

gas LF[13,41] $\tilde{b}-\tilde{a}$ 510–610 nm

$\tau(0,16,0)$ = 6.0(7) μs LF[13]

$\tilde{a}$ $^1A_1$ [b] C_{2v}

T_0 = 3140(50) gas PE[23]LF[41]SEP[41] $\tilde{b}-\tilde{a}$ 510–610 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	1005(1)	gas	LF	13

A_0 = 11.37(32); B_0 = 5.476(48); C_0 = 3.701(45) LF[41]SEP[41]

$\tilde{X}$ $^3B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	752.37	gas	DL	19

A_0 = 37.787; $\frac{1}{2}(B+C)_0$ = 3.962; $\frac{1}{2}(B-C)_0$ = 0.267 LMR[18,22]

[a] Value given for $^{13}CH_2$.

[b] The aA_1 and $\tilde{b}\ ^1B_1$ states are perturbed by strong Renner-Teller interaction.[13,14,29] They are also strongly perturbed by interaction with the $\tilde{X}\ ^3B_1$ state.[27,28,35]

[c] Calculated value.[21]

[d] From analysis of perturbations involving combination bands.[31]

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SiH_2

$\tilde{A}$ $^1B_1$ [a] C_{2v} Structure: AB[1,2]

T_0 = 15530.4(5) gas AB[1,2]LF[10,11,13] $\tilde{A}-\tilde{X}$ 480–650 nm

Onset of predissociation into Si (^1D) + H_2 near 21450.[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1990	gas	LF	13
	2	Bend	854	gas	AB,LF	1,11,13

τ_0 = 1.10(17) μs gas LF[6,7,11]

A_0 = 17.75[b]; B_0 = 4.9[b]; C_0 ≅ 2.8[b] AB[2]

Barrier to linearity ≅ 8000 [3]

$\tilde{a}$ $^3B_1$ C_{2v}

T_0 = 7340(240)[c] gas PI[8]

Barrier to predissociation into Si (^3S) + H_2 between 17070 and 17690.[11]

$\tilde{X}\ ^1A_1$ [a] C_{2v} Structure: AB[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1975.2[d]	gas	LF	10,13
			1964[d]	Ar	IR	5
	2	Bend	998.62	gas	AB,LF DL	2,4,9,13
			995	Ar	IR	5
b_2	3	Asym. stretch	1954[e]	gas	LF	10,13
			1973	Ar	IR	5

A_0 = 8.099; B_0 = 7.024; C_0 = 3.703 AB^2DL[9]

SiD_2

$\tilde{A}\ ^1B_1$ [a] C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	610	gas	AB,LF	1,11

τ_0 = 0.93(38) μs gas LF[11]

$\tilde{X}\ ^1A_1$ [a] C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1427[d]	Ar	IR	5
	2	Bend	731	gas	LF	11
			720	Ar	IR	5
b_2	3	Asym. stretch	1439	Ar	IR	5

[a] The $\tilde{A}\ ^1B_1$ and $\tilde{X}\ ^1A_1$ states are perturbed by strong Renner-Teller interaction.[3] The combined effects of Renner-Teller and spin-orbit interaction have been considered in detail by Ref. 12.
[b] Extrapolated values.[2]
[c] Possibly 6290(240).[8]
[d] In Fermi resonance with $2\nu_2$, observed for SiH_2 at 2002.7 (gas) and 1993 (Ar) and for SiD_2 at 1445 (Ar).
[e] $\frac{1}{2}(2\nu_3)$.

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GeH_2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		GeH stretch	1887wm	Ar	IR	1
		GeH stretch	1864wm	Ar	IR	1
		Bend	920wm	Ar	IR	1

GeD_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		GeD stretch	1338ms 1329vs 1325vs	Ar	IR	1
		Bend	658m	Ar	IR	1

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NH_2^+

$\tilde{b}\ ^1B_1$ C_{2v}
$T_0 \leq 20490(160)$[a] gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	920(150)	gas	PE	1

$\tilde{a}\ ^1A_1$ C_{2v}
T_0 = 10530(80) gas PI[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	2900(50)	gas	PE	1
	2	Bend	1350(50)	gas	PE	1

$\tilde{X}\ ^3B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	840(50)	gas	PE	1
b_2	3	Asym. stretch	3359.9	gas	LD	3

B_0 = 8.273; C_0 = 7.644 LD[3]

ND_2^+

$\tilde{b}\ ^1B_1$ C_{2v}

$\tilde{a}\ ^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	2210(50)	gas	PE	1
	2	Bend	940(50)	gas	PE	1

$\tilde{X}\ ^3B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	660(50)	gas	PE	1

[a] Corrected for revision[2] of first adiabatic ionization potential of NH_2.

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PH_2^+

$\tilde{a}\ ^3B_1$ C_{2v}

$T_0 \cong 5650$ gas PI[1,2]

$\tilde{X}\ ^1A_1$ C_{2v}

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CH_2^-

Threshold for electron detachment from ground-state CH_2^- is 5260(50).[1,2]

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	1230(30)	gas	PE	1,2

CD_2^-

Threshold for electron detachment from ground-state CD_2^- is 5200(50).[1]

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	940(30)	gas	PE	1

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SiH_2^-

Threshold for electron detachment from ground-state SiH_2^- is 9070(160).[1]

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	1200(160)	gas	PE	1

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NH_2

Rydberg series with members at 93054, 95753, 97193, and 98049, converging to NH_2^+ ($\tilde{A}\ ^1A_1$) at 100410. PI[19]

$\tilde{A}\ ^2A_1(\Pi_u)$ [a] C_{2v} Structure: AB[1,4]

T_0 = 11122.6 gas AB[1,8,22]LF[6,21,25,26]EM[25] $\tilde{A}-\tilde{X}$ 342-2700 nm
Ne,Ar,Kr,Xe[b] AB[2,3,5,27] $\tilde{A}-\tilde{X}$ 344–880 nm
N_2[b] AB[5] $\tilde{A}-\tilde{X}$ 480–620 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	3325	gas	AB	1
	2	Bend	633	gas	AB	1

$\tau_{090\Sigma}$ = 10.0(1.7) μs gas LF[7]
τ_{08011} = 10(3) μs gas LF[17]

Approximate ν^3 dependence.[7,17] In another LF study,[12] τ varied from 25 to 46 μs for relatively unperturbed rotational sublevels, and there was a weaker ca. 100 μs component associated with levels which are substantially perturbed.
B_0 = 8.78 AB[1]
Barrier to linearity = 730 [14]

$\tilde{X}\ ^2B_1$ [a] C_{2v} Structure: AB[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	3219.37	gas	LF,EM	6,15,16
					LD,IR	21,23
			3220w[c]	N_2	IR	5
	2	Bend	1497.32	gas	UV,LF	1,6,8-10
					LMR,IR	13,20
			1499m	N_2	IR	5
b_2	3	Asym. stretch	3301.11	gas	LD,LF	16,21
					IR	23

A_0 = 23.693; B_0 = 12.952; C_0 = 8.173 AB[1,8]LMR[13]IR[20]
Barrier to linearity = 12024 [14]

ND_2

$\tilde{A}\ ^2A_1(\Pi_u)$ [a] C_{2v}

gas AB[1] $\tilde{A}-\tilde{X}$ 500–680 nm

Ar AB[27] $\tilde{A}-\tilde{X}$ 380–825 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	2520T	gas	AB	1
	2	Bend	430	gas	AB	1

B_0 = 4.41 AB[1]

$\tilde{X}\ ^2B_1$ [a] C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	1108.75	gas	LMR	11,18
			1110m	N_2	IR	5

A_0 = 13.342; B_0 = 6.487; C_0 = 4.290 AB[1,18]LMR[11]MW[24]

[a] The $\tilde{A}\ ^2A_1$ and $\tilde{X}\ ^2B_1$ states are perturbed by strong Renner-Teller interaction.

[b] A detailed comparison of the argon-matrix data with gas-phase data has been given in Refs. 22 and 27. Rotational structure is resolved in the rare-gas matrices. In nitrogen,[5] bands are very broad and red-shifted by approximately 400 cm^{-1}, with no evidence for rotational structure.

[c] Assigned[5] in matrix studies to ν_3. Gas-phase observation of ν_1 at 3219.37 cm^{-1} and demonstration[16] that ν_1 is more intense than ν_3 dictate reassignment to ν_1.

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PH_2

$\tilde{A}\ ^2A_1$ [a] C_{2v} Structure: AB[4]

T_0 = 18276.59(3) gas AB[1,4,6]EM[2,3,5] $\tilde{A}-\tilde{X}$ 360–880 nm

18215(4) Ar AB[13,19] $\tilde{A}-\tilde{X}$ 405–550 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	949.12	gas	UV	2,6
			949(7)	Ar	AB	13,19

τ = 4(1) μs gas LF[11,20]EM[12]

A_0 = 20.41; B_0 = 5.60; C_0 = 4.295(3) AB[4,6]EM[5]

Barrier to linearity = 6840 [7]

$\tilde{X}\ ^2B_1$ [a] C_{2v} Structure: AB[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	2310(2)	gas	PE,Ra	10,21
	2	Bend	1101.91	gas	UV,LMR	2,4,14
			1103m	Ar	IR	13

A_0 = 9.132; B_0 = 8.084; C_0 = 4.214 AB[4,16]LMR[8,14,15]MW[17,18]

Barrier to linearity = 25100 [7]

PD_2

$\tilde{A}\ ^2A_1$ [a] C_{2v}

T_0 = 18282.1 gas AB[1]EM[2,3] $\tilde{A}-\tilde{X}$ 360–880 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	689.5	gas	EM	2
			665(25)	Ar	UV	13

$\tilde{X}\ ^2B_1$ [a] C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	795.5	gas	EM	2,3
			797w	Ar	IR	13

A_0 = 4.857(2); B_0 = 4.044(4); C_0 = 2.180(2) AB[9]

[a] The $\tilde{A}\ ^2A_1$ and $\tilde{X}\ ^2B_1$ states are perturbed by strong Renner-Teller interaction.

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AsH_2

$\tilde{A}\ ^2A_1$ [a] C_{2v} Structure: AB^1

T_0 = 19907.8 gas AB^1EM^2 $\tilde{A}$–$\tilde{X}$ 390–650 nm

Predissociated above 23300 [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	851.4	gas	AB	1

τ = 130(20) ns gas EM^2

A_{010} = 19.48(1); B_{010} = 4.97(1); C_{010} = 3.71 AB^1

$\tilde{X}\ ^2B_1$ C_{2v} Structure: AB^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	981	gas	EM	2

A_0 = 7.549(4); B_0 = 7.162(4); C_0 = 3.617(3) AB^1

AsD_2

$\tilde{A}\ ^2A_1$ C_{2v}

T_0 = 19904.9 gas AB^1 $\tilde{A}$–$\tilde{X}$ 390–490 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	615.9	gas	AB	1

$\tilde{X}\ ^2B_1$ C_{2v}

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SbH_2

$\tilde{A}\ ^2A_1$ C_{2v}

T_0 = 19438 gas AB^1EM^2 $\tilde{A}$–$\tilde{X}$ 403–700 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	695(3)	gas	AB	1

τ = 70(20) ns gas EM^2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	SbH_2 a-stretch	1840.5	Ar	IR	3

SbD_2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	SbD_2 a-stretch	1320.2	Ar	IR	3

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H_2O^+

$\tilde{B}\ ^2B_2$ C_{2v}

T_0 = 36757(12) gas PE[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	2968[a]	gas	PE	9
	2	Bend	1596[a]	gas	PE	9

$\tilde{A}\ ^2A_1(\Pi_u)$ [b] $D_{\infty h}$ Structure: PE[4,7]EM[7]

T_{050} = 13409.3 gas EM[1,5]AB[14] $\tilde{A}$–$\tilde{X}$ 400–750 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	3547(16)	gas	PE	9
	2	Bend	876.8[b]	gas	EM,PE	5,9

τ = 10.5(1.0) μs gas EF[6]

B_{050} = 8.57 EM[5]

$\tilde{X}\ ^2B_1$ [b] C_{2v} Structure: EM[5,7]LMR[8]LD[11]CC[15]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	3212.86	gas	PE,LD	9,11
					PI,CC	13,15
			3182.7	Ne	IR	16
	2	Bend	1408.42	gas	EM,PE	1,5,9
					DL	12
			1401.7	Ne	IR	16
b_2	3	Asym. stretch	3259.04	gas	LD,CC	11,15
			3219.5	Ne	IR	16

A_0 = 29.036(2); B_0 = 12.423; C_0 = 8.469 LMR[8]LD[11]DL[12]CC[15]

Barrier to linearity = 9187 [7]

D_2O^+

$\tilde{B}\ ^2B_2$ C_{2v}

T_0 = 37430(50) gas PE[2,4]

38498(12) gas PE[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	2282[a]	gas	PE	2,9
	2	Bend	1099[a]	gas	PE	9

$\tilde{A}\ ^2A_1(\Pi_u)$ [b] $D_{\infty h}$

T_{030} = 10456(30) gas PE[2,4]EM[10] $\tilde{A}$–$\tilde{X}$ 490–670 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	2531(8)	gas	PE	9
	2	Bend	640(9)	gas	PE	9

τ is ca. 12% greater than for H_2O^+.[3]

$\tilde{X}\ ^2B_1$ [b] C_{2v} Structure: EM[10]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	2344(6)	gas	PE	2,4,9
			2326.7	Ne	IR	16
	2	Bend	1044.27(5)	gas	EM	10
			1040.5	Ne	IR	16
b_2	3	Asym. stretch	2392.7	Ne	IR	16

A_0 = 16.03; B_0 = 6.240(3); C_0 = 4.407(3) EM[10]

[a] Best fit of simulated photoelectron spectrum.

[b] The $\tilde{A}\ ^2A_2\ (\Pi_u)$ and $\tilde{X}\ ^2B_1$ states are perturbed by strong Renner-Teller interaction.

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H_2S^+

$\tilde{B}\ ^2B_2$ C_{2v}

T_0 = 34770(160) gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	2259T	gas	PE	5

$\tilde{A}\ ^2A_1$ [a] C_{2v} Structure: EF^3

T_0 = 18518 gas $EF^{1,3}PE^{2,5}$ $\tilde{A}$–$\tilde{X}$ 400–500 nm

Predissociated above 23300 into $H_2 + S^+$.[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	910(20)	gas	PE	2,5

τ = 4.2(4) μs gas EF^4

B_{020} = 5.03 EF^3

Barrier to linearity ≅ 4600 [1]

$\tilde{X}\ ^2B_1$ [a] C_{2v} Structure: $EF^{1,3}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	2570(40)	gas	PE	5
	2	Bend	1159.0	gas	EF	3

A_0 = 10.18(2); B_0 = 8.63(1); C_0 = 4.60(6) EF^3

D_2S^+

$\tilde{A}\ ^2A_1$ C_{2v}

T_0 = 18574 gas EF^3 $\tilde{A}$–$\tilde{X}$ 400–500 nm

B_{030} = 2.46 EF^3

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	838.6	gas	EF	3

A_0 = 5.37(2); B_0 = 4.32(1); C_0 = 2.34(2) EF^3

[a] The $\tilde{A}\ ^2A_1$ and $\tilde{X}\ ^2B_1$ states are perturbed by strong Renner-Teller interaction.

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H_2Se^+

$\tilde{B}\ ^2B_2$ C_{2v}

T_0 = 34060(40) gas $PE^{1,2}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1950(40)	gas	PE	2
	2	Bend	580(100)	gas	PE	2

$\tilde{A}\ ^2A_1$ C_{2v}

T_0 = 20270(70) gas $PE^{1,2}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	863(100)	gas	PE	1,2

Barrier to linearity ≅ 6450 [2]

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	2267(40)	gas	PE	1,2
	2	Bend	1017(60)	gas	PE	2

References

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H_2Te^+

$\tilde{B}\ ^2B_2$ C_{2v}

T_0 = 31470(160) gas PE^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1694(100)	gas	PE	1

$\tilde{A}\ ^2A_1$ C_{2v}

T_0 = 20090(160) gas PE^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	702(20)	gas	PE	1

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	2100(200)	gas	PE	1

References

[1]A. W. Potts and W. C. Price, Proc. Roy. Soc. (London) **A326**, 181 (1972).

NH_2^-

Threshold for electron detachment from ground-state NH_2^- is 6220(40).[1-3,7]

$\tilde{X}\ ^1A_1$ C_{2v} Structure: CC[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	3121.93	gas	CC	4,5
	2	Bend	1523	Ar	IR	6
b_2	3	Asym. stretch	3190.29	gas	CC	5
			3152	Ar	IR	6

A_0 = 23.051(2); B_0 = 13.068(2); C_0 = 8.115 CC[4,5]

References

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H_2F^+

$\tilde{X}$ C_{2v} Structure: CC[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	3348.71	gas	CC	1,2
b_2	3	Asym. stretch	3334.69	gas	CC	1,2

A_0 = 34.511; B_0 = 12.885; C_0 = 9.080 CC[1,2]

References

[1]E. Schafer and R. J. Saykally, J. Chem. Phys. **80**, 2973 (1984).
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H_2Cl^+

C_{2v} Structure: $DL^1MW^2LD^3$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	2643.22	gas	LD	3
	2	Bend	1184.13	gas	DL	1
b_2	3	Asym. stretch	2630.14	gas	LD	3

A_0 = 11.253; B_0 = 9.124; C_0 = 4.941 $DL^1MW^2LD^3$

References

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6.2. Triatomic Monohydrides

Li_2H

$\tilde{B}$ C_{2v} Structure: MPI[1]
T_0 = 18940 gas MPI[1] $\tilde{B}$–$\tilde{X}$ 457–528 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1		332	gas	MPI	1
	2		195	gas	MPI	1
b_2	3		309	gas	MPI	1

A_0 = 6.87; B_0 = 0.455; C_0 = 0.427 MPI[1]

$\tilde{X}$ C_{2v} Structure: MPI[1]
A_0 = 13.250; B_0 = 0.750; C_0 = 0.710 MPI[1]

References

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CrCrH

$\tilde{X}\ ^2\Sigma^+$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CrH stretch	1507(5)	gas	PE	1
Π	2	Bend	215(15)	gas	PE	1
Σ^+	3	CrCr stretch	532(5)	gas	PE	1

CrCrD

$\tilde{X}\ ^2\Sigma^+$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CrD stretch	1092(5)	gas	PE	1
Π	2	Bend	170(15)	gas	PE	1
Σ^+	3	CrCr stretch	532(5)	gas	PE	1

References

[1]S. M. Casey and D. G. Leopold, Chem. Phys. Lett. **201**, 205 (1993).

$CrCrH^-$

Threshold for electron detachment from ground-state $CrCrH^-$ = 11890(40) gas PE[1]

$\tilde{X}\ ^1\Sigma^+$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CrH stretch	1170(150)	gas	PE	1
Π	2	Bend	100(20)	gas	PE	1
Σ^+	3	CrCr stretch	414(5)	gas	PE	1

$CrCrD^-$

Threshold for electron detachment from ground-state $CrCrD^-$ = 11810(40) gas PE[1]

$\tilde{X}\ ^1\Sigma^+$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CrD stretch	840(100)	gas	PE	1
Π	2	Bend	70(10)	gas	PE	1
Σ^+	3	CrCr stretch	407(8)	gas	PE	1

References

[1]S. M. Casey and D. G. Leopold, Chem. Phys. Lett. **201**, 205 (1993).

$NaOH^+$

$\tilde{A}\ ^2\Sigma^+$ $C_{\infty v}$
T_0 = 28400(1200) gas PE[1]

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$

References

[1]J. M. Dyke, M. Feher, and A. Morris, J. Electron Spectrosc. Relat. Phenom. **41**, 343 (1986).

KOH^+

$A\ ^2\Sigma^+$ $C_{\infty v}$
T_0 = 31000(1200) gas PE[1]

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$

References

[1]J. M. Dyke, M. Feher, and A. Morris, J. Electron Spectrosc. Relat. Phenom. **41**, 343 (1986).

YNH

$\tilde{B}\ ^2\Sigma$ $D_{\infty h}$
T_0 = 16992.5 gas LF[1] $\tilde{B}$–$\tilde{X}$ 585–650 nm

$\tilde{X}\ ^2\Sigma$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	510	gas	LF	1
Σ^+	3	YN stretch	810	gas	LF	1

$A \cong 440$ gas LF[1]

YND

$\tilde{B}\ ^2\Sigma$ $D_{\infty h}$
T_0 = 16950.0 gas LF[1] $\tilde{B}$–$\tilde{X}$ 585–650 nm

$\tilde{X}\ ^2\Sigma$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	ND stretch	2230	gas	LF	1
Π	2	Bend	400	gas	LF	1
Σ^+	3	YN stretch	770	gas	LF	1

References

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MgOH

$\tilde{X}$
B_0 = 0.494 MW[1]

MgOD

$\tilde{X}$
B_0 = 0.450 MW[1]

References

[1]W. L. Barclay Jr., M. A. Anderson, and L. M. Ziurys, Chem. Phys. Lett. **196**, 225 (1992).

CaOH

$\tilde{C}\ ^2\Delta$ $C_{\infty v}$
T_0 = 21896T gas LF[12,14] $\tilde{C}$–$\tilde{X}$ 440–470 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	312	gas	LF	12
Σ^+	3	CaO stretch	528	gas	LF	12

$B_{010\,\Pi}$ = 0.322 LF[12]

$\tilde{B}\ ^2\Sigma^+$ $C_{\infty v}$ Structure: LF[7]
T_0 = 18022.268(1) gas $CL^2LF^{4,6,10}$ $\tilde{B}$–$\tilde{X}$ 555 nm
Absorption maximum at 18236(15) in a krypton matrix.[5]
B_0 = 0.339 LF[4,6]

$\tilde{A}\ ^2\Pi$ $C_{\infty v}$ Structure: LF[3]
T_0 = 15998.128(1) gas $CL^2LF^{3,6,8,10,13}$ $\tilde{A}$–$\tilde{X}$ 600–650 nm
Absorption maximum at 16096(15) in a krypton matrix.[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	361.53[a]	gas	LF	13
Σ^+	3	CaO stretch	630.68[a]	gas	LF	13

A = 66.795(1) gas LF[3,6]
$\epsilon\omega_2$ = −36.57 gas LF[13]
B_0 = 0.341 LF[3,6]

BaOH

$\tilde{B}\ ^2\Sigma^+$ $C_{\infty v}$

T_0 = 13200.007(2) gas LF[4,6] $\tilde{B}$–$\tilde{X}$ 710–757 nm

Absorption maximum at 13105(15) in a krypton matrix.[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	BaO stretch	461.0(3)	gas	LF	4

B_0 = 0.213 LF[4]

$\tilde{A}\ ^2\Pi$ $C_{\infty v}$

T_0 = 11760(2) gas LF[5] $\tilde{A}$–$\tilde{X}$ 827–874 nm

Absorption maximum at 11892(15) in a krypton matrix.[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	352	gas	LF	5
Σ^+	3	BaO stretch	458	gas	LF	5

A = 635(1) LF[4]

$\tilde{A}'\ ^2\Delta$ $C_{\infty v}$

gas LF[5] $\tilde{A}'$–$\tilde{X}$ 848–888 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	342	gas	LF	5
Σ^+	3	BaO stretch	468	gas	LF	2

$\tilde{X}\ ^2\Sigma^+$ $C_{\infty v}$ Structure: LF[4]MW[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	341.6(6)	gas	LF	4
Σ^+	3	BaO stretch	492.4(8)	gas	LF	4
			430.1	Ar	IR	3

B_0 = 0.217 LF[4]MW[7]

BaOD

$\tilde{B}\ ^2\Sigma^+$ $C_{\infty v}$

T_0 = 13177.318(3) gas LF[4] $\tilde{B}$–$\tilde{X}$ 730–759 nm

B_0 = 0.19 gas LF[4]

$\tilde{A}\ ^2\Pi$ $C_{\infty v}$

T_0 = 11754(2) gas LF[5] $\tilde{A}$–$\tilde{X}$ 828–878 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	268	gas	LF	5
Σ^+	3	BaO stretch	451	gas	LF	5

$\tilde{A}'\ ^2\Delta$ $C_{\infty v}$

gas LF[5] $\tilde{A}'$–X 886–889 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	258	gas	LF	5
Σ^+	3	BaO stretch	469	gas	LF	5

$\tilde{X}\ ^2\Sigma^+$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	257.6(4)	gas	LF	4
Σ^+	3	BaO stretch	482.4(2)	gas	LF	4
			413.6	Ar	IR	3

B_0 = 0.196 LF[4]MW[7]

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ScOD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	3	ScO stretch	699.2	Ar	IR	1

References

[1]J. W. Kauffman, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **89**, 3547 (1985).

NiOH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OH stretch	3648.7	Ar	IR	1
	3	NiO stretch	682.7	Ar	IR	1

NiOD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OD stretch	2712.4	Ar	IR	1
	3	NiO stretch	644.3	Ar	IR	1

References

[1]M. Park, R. H. Hauge, and J. L. Margrave, High Temp. Sci. **25**, 1 (1988).

CuOH

$\tilde{B}\ ^1A''$ C_s Structure: LF[1,3]

T_0 = 18406.779 gas CL'LF[1,3] $\tilde{B}-\tilde{X}$ 500–560 nm

A_0 = 25.898; B_0 = 0.382; C_0 = 0.376 LF[1,3]

$\tilde{A}\ ^1A'$ C_s Structure: LF[4]

T_0 = 15911.546 gas LF[4]

A_0 = 18.316; B_0 = 0.388; C_0 = 0.378 LF[4]

$\tilde{X}\ ^1A'$ C_s Structure: LF[1,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	743(1)	gas	LF	1
			727.7	Ar	IR	2
	3	CuO stretch	632.7	Ar	IR	2

A_0 = 23.039; B_0 = 0.392; C_0 = 0.385 LF[1,3]

CuOD

$\tilde{B}\ ^1A''$ C_s

T_0 = 18422.335 gas LF[1,3] $\tilde{B}-\tilde{X}$ 500–560 nm

A_0 = 14.235; B_0 = 0.354; C_0 = 0.344 LF[1,3]

$\tilde{A}\ ^1A'$ C_s

T_0 = 15911.095(3) gas LF[4]

A_0 = 10.714; B_0 = 0.361; C_0 = 0.346 LF[4]

$\tilde{X}\ ^1A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	537(1)	gas	LF	1
			533.6	Ar	IR	2
	3	CuO stretch	635.1	Ar	IR	2

A_0 = 12.426; B_0 = 0.366; C_0 = 0.354 LF[1,3]

References

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[4]C. N. Jarman, W. T. M. L. Fernando, and P. F. Bernath, J. Mol. Spectrosc. **145**, 151 (1991).

ZnOH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		^{64}ZnO stretch	649.6	Ar	IR	1

ZnOD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		^{64}ZnO stretch	648.1	Ar	IR	1

References

[1]J. W. Kauffman, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **89**, 3541 (1985).

HNB

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NH stretch	3675m	Ar	IR	1
	3	NB stretch	2035s	Ar	IR	1

DNB

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	ND stretch	2770m	Ar	IR	1
	3	NB stretch	1963s	Ar	IR	1

References

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HBS^+

$\tilde{B}\ ^2\Sigma^+$ $C_{\infty v}$

T_0 = 38000(1000) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BH stretch	2190(100)	gas	PE	1,2

$\tilde{A}\ ^2\Sigma^+$ $C_{\infty v}$

T_0 = 19827 gas EF[3] $\tilde{A}$–$\tilde{X}$ 479–635 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BH stretch	2214.8(4)	gas	EF	3
Σ^+	3	BS stretch	1050.9(4)	gas	EF	3

$\tau \geq$ 2300(200) ns gas EF[4]

$\tilde{X}\ ^2\Pi_{3/2}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BH stretch	2746.8(4)	gas	EF	3
Π	2	Bend	659(1)	gas	EF	3
Σ^+	3	BS stretch	984.1(4)[a]	gas	EF	3

$A_{010} = -321.4$, $\epsilon\omega_2 = -45(1)$.[3]

DBS^+

$\tilde{A}\ ^2\Sigma^+$ $C_{\infty v}$

T_0 = 19913 gas EF[3] $\tilde{A}$–$\tilde{X}$ 462–646 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BD stretch	1706.6(4)	gas	EF	3
Σ^+	3	BS stretch	1011.1(4)	gas	EF	3

$\tilde{X}\ ^2\Pi_{3/2}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BD stretch	2071.1(4)	gas	EF	3
Σ^+	3	BS stretch	933.9(4)[b]	gas	EF	3

[a] 975.9(4) in $\tilde{X}\ ^2\Pi_{1/2}$ state.

[b] 937.4(4) in $\tilde{X}\ ^2\Pi_{1/2}$ state.

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HCC

3pσ Rydberg state[a] $C_{\infty v}$

T_0 = 72100(1300) gas MPI[34]

T_0 = 51387(25)T Ar AB[8] 195–160 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CC stretch	2175(25)	Ar	AB	8
		Bend	630(25)[b]	Ar	AB	8

$2\ ^2\Pi$? $D_{\infty h}$ $2\ ^2\Pi$–$\tilde{X}$ 250–313 nm

T_0 = 39176 gas LF[35,36]

The observed bands can be assigned[36] to transitions between a common $^2\Pi$ upper state and HCC $\tilde{X}(0n0)$, n = 1, 3, 5, 7.

$\tau \cong$ 120 ns gas LF[36]

$T_0 \leq$ 29360 Ar AB[2,8]

An absorption band system between 340 and 246 nm, with band spacings of approximately 2700, 1300 and 840 cm^{-1}, which has been observed on vacuum UV photolysis of C_2H_2 in an argon matrix is tentatively attributed to HCC.

$\tilde{A}\ ^2\Pi$ $C_{\infty v}$

$T_0 >$ 3400 gas PE[32]

$T_0 <$ 3800 Ar AB[21]

In an argon matrix, a complicated absorption band system of HCC extends from approximately 3600 to 7800.[21] This band system is extensively perturbed by high vibrational levels of the ground state. A few of the individual bands have been observed in the gas phase by color-center laser absorption[10,14,29], by high resolution emission spectroscopy,[24] or by time-resolved emission spectroscopy.[30] Because of the extensive perturbations and because of the high energy input in the gas-phase studies, high ground-state vibrational levels are prominent both in the gas phase[10,14,19,26,27,32] and in an argon matrix.[20,21]

Quasicontinuous 400–900 nm emission results on 136–110 nm photolysis of C_2H_2 or HCCBr in the gas phase.[5,11,13,17] The fluorescence lifetimes vary from 6 to 20 μs.[11,13,17] Unstructured emission from 1 to 5 μm has been detected[18] upon 193-nm photolysis of gas-phase C_2H_2, with maximum intensity between 3600 and 5000. The HCC fluorescence resulting from the 193-nm photolysis of HCCBr extends from 500 nm to 5 μm,[18] with lifetime increasing from ca. 5 μs near 500 nm to ca. 60 μs near 4000. Unstructured HCC emission between 400 and 500 nm has also been observed[15] on vacuum UV irradiation of C_2H_2 isolated in the solid rare gases.

$\tilde{X}\ ^2\Sigma^+$ $C_{\infty v}$ Structure: MW[31]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	371.60[c]	gas	DL	26,27
Σ^+	3	CC stretch	1840.57	gas	DL	23
			1846.2m	Ar	IR	1,3,20, 21

$A \cong$ 10 IR[14]

B_{000} = 1.457 MW[4,6,7,9] LMR[12]

B_{020} = 1.451 LMR[28]

DCC

3pσ Rydberg state[a] $C_{\infty v}$

T_0 = 72100(1300) gas MPI[34]

T_0 = 51493(25)T Ar AB[8] 194–170 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CC stretch	2183(25)	Ar	AB	8
		Bend	520(25)[b]	Ar	AB	8

Fluorescence observed on laser excitation between 34500 and 40000 (250–290 nm) of gas-phase DCC from 2 to 10 μs after its formation by 193 nm photolysis of C_2D_2 has been attributed[35] to transitions of DCC between high vibrational levels of the ground state and an undetermined excited state, possibly $2\ ^2\Pi$.

$\tilde{A}\ ^2\Pi$ $C_{\infty v}$

$T_0 < 3800$ Ar AB[21]

A complicated absorption band system extends to approximately 7500 in argon-matrix studies of DCC.[21] As for HCC, the band system is extensively perturbed by high vibrational levels of the ground state. A few of the bands, some of which arise from excited ground-state vibrational energy levels, have been studied in the gas phase using infrared laser absorption.[22,29,33]

$\tilde{X}\ ^2\Sigma^+$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
Σ^+	3	CC stretch	1743.18	gas	DL	25
			1746.3m	Ar	IR	1,3,20,21

$B_0 = 1.203$ MW[16]

[a] Tentative assignment.
[b] Observed band spacing; $2\nu_2$ if upper state is linear.
[c] Derived from $(\nu_2 + \nu_3) - [(\nu_2 + \nu_3) - \nu_2]$. The detailed assignment of $(\nu_2 + \nu_3)$ is given in Ref. 27 and that of $(\nu_2 + \nu_3) - \nu_2$ in Ref. 26.

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HCN^+

$\tilde{B}\ ^2\Sigma^-$ $C_{\infty v}$

$T_0 \leq 42380(40)$ gas PE[2]

A progression with irregular vibrational spacings spanning almost 2 eV in the photoelectron spectrum of HCN has been assigned to this state of HCN^+. A wave packet analysis has been conducted[3] to provide insight into the structure of the transition.

$\tilde{A}\ ^2\Sigma^+$ $C_{\infty v}$

$T_0 = 3260(30)$ gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
Σ^+	1	CH stretch	3106(40)	gas	PE	2
Π	2	Bend	428(30)H	gas	PE	2
Σ^+	3	CN stretch	2098(30)	gas	PE	2

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
Σ^+	1	CH stretch	3070(30)	gas	PE	1
			3049.9	Ne	IR	4
Π	2	Bend	760(30)T[a]	gas	PE	1
Σ^+	3	CN stretch	1800(30)	gas	PE	1,2

DCN^+

$\tilde{B}\ ^2\Sigma^-$ $C_{\infty v}$

$T_0 \leq 41986(40)$ gas PE[2]

$\tilde{A}\ ^2\Sigma^+$ $C_{\infty v}$

T_0 = 3114(30) gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2566(40)	gas	PE	2
Π	2	Bend	323(30)H	gas	PE	2
Σ^+	3	CN stretch	1904(30)	gas	PE	2

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2374.1	Ne	IR	4
Σ^+	3	CN stretch	1686(30)	gas	PE	2

[a] Ref. 2 gives 298(30) for HCN^+ and 234(30) for HNC^+.

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HCP^+

$\tilde{A}\ ^2\Sigma^+$ $C_{\infty v}$

T_0 = 16766.4(2) gas EF^{2-4} $\tilde{A}$–$\tilde{X}$ 555–755 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	2985.6(4)	gas	EF	4
Π	2	Bend	706.4(1.0)	gas	EF	4
Σ^+	3	CP stretch	1275.4(4)	gas	EF	4

$\tau \geq 1.2(1)$ μs gas EF^2
B_0 = 0.669(2) EF^3

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3125.1(4)	gas	EF	4
Π	2	Bend	642.3(1.0)	gas	EF	4
Σ^+	3	C≡P stretch	1147.1(4)[a]	gas	EF	2–4

A = −146.97(3) EF^3, $\epsilon\omega_2$ = −26.4(6) EF^4
B_0 = 0.622(2) EF^3

DCP^+

$\tilde{A}\ ^2\Sigma^+$ $C_{\infty v}$

T_0 = 16769.9(2) gas EF^3 $\tilde{A}$–$\tilde{X}$ 520–825 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2274.4(4)	gas	EF	4
Π	2	Bend	552.0(1.0)	gas	EF	4
Σ^+	3	C≡P stretch	1218.1(4)	gas	EF	4

B_0 = 0.568 EF^3

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2356.5(4)	gas	EF	4
Π	2	Bend	499.1(1.0)	gas	EF	4
Σ^+	3	C≡P stretch	1112.4(4)	gas	EF	2–4

A = −146.71(1) EF^3, $\epsilon\omega_2$ = −18.7(6) EF^4
B_0 = 0.528 EF^3

[a]1159.9 for $\tilde{X}\ ^2\Pi_{1/2}$.

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HNC^+

In a neon matrix, threshold for photoisomerization to HCN^+ near 17200.[1]

$\tilde{X}\ ^2\Sigma^+$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NH stretch	3365.0s	Ne	IR	1
Π	2	Bend	577.6m	Ne	IR	1
Σ^+	3	NC stretch	2195.2w	Ne	IR	1

DNC^+

$\tilde{X}\ ^2\Sigma^+$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	ND stretch	2664.9	Ne	IR	1
Σ^+	3	NC stretch	2028.1	Ne	IR	1

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HFeF

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		HFe stretch	1753.2	Ar	IR	1
		FeF stretch	650.0	Ar	IR	1

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HFeCl

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		FeH stretch	1755	Ar	IR	1
			1739	Kr	IR	1

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HFeBr

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		FeH stretch	1738	Kr	IR	1

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HFeI

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		FeH stretch	1754	Ar	IR	1

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HBO

$\tilde{X}$ $C_{\infty v}$ Structure: $MW^{3,4}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	754.42	gas	DL	6
			756.1m	Ar	IR	1,7,8
Σ^+	3	BO stretch	1825.56	gas	DL	2
			1822.3s	Ar	IR	1,7,8

B_0 = 1.308 $DL^2MW^{3,4}$

DBO

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BD stretch	2253.53	gas	DL	5
			2258.9w	Ar	IR	1,8
Π	2	Bend	607.6m	Ar	IR	1,8
Σ^+	3	BO stretch	1647.69	gas	DL	5
			1650.2m	Ar	IR	1,8

B_0 = 1.049 gas MW^4

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HBS

$\tilde{X}$ $C_{\infty v}$ Structure: MW^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BH stretch	2735.80	gas	IR	2
			2724	Ar	IR	4
	3	BS stretch	1172.39	gas	IR	3
			1168	Ar	IR	4

DBS

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BD stretch	2077.71	gas	IR	3
	3	BS stretch	1119.98[a]	gas	IR	3

[a] In Fermi resonance with $2\nu_2$, at 1098.60 cm^{-1}.

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AlOH

$\tilde{B}$

T_0 = 41747 gas MPI[4] $\tilde{B}$–$\tilde{X}$ 230–240 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			760.3	gas	MPI	4
			581.0	gas	MPI	4

$\tilde{A}$

T_0 = 40073 gas MPI[4] $\tilde{A}$–$\tilde{X}$ 227–255 nm
Kr AB[2,3] $\tilde{A}$–$\tilde{X}$ 245–252 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3258.4T	gas	MPI	4
			807.6	gas	MPI	4
			636.6	gas	MPI	4

$\tilde{X}\ ^1\Sigma^+$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	OH stretch	3790	Ar	IR	1
	3	AlO stretch	895	gas	MPI	4
			810.3	Ar	IR	1

AlOD

$\tilde{B}$

T_0 = 41706 gas MPI[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			570.8[a]	gas	MPI	4

$\tilde{A}$

T_0 = 40025 gas MPI[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			667.5	gas	MPI	4
			569.3	gas	MPI	4

$\tilde{X}\ ^1\Sigma^+$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	AlO stretch	795.2	Ar	IR	1

[a] ω.

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GaOH

$\tilde{A}\ ^1\Pi$? $C_{\infty v}$

A broad absorption with maximum near 256 nm observed in argon and krypton matrices has been assigned[2] to this transition of GaOH.

$\tilde{X}\ ^1\Sigma^+$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	OH stretch	3692	Ar	IR	1
Π	2	Bend	424.4	Ar	IR	1
Σ^+	3	^{69}GaO stretch	613.0	Ar	IR	1

GaOD

$\tilde{X}\ ^1\Sigma^+$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	OD stretch	2721	Ar	IR	1
	3	^{69}GaO stretch	595.8	Ar	IR	1

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InOH

$\tilde{A}\ ^1\Pi$ $C_{\infty v}$

A broad absorption with maximum near 271 nm observed in a krypton matrix has been assigned[2] to this transition of InOH.

$\tilde{X}\ ^1\Sigma^+$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	421.8	Ar	IR	1
Σ^+	3	InO stretch	522.8	Ar	IR	1

InOD

$\tilde{X}\ ^1\Sigma^+$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	InO stretch	595.7	Ar	IR	1

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HBF^+

$\tilde{X}$ $C_{\infty v}$ Structure: $MW^{2,3}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	BF stretch	1633.22	gas	DL	1

B_0 = 1.212 $IR^1MW^{2,3}$

DBF^+

B_0 = 0.972 $MW^{2,3}$

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HCC^-

Threshold for electron detachment from ground-state HCC^- = 23950(50) gas PE^1

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	505(20)	gas	PE	1
Σ^+	3	CC stretch	1800(20)	gas	PE	1
			1773.0T	Ne	IR	2

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HCO^+

$\tilde{X}$ $C_{\infty v}$ Structure: MW^{2-4}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3088.74	gas	LD,CC	5,6,15,16
Π	2	Bend	829.72	gas	DL	10,11
Σ^+	3	CO stretch	2183.95	gas	DL	7,8,14

B_0 = 1.488 MW^{2-4}

DCO^+

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2584.56	gas	DL	12
Π	2	Bend	647(25)	gas	PE	1,13
Σ^+	3	CO stretch	1904.06	gas	DL	9

B_0 = 1.201 MW^{2-4}

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HCS^+

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3141.68	gas	CC	4,5
Π	2	Bend	766.45	gas	DL	3

B_0 = 0.712 MW[1,2]DL[3]CC[4,5]

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HNC

$\tilde{A}$ [a]

T_0 = 32850 gas AB[7] $\tilde{A}$–$\tilde{X}$ 250–305 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CN stretch	1005	gas	UV	7

$\tilde{X}$ $C_{\infty v}$ Structure: MW[4,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NH stretch	3652.66	gas	IR	3,6,8
			3643.1	Ne	IR	9
			3620s	Ar	IR	2
			3583s N_2	Ar	IR	1,2
			3567s	N_2	IR	2
Π	2	Bend	464.24	gas	IR	8
			477s	Ar	IR	2
			535s N_2	Ar	IR	1
			559s	N_2	IR	2
Σ^+	3	NC stretch	2023.86	gas	IR	8
			2025.4	Ne	IR	9
			2029w	Ar	IR	2
			2032w N_2	Ar	IR	1
			2035w	N_2	IR	2

B_0 = 1.512 MW[4]IR[8]

DNC

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	ND stretch	2787.07	gas	IR	3,6
			2780.7	Ne	IR	9
			2769s	Ar	IR	2
			2733s N_2	Ar	IR	1
			2728s	N_2	IR	2
Π	2	Bend	374s	Ar	IR	2
			413s N_2	Ar	IR	1
			432s	N_2	IR	2
Σ^+	3	NC stretch	1938.7	NEs	IR	9
			1940w	Ar	IR	2
			1940w N_2	Ar	IR	1
			1937w	N_2	IR	2

B_0 = 1.273 MW[4]

[a] Tentative identification.

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HNSi

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NH stretch	3588.44	gas	EM	2
			3583	Ar	IR	1
Π	2	Bend	523	Ar	IR	1
Σ^+	3	NSi stretch	1198	Ar	IR	1

B_0 = 0.634 gas EM[2]MW[3]

DNSi

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	ND stretch	2669	Ar	IR	1
Π	2	Bend	395	Ar	IR	1
Σ^+	3	NSi stretch	1166	Ar	IR	1

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HN_2^+

$\tilde{X}$ $C_{\infty v}$ Structure: MW^4IR^{10}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NH stretch	3233.96	gas	CC,IR	5,11,12,14
Π	2	Bend	686.80	gas	DL	8,10
Σ^+	3	NN stretch	2257.87	gas	DL	6

B_0 = 1.541 $MW^{1,4,13}DL^{10}IR^{12}$

DN_2^+

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	ND stretch	2636.98	gas	LD	7
Π	2	Bend	543.18	gas	DL	9,10
Σ^+	3	NN stretch	2024.04	gas	DL	6,10

B_0 = 1.286 $MW^{2,3}$

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HOC^+

$\tilde{X}$ $C_{\infty v}$ Structure: MW^{1-3}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	OH stretch	3268.03	gas	LD	4

B_0 = 1.492 $MW^{1,2}LD^4$

DOC^+

$\tilde{X}$ $C_{\infty v}$
B_0 = 1.274 MW^3

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$HOSi^+$

$\tilde{X}$ $C_{\infty v}$ Structure: LD,DL^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	OH stretch	3662.36	gas	LD	1
	3	SiO stretch	1127.01	gas	DL	2

B_0 = 0.609 LD^1DL^2

$DOSi^+$

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	OD stretch	2716.56	gas	LD	1
	3	SiO stretch	1103.11	gas	DL	2

B_0 = 0.541 LD^1DL^2

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HCO

$3p\,^2\Pi$ $C_{\infty v}$

T_0 = 45540.1(3.3) gas MPI[19,20,28] $3p^2\Pi$–$\tilde{X}$ 187–222 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	799.9(1.4)[a]	gas	MPI	28
Σ^+	3	CO stretch	2177(3)	gas	MPI	20

A = 0.9(3); ϵ = 0.071 gas MPI[28]
B = 1.492(12) MPI[28]

$\tilde{B}\,^2A'$ C_s

T_0 = 38695.453(3) gas EM[6]LF[25,30]MPI[29]SEP[30] $\tilde{B}$–$\tilde{X}$ 235–410 nm
38595(35) Ar AB[5,11] $\tilde{B}$–$\tilde{X}$ 210–260 nm
38567(35) CO AB[5] $\tilde{B}$–$\tilde{X}$ 210–260 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	2597.1(2.0)	gas	EM,LF	6,25,30
					MPI	29
			2570(29)	Ar	AB	5,11
			2570(29)	CO	AB	5
	2	Mixed	1381.6(2.0)	gas	LF,MPI	25,29,30
			1375(35)	Ar	AB	5,11
			1375(35)	CO	AB	5
	3	Mixed	1065.6(2.8)	gas	LF,MPI	25,29,30
			1035(35)	Ar	AB	5,11
			1035(35)	CO	AB	5

A_0 = 16.039(5); $\frac{1}{2}(B_0 + C_0)$ = 1.151; $\frac{1}{4}(B_0 - C_0)$ = 0.022 LF[30]
τ_0 = 43(2) ns gas LF[27]

$\tilde{A}\,^2A''(\Pi)$ $C_{\infty v}$

T_0 = 9297(3) gas AB[1,3,8]LF[24,26] $\tilde{A}$–$\tilde{X}$ 460–860 nm
Bands with K′ > 0 are diffuse.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	3319(3)	gas	AB	1,3,8
	2	Bend	805	gas	AB	1,3,8
	3	CO stretch	1812.2	gas	AB	1,3,8

τ_{090} = 46(4) ns LF[15]
B_0 = 1.34 UV[1,3,8]

$\tilde{X}\,^2A'$ C_s Structure: MW[7] UV[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	2434.48	gas	LF,PE	17,18,25
					DL,LD	22,26
					IR	23
			2483m	Ar	IR	5
			2488m	CO	IR	4

$\tilde{X}\,^2A'$—Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	Bend	1080.76	gas	UV	1,3,8
					LS,LMR	9,10
					LF	25,26
			1087s	Ar	IR	5
			1090s	CO	IR	2,4
	3	CO stretch	1868.17	gas	IR	12,23
					LMR	13,25
			1863vs	Ar	IR	5
			1861vs	CO	IR	2,4

A_0 = 24.329; B_0 = 1.494; C_0 = 1.399 UV[1,3,8]MW[16]

DCO

$3p\,^2\Pi$ $C_{\infty v}$

T_0 = 45444.0(3.6) gas MPI[20,28] $3p^2\Pi$–$\tilde{X}$ 187–229 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	645.5(1.6)[a]	gas	MPI	28
Σ^+	3	CO stretch	1900(5)	gas	MPI	20

A = 0.9(3); ϵ = 0.069 MPI[28]
B = 1.221(12) MPI[28]

$\tilde{B}\,^2A'$ C_s

T_0 = 38628.4(2.0) gas MPI[29]
38568(70) Ar AB[5] $\tilde{B}$–$\tilde{X}$ 200–260 nm
38569(35) CO AB[5] $\tilde{B}$–$\tilde{X}$ 204–260 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CD stretch	1944.2(2.0)	gas	MPI	29
	2	Mixed	1212.9(2.5)	gas	MPI	29
			1150(35)	Ar	AB	5
			1150(35)	CO	AB	5
	3	Mixed	922.1(1.6)	gas	MPI	29
			925(35)	Ar	AB	5
			925(35)	CO	AB	5

$\tilde{A}\,^2A''$ (Π) $C_{\infty v}$

T_0 = 9162(3) gas UV[1,3,8]LF[24,26] $\tilde{A}$–$\tilde{X}$ 460–860 nm
Bands with K′ > 0 are diffuse.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2547(2)	gas	UV	1,3,8
Π	2	Bend	641.7(7)	gas	UV	1,3,8

B_0 = 1.10 UV[1,3,8]

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CD stretch	1909.77	gas	LMR,LF	14,26
			1926s	Ar	IR	5
			1937s	CO	IR	4
	2	Bend	846.5	gas	UV,LF	1,3,8,26
			850s	Ar	IR	5
			852s	CO	IR	2,4
	3	CO stretch	1794.59	gas	LMR,LF	14,26
			1803m	Ar	IR	5
			1800m	CO	IR	2,4

$A_0 = 14.734$; $B_0 = 1.281$; $C_0 = 1.171$ $UV^{1,3,8}MW^{21}$

[a] ω_2.

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HCF^+

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CF stretch	1368m	Ar	IR	1

DCF^+

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CF stretch	1369m	Ar	IR	1

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HNO^+

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	1090(40)	gas	PE	1
	3	NO stretch	1960(29)	gas	PE	1

DNO^+

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	870(40)	gas	PE	1
	3	NO stretch	1920(40)	gas	PE	1

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HCF

$\tilde{A}\ ^1A''$ C_s Structure: $AB^1LF^{5,6}$

T_0 = 17277.47 gas $AB^1CL^3LF^{5,10}$ $\tilde{A}-\tilde{X}$ 429–635 nm
17320(15) Ar AB^2 $\tilde{A}-\tilde{X}$ 469–546 nm

Evidence has been obtained[8,9] for perturbation of the $\tilde{A}$ state by high vibrational levels of the ground state and by the low-lying triplet state.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	1021.26	gas	AB,LF	1,7
			1000(20)	Ar	AB	2

A_0 = 25.69; B_0 = 1.162; C_0 = 1.107 AB^1LF^5
τ_0 = 2.45(10) μs gas LF^4
τ_1 = 2.57(16) μs; τ_2 = 12.5(8) μs gas EM^{13}

$\tilde{a}\ ^3A''$ C_s

T_0 = 5210(140) gas $PE^{12,14}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	1047(25)	gas	PE	14
	3	CF stretch	1232(25)	gas	PE	14

$\tilde{X}\ ^1A'$ C_s Structure: $AB^1LF^{5,6}SEP^{11}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	2643.04	gas	SEP	11
	2	Bend	1403.20	gas	AB,LF	1,7
					SEP	11
			1406vw	Ar	IR	2
	3	CF stretch	1189(25)	gas	PE	12,14
			1181.5m	Ar	IR	2

A_0 = 15.563; B_0 = 1.223; C_0 = 1.129 $AB^1LF^5SEP^{11}$

DCF

$\tilde{A}\ ^1A''$ C_s

T_0 = 17293.426(3) gas CL^3LF^6 $\tilde{A}-\tilde{X}$ 460–585 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	780(5)	gas	CL	3

A_0 = 15.10; B_0 = 1.014; C_0 = 0.945 LF^6

$\tilde{a}\ ^3A'$ C_s

T_0 < 5140(700) gas PE^{12}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	834(25)	gas	PE	12,14
	3	CF stretch	1216(25)	gas	PE	12,14

$\tilde{X}\ ^1A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	1046m	Ar	IR	2
	3	CF stretch	1193(25)	gas	PE	12,14
			1183m	Ar	IR	2

A_0 = 8.828; B_0 = 1.120; C_0 = 0.990 LF^6

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HCCl

$\tilde{A}\ ^1A''$ C_s

T_0 = 12274 gas AB^1LF^4 $\tilde{A}-\tilde{X}$ 550–820 nm
Ar AB^2 $\tilde{A}-\tilde{X}$ 570–750 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	865T	gas	AB	1
			855(50)	Ar	AB	2

Barrier to linearity = 2250 [1]

$\tilde{a}\ ^3A''$ C_s

T_0 = 1470(880) gas $PE^{5,6}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CCl stretch	850(60)	gas	PE	5,6

$\tilde{X}\ ^1A'$ C_s Structure: AB^1LF^3

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	1201wm	Ar	IR	2
	3	CCl stretch	810(25)	gas	PE	5,6
			815s	Ar	IR	2

A_0 = 15.759; B_0 = 0.605; C_0 = 0.581 AB^1LF^3

DCCl

$\tilde{A}\ ^1A''$ C_s

T_0 = 12274 gas AB[1] $\tilde{A}-\tilde{X}$ 550–820 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	657.2	gas	AB	1

$\tilde{X}\ ^1A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CCl stretch	805s	Ar	IR	2

A_0 = 8.75; B_0 = 0.557; C_0 = 0.525 AB[1]

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HCBr

$\tilde{a}\ ^3A''$ C_s

T_0 = 910(770) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CBr stretch	725(70)	gas	PE	2

$\tilde{X}\ ^1A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CBr stretch	683(25)	gas	PE	1,2

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HCl

$\tilde{a}\ ^1A'$ C_s

T_0 < 3150(700) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	Cl stretch	637(80)	gas	PE	2

$\tilde{X}\ ^3A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	Cl stretch	578(25)	gas	PE	1,2

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HSiF

$\tilde{A}\ ^1A''$ C_s Structure: LF[3,4]

T_0 = 23260.02 gas LF[2–4] $\tilde{A}-\tilde{X}$ 390–470 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	560T	gas	LF	2

τ_0 = 185(10) ns gas LF[2]
A_0 = 9.319; B_0 = 0.549; C_0 = 0.516 LF[3,4]

$\tilde{X}\ ^1A'$ C_s Structure: LF[3,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SiH stretch	1913s	Ar	IR	1
	2	Bend	860T	gas	LF	2
			859m	Ar	IR	1
	3	SiF stretch	834s	Ar	IR	1

A_0 = 7.58; B_0 = 0.564; C_0 = 0.524 LF[3,4]

DSiF

$\tilde{X}\ ^1A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SiD stretch	1387m	Ar	IR	1
	2	Bend	638w	Ar	IR	1
	3	SiF stretch	833m	Ar	IR	1

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HSiCl

$\tilde{A}\ ^1A''$ [a] C_s Structure: UV^1
$T_0 = 20717.65$ gas UV^1 $\tilde{A}-\tilde{X}$ 410–600 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SiH stretch	1250[b]	gas	UV	1
	2	Bend	568	gas	UV	1
	3	SiCl stretch	533	gas	UV	1

$\tau \cong 250$ ns gas LF^4
$A_0 = 9.857$; $B_0 \cong 0.246$; $C_0 \cong 0.240$ UV^1

$\tilde{X}\ ^1A'$ C_s Structure: UV^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	808	gas	UV	1
	3	SiCl stretch	522	gas	UV	1

$A_0 = 7.587$; $B_0 \cong 0.246$; $C_0 \cong 0.238$ UV^1

DSiCl

$\tilde{A}\ ^1A''$ C_s
$T_0 = 20718$ gas UV^1 $\tilde{A}-\tilde{X}$ 410–600 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	409	gas	UV	1

$A_0 \cong 3.99$; $B_0 \cong 0.238$; $C_0 \cong 0.155$ UV^1

$\tilde{X}\ ^1A'$ C_s
$A_0 \cong 5.26$; $B_0 \cong 0.235$; $C_0 \cong 0.225$ UV^1

[a] See Ref. 2.
[b] Alternate assignment[1] giving $\nu_1 = 1756$ is supported by analysis given in Ref. 3.

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HSiBr

$\tilde{A}\ ^1A''$ [a] C_s Structure: UV^1
$T_0 = 19903.0$ gas UV^1 $\tilde{A}-\tilde{X}$ 429–620 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SiH stretch	1270[b]	gas	UV	1
	2	Bend	540	gas	UV	1
	3	SiBr stretch	412	gas	UV	1

$A_0 = 9.906$; $B_0 \cong 0.159$; $C_0 \cong 0.156$ UV^1

$\tilde{X}\ ^1A'$ C_s Structure: UV^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SiH stretch	1548	gas	UV	1
	2	Bend	774	gas	UV	1
	3	SiBr stretch	408	gas	UV	1

$A_0 = 7.580$; $B_0 \cong 0.158$; $C_0 \cong 0.155$ UV^1

[a] See Ref. 2.
[b] Alternate assignment[1] giving $\nu_1 = 1785$ is supported by analysis given in Ref. 3.

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HSiI

$\tilde{A}\ ^1A''$ C_s Structure: AB^1
$T_0 = 18259.01$ gas AB^1 $\tilde{A}-\tilde{X}$ 460–560 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SiH stretch	1360	gas	AB	1
	2	Bend	485	gas	AB	1

$A_0 = 9.795$; $B_0 = 0.118$; $C_0 = 0.117$ AB^1

$\tilde{X}\ ^1A'$ C_s Structure: AB^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	727	gas	AB	1

$A_0 = 7.557$; $B_0 = 0.118$; $C_0 = 0.116$ AB^1

DSiI

$\tilde{A}\ ^1A''$ C_s
$T_0 = 18671.1$ gas AB^1 $\tilde{A}-\tilde{X}$ 460–560 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	356	gas	AB	1

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HGeCl

$\tilde{A}\ ^1A''$ C_s Structure: LF^3

T_0 = 21291.23(7) gas CL^2LF^3 $\tilde{A}-\tilde{X}$ 439–520 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	431.1	gas	CL,LF	2,3
	3	GeCl stretch	386.4	gas	CL	2

$\tilde{X}\ ^1A'$ C_s Structure: LF^3

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	GeH stretch	1862w	Ar	IR	1
	2	Bend	706	gas	CL	2
	3	GeCl stretch	439.2	gas	CL	2

DGeCl

$\tilde{A}\ ^1A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	360T	gas	CL	2

$\tilde{X}\ ^1A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	GeD stretch	1343vw	Ar	IR	1

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HGeBr

$\tilde{A}\ ^1A''$ C_s Structure: LF^2

T_0 = 20660.5(2) gas LF^2 $\tilde{A}-\tilde{X}$ 450–500 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	419.3(3)	gas	LF	2

$\tilde{X}\ ^1A'$ C_s Structure: LF^2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	GeH stretch	1858vs	Ar	IR	1
	2	Bend	695T	gas	LF	2
			701m	Ar	IR	1
	3	GeBr stretch	283s	Ar	IR	1

DGeBr

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	GeD stretch	1336vs	Ar	IR	1
	2	Bend	502m	Ar	IR	1
	3	GeBr stretch	281ms	Ar	IR	1

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HNO

T_0 = 48240 gas AB^5 198–208 nm
Diffuse bands.

$\tilde{A}\ ^1A''$ C_s Structure: $AB^{1,4}$

T_0 = 13154.4 gas $AB^{1,4}LF^{13,21}$ $\tilde{A}-\tilde{X}$ 550–770 nm
13118(2) Ar $AB^{2,3}$ $\tilde{A}-\tilde{X}$ 590–762 nm

Onset of predissociation at 16450(10). LF^{13}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH stretch	2854.17	gas	AB	4
	2	Bend	981.18	gas	AB	1
			982	Ar	AB	2,3
	3	NO stretch	1420.77	gas	AB	1
			1422	Ar	AB	2,3

τ = 25(4) μs $LF^{12,14,23}$
A_0 = 22.156; B_0 = 1.325; C_0 = 1.242 $AB^{1,4}MODR^{11,17}$

$\tilde{a}\ ^3A''$ C_s

T_0 = 6280(160) gas PE^{15}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	992(150)	gas	PE	15
	3	NO stretch	1468(140)	gas	PE	15

$\tilde{X}\ ^1A'$ C_s Structure: AB^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	1	NH stretch	2683.95	gas	IR,EM	9,16,22
			2716.3wm[a]	Ar	IR	8
			2756m	N_2	IR	8
	2	Bend	1500.82	gas	LS	10
			1505w	Ar	IR	8
			1511w	N_2	IR	8
	3	NO stretch	1565.34	gas	LS	10
			1563.2vs[a]	Ar	IR	8
			1568.5s	N_2	IR	8

A_0 = 18.476; B_0 = 1.411; C_0 = 1.296 $AB^1MW^{7,19}IR^{10,16,22}$

DNO

T_0 = 48400 gas AB^5 $\tilde{A}-\tilde{X}$ 196–206 nm
Diffuse bands.

$\tilde{A}\ ^1A''$ C_s
T_0 = 13180.3 gas AB^1 $\tilde{A}-\tilde{X}$ 550–770 nm
Onset of predissociation at 17010(10) $LF^{18,20}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	1	ND stretch	2176.49	gas	AB	4
	2	Bend	755.31	gas	AB	1
	3	NO stretch	1401.28	gas	AB	1

τ_{011} = 32.4(1.6) μs gas LF^{23}
A_0 = 12.629; B_0 = 1.199; C_0 = 1.088 $AB^{1,4}$

$\tilde{a}\ ^3A''$ C_s
T_0 = 6329(160) gas PE^{15}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	2	Bend	750(140)	gas	PE	15
	3	NO stretch	1452(140)	gas	PE	15

$\tilde{X}\ ^1A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	1	ND stretch	2025.14	gas	LS,IR	10,16
			2043wm	Ar	IR	8
			2074m	N_2	IR	8
	2	Bend	1153s	Ar	IR	8
			1158.5m	N_2	IR	8
	3	NO stretch	1546.88	gas	LS	10
			1547vs	Ar	IR	8
			1548vs	N_2	IR	8

A_0 = 10.524; B_0 = 1.292; C_0 = 1.146 $AB^1MW^{6,19}IR^{10,16}$

[a]Refined value from unpublished Fourier transform spectra.

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HPO

$\tilde{A}\ ^1A''$ C_s Structure: EM^6
T_0 = 19032.778(7) gas $EM^{1-4,6}$ $\tilde{A}-\tilde{X}$ 460–680 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	2	Bend	565.6	gas	EM	4
	3	PO stretch	857.7	gas	EM	4

A_0 = 8.269; B_0 = 0.643; C_0 = 0.594 $EM^{3,6}$

$\tilde{X}\ ^1A'$ C_s Structure: EM^6

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	1	PH stretch	2095ms	Ar	IR	5
	2	Bend	985.54(3)	gas	EM	2,6
			998.0w[a]	Ar	IR	8
	3	PO stretch	1188.04(3)	gas	EM	2,6
			1188s	Ar	IR	5

A_0 = 8.850; B_0 = 0.703; C_0 = 0.649 $EM^{3,6}MW^7$

DPO

$\tilde{A}\ ^1A''$ C_s

T_0 = 19116 gas EM[2-4] $\tilde{A}$–$\tilde{X}$ 460–680 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	2	Bend	438(5)	gas	EM	4
	3	PO stretch	846(5)	gas	EM	5

$\tilde{X}\ ^1A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	1	PD stretch	1529m	Ar	IR	5
	2	Bend	745	gas	EM	2
			750w	Ar	IR	5
	3	PO stretch	1177	gas	EM	2
			1186s	Ar	IR	5

[a] Formed from photodecomposition of $H_3P{\cdots}O_3$; O_2 or, possibly, H_2O trapped in adjacent site.

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HO_2^+

$\tilde{X}\ ^3A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	3	OO stretch	1560(50)[a]	gas	PE	1

DO_2^+

$\tilde{X}\ ^3A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	3	OO stretch	1595(50)[b]	gas	PE	1

[a] ω_e; $\omega_e x_e$ = 15(20) cm^{-1}.
[b] ω_e; $\omega_e x_e$ = 25(10) cm^{-1}.

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HCF^-

Threshold for electron detachment from ground-state HCF^- = 4370(40) gas PE[1,2]

$\tilde{X}\ ^2A''$ C_s Structure: PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	3	CF stretch	720(25)	gas	PE	1,2

DCF^-

Threshold for electron detachment from ground-state DCF^- = 4320(40) gas PE[2]

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	3	CF stretch	709(25)	gas	PE	1,2

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[1]K. K. Murray, D. G. Leopold, T. M. Miller, and W. C. Lineberger, J. Chem. Phys. **89**, 5442 (1988).
[2]M. K. Gilles, K. M. Ervin, J. Ho, and W. C. Lineberger, J. Phys. Chem. **96**, 1129 (1992).

$HCCl^-$

Threshold for electron detachment from ground-state $HCCl^-$ = 9760(40) gas PE[1,2]

$\tilde{X}\ ^2A''$ C_s Structure: PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	3	CCl stretch	445(25)	gas	PE	1,2

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[1]K. K. Murray, D. G. Leopold, T. M. Miller, and W. C. Lineberger, J. Chem. Phys. **89**, 5442 (1988).
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$HCBr^-$

Threshold for electron detachment from ground-state $HCBr^-$ = 11729(40) gas PE[1,2]

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	3	CBr stretch	393(25)	gas	PE	1,2

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[1]K. K. Murray, D. G. Leopold, T. M. Miller, and W. C. Lineberger, J. Chem. Phys. **89**, 5442 (1988).
[2]M. K. Gilles, K. M. Ervin, J. Ho, and W. C. Lineberger, J. Phys. Chem. **96**, 1129 (1992).

HCl^-

Threshold for formation of HCl ($\tilde{a}\,^1A'$) by electron detachment from ground-state HCl^- = 13550(40) gas PE[1,2]

Threshold for formation of HCl ($\tilde{X}\,^3A''$) by electron detachment from ground-state HCl^- = 11460(1380) gas PE[2]

$\tilde{X}\,^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	3	Cl stretch	370(25)	gas	PE	1,2

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[1]K. K. Murray, D. G. Leopold, T. M. Miller, and W. C. Lineberger, J. Chem. Phys. **89**, 5442 (1988).
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HNO^-

Threshold for electron detachment from ground-state HNO^- = 2729(120) PE[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	1	NH stretch	2750.78	gas	PD	2
	3	NO stretch	1153(170)	gas	PE	1

A_0 = 15.233; $\frac{1}{2}(B_0 + C_0)$ = 1.097; $\frac{1}{2}(B_0 - C_0)$ = 0.034 PD[2]

DNO^-

Threshold for electron detachment from ground-state DNO^- = 2660(120) PE[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	3	NO stretch	1113(170)	gas	PE	1

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HNF

$\tilde{A}\,^2A'$ C_s Structure: AB^3LF^5

T_0 = 20141.26(1) gas $AB^{1,3}CL^4LF^5$ $\tilde{A}-\tilde{X}$ 380–650 nm
20140(20) Ar AB^2 $\tilde{A}-\tilde{X}$ 395–497 nm

Onset of predissociation into NH + F identified at 23800(500) gas LF^5PF^6

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	2	Bend	1074	gas	AB	3
			1033[a]	Ar	AB	2
	3	NF stretch	1121(5)	gas	AB	3

τ_0 = 3.6 μs gas LF^5
A_0 = 27.570(5); B_0 = 1.033; C_0 = 0.992 AB^3

$\tilde{X}\,^2A''$ C_s Structure: AB^3LF^5

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	2	Bend	1419	gas	CL	4
			1432m	Ar	IR	2
	3	NF stretch	1000s	Ar	IR	2

A_0 = 17.688(8); B_0 = 1.039; C_0 = 0.978 AB^3

DNF

$\tilde{A}\,^2A'$ C_s

T_0 = 20168.4(8) gas LF^5 $\tilde{A}-\tilde{X}$ 400–500 nm
20220 Ar AB^2 $\tilde{A}-\tilde{X}$ 413–495 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	2	Bend	837.4(8)[a]	gas	LF	5
			798[b]	Ar	AB	2
	3	NF stretch	1124[c]	gas	LF	5

τ_0 = 3.5(2) μs gas LF^5
B^b = 0.894(2) LF^5

$\tilde{X}\,^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	2	Bend	1069[d]	Ar	IR	2
	3	NF stretch	1000s	Ar	IR	2

B^b = 0.946(2) LF^5

[a] $\omega_2 + 0.5x_{12}$.
[b] Average value.
[c] $\omega_3 + 2x_{33} + 0.5x_{13}$.
[d] Overlapped by NF_2 absorption.

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HO_2

Broad, unstructured gas–phase absorption between 200 and 280 nm, with maximum near 205 nm.[2,3,5,6,37]

$\tilde{A}\ ^2A'$ C_s

T_0 = 7029.684(2) gas AB[9,15]EM[10,16,19,20,35] $\tilde{A}$–$\tilde{X}$ 1.13–2.12 μm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	1	OH stretch	3268.5	gas	EM	35
	2	Bend	1285	gas	EM	35
	3	OO stretch	929.068	gas	AB,EM	15,19,28 35

A_0 = 20.486; B_0 = 1.021; C_0 = 0.968 EM[16,20,35]

$\tilde{X}\ ^2A''$ C_s Structure: MW[14]UV[21]LMR[23]ESR[23]IR[31,33]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	1	OH stretch	3436.20	gas	LD	26
			3415.1	Ne	IR	36
			3412.5s[a]	Ar	IR	1,4,7
			3400	O_2	IR	32
	2	Bend	1391.75	gas	DL,IR	24,39
			1397.8	Ne	IR	36
			1388.5vs[a]	Ar	IR	1,4,7
			1392	O_2	IR	32
	3	OO stretch	1097.63	gas	LMR	18,29
					DL,IR	29,38,39
			1100.3	Ne	IR	36
			1101.1s[a]	Ar	IR	1,4,7
			1109	O_2	IR	32

A_0 = 20.356; B_0 = 1.118; C_0 = 1.056 LMR[8,11,12,18]MW[13,17,25]EM[16]

DO_2

$\tilde{A}\ ^2A'$ C_s

T_0 = 7041.1(1) gas AB[9]EM[10,19,21] $\tilde{A}$–$\tilde{X}$ 1.13–2.12 μm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	3	OO stretch	940(28)	gas	AB,EM	8,19

A_0 = 11.147(7); B_0 = 0.970; C_0 = 0.887 EM[21]

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	1	OD stretch	2549.22	gas	LD,DL	31
			2529.2	Ne	IR	36
			2529.5m[a]	Ar	IR	1,4,7
			2521	O_2	IR	32
	2	Bend	1020.16	gas	LMR,DL	22,33
			1027.3	Ne	IR	36
			1019.9s[a]	Ar	IR	1,4,7
			1024	O_2	IR	32
	3	OO stretch	1121.47	gas	LMR,DL	22,33
			1124.7	Ne	IR	36
			1122.9vw[a]	Ar	IR	7

A_0 = 11.194; B_0 = 1.056; C_0 = 0.961 MW[14,27,34]EM[21]LMR[22,23,34]ESR[23]

[a] Refined value from unpublished Fourier transform spectra.

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HSO

$\tilde{A}\ ^2A'$ C_s Structure: LF[2,3]

T_0 = 14367 gas CL[1] $\tilde{A}-\tilde{X}$ 520–960 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	3	SO stretch	702(5)	gas	CL	1

τ_{001} = 74(1) μs gas LF[6]
Values decrease steadily as v_3' increases.
A_{003} = 9.735; B_{003} = 0.565; C_{003} = 0.527 LF[2]

$\tilde{X}\ ^2A''$ C_s Structure: LF[2,3]MW[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	2	Bend	1063(5)	gas	CL	1
	3	SO stretch	1009.36	gas	LMR	5

A_0 = 9.990; B_0 = 0.684; C_0 = 0.638 LF[2]MW[4]

DSO

$\tilde{A}\ ^2A'$ C_s

T_0 = 14371 gas CL[1]LF[8] $\tilde{A}-\tilde{X}$ 520–960 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	2	Bend	575(10)	gas	LF	7
	3	SO stretch	702(10)	gas	CL	1

τ^a = 76 μs gas LF[6]
A_0^b = 4.969(7); B_0^b = 0.566; C_0^b = 0.507 LF[7,8]

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	2	Bend	770(10)	gas	CL	1
	3	SO stretch	1029(15)	gas	CL	1

A_0 = 5.295; B_0 = 0.662; C_0 = 0.586 LF[3]MW[4]

[a] Measured at 606.0 nm.
[b] Extrapolated from values for 021 and 022.

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HS_2

gas AB[1-3] 297–380 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	1	SH stretch	2500T	gas	AB	3
	2	Bend	900T	gas	AB	3
	3	SS stretch	600T	gas	AB	3

$\tilde{A}\ ^2A'$ C_s

T_0 = 7255(7) gas CL[4] $\tilde{A}-\tilde{X}$ 950–2100 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	3	SS stretch	504(4)	gas	CL	4

A_0 = 9.7(5) CL[4]

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	2	Bend	904(8)	gas	CL	4
	3	SS stretch	595(4)	gas	CL	4

A_0 = 9.7(5) CL[4]

DS_2

$\tilde{A}\ ^2A'$ C_s

T_0 = 7264(15) gas CL[4] $\tilde{A}-\tilde{X}$ 950–2100 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	3	SS stretch	502(15)	gas	CL	4

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	2	Bend	696(20)	gas	CL	4
	3	SS stretch	591(10)	gas	CL	4

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HOF^+

$\tilde{B}\ ^2A'$ C_s

T_0 = 25740(500) gas PE[1]

$\tilde{A}\ ^2A'$ C_s

T_0 = 14440(320) gas PE[1]

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	3	OF stretch	946[a]	gas	PE	1

[a] Average value.

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$HOCl^+$

$\tilde{C}\ ^2A'$ C_s

T^a = 36150(900) gas PE[1]

$\tilde{B}\ ^2A''$ C_s

T^a = 28080(900) gas PE[1]

$\tilde{A}\ ^2A'$ C_s

T_0 = 7829(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	2	Bend	1250(80)	gas	PE	1
	3	OCl stretch	700(50)	gas	PE	1

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	3	OCl stretch	829(50)	gas	PE	1

[a] From vertical ionization potential.

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HO_2^-

Threshold for electron detachment from ground-state HO_2^- is 8700(140).[1]

$\tilde{X}\ ^1A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	3	OO stretch	775(250)	gas	PE	1

DO_2^-

Threshold for electron detachment from ground-state DO_2^- is 8790(140).[1]

$\tilde{X}\ ^1A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	3	OO stretch	900(250)	gas	PE	1

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HOF

In the gas phase, unstructured absorption occurs, with a threshold near 380 nm and with constantly increasing intensity out to the 200 nm observation limit.[6,8]

$\tilde{X}$ C_s Structure: $MW^{3,5}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	1	OH stretch	3577.93	gas	IR	4,10
			3572ms	Ar	IR	8
			3537.1s	N_2	IR	2,8
			3550s	O_2	IR	8
	2	Bend	1353.40	gas	IR	4,7
			1350vs	Ar	IR	8
			1359.0vs	N_2	IR	2,8
			1350vs	O_2	IR	8
	3	OF stretch	889.08	gas	IR	4,7
			888ms	Ar	IR	8
			886.0wm	N_2	IR	1,2,8
			884ms	O_2	IR	8

A_0 = 19.535; B_0 = 0.893; C_0 = 0.851 $MW^{3,5}IR^{7,9}$

DOF

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	1	OD stretch	2643.5	gas	IR	4
			2573wm[a]	N_2	IR	1
	2	Bend	1002.01	gas	IR	4,7
			1029.5m[a]	N_2	IR	1
	3	OF stretch	891.00	gas	IR	4,7
			885.5w[a]	N_2	IR	1

A_0 = 10.544; B_0 = 0.854; C_0 = 0.787 $MW^{3,5}IR^{7}$

[a] DOF··DF.

References

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HOCl

$\tilde{X}$ C_s Structure: $IR^{2,14}MW^{4,12}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	1	OH stretch	3609.48	gas	IR	2,6,7,11
			3581	Ar	IR	3
	2	Bend	1238.62	gas	IR	1,5,6,8,9 11,13
			1239	Ar	IR	3
	3	OCl stretch	724.36	gas	IR	5,6,8,11 13
			728	Ar	IR	3

A_0 = 20.464; B_0 = 0.504; C_0 = 0.491 $IR^{2,11}MW^{4,10}$

DOCl

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	1	OD stretch	2665.58	gas	IR	1,2,11,14
			2647	Ar	IR	3
	2	Bend	909.63	gas	IR	1,11,14
			911	Ar	IR	3
	3	OCl stretch	723.25	gas	IR	11,14
			728	Ar	IR	3

A_0 = 11.052; B_0 = 0.477; C_0 = 0.456 $IR^{2,14}MW^{4,12}$

References

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[13]W. J. Lafferty and W. B. Olson, J. Mol. Spectrosc. **120**, 359 (1986).
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HOBr

$\tilde{X}$ C_s Structure: MW^3

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	1	OH stretch	3610	gas	IR	2
			3590	Ar	IR	1
	2	Bend	1162.57	gas	IR	4
			1164	Ar	IR	1
	3	OBr stretch	620.2	gas	IR	2,4,5
			626.0	Ar	IR	1

A_0 = 20.470; B_0 = 0.353; C_0 = 0.346 MW^3

DOBr

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	1	OD stretch	2652	Ar	IR	1
	2	Bend	854	Ar	IR	1
	3	OBr stretch	621.8	Ar	IR	1

A_0 = 11.027; B_0 = 0.331; C_0 = 0.321 MW^3

References

[1]I. Schwager and A. Arkell, J. Am. Chem. Soc. **89**, 6006 (1967).
[2]I. Barnes, V. Bastian, K. H. Becker, R. Overath, and T. Zhu, Int. J. Chem. Kinet. **21**, 499 (1989).
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HOI

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	1	OH stretch	3620	gas	IR	2
			3597m	N_2	IR	1
	2	Bend	1069.8	gas	IR	2
			1075	Ar	IR	1
			1103m	N_2	IR	1
	3	OI stretch	577	Ar	IR	1
			575m	N_2	IR	1

DOI

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	1	OD stretch	2653	N_2	IR	1
	2	Bend	808	N_2	IR	1
	3	OI stretch	571	N_2	IR	1

References

[1]N. Walker, D. E. Tevault, and R. R. Smardzewski, J. Chem. Phys. **69**, 564 (1978).
[2]I. Barnes, K. H. Becker, and J. Starcke, Chem. Phys. Lett. **196**, 578 (1992).

HS_2^-

Threshold for electron detachment from ground-state HS_2^- = 15390(185) gas PE[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	3	SS stretch	610(80)	gas	PE	1

DS_2^-

Threshold for electron detachment from ground-state DS_2^- = 15429(120) gas PE[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	3	SS stretch	580(90)	gas	PE	1

References

[1]S. Moran and G. B. Ellison, J. Phys. Chem. **92**, 1794 (1988).

XeOH

Unstructured gas-phase emission[1] between 225 and 240 nm, with maximum near 234 nm.
$\tau \leq 4$ ns gas EM[1]

References

[1]M. H. R. Hutchinson, Chem. Phys. Lett. **54**, 359 (1978).

FHF^-

$\tilde{X}$ $D_{\infty h}$ Structure: DL[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
Σ_g^+	1	Sym. stretch	583.05	gas	DL	5
Π_u	2	Bend	1286.03	gas	DL	5
			1217m Cs	Ar	IR	1,2
Σ_u^+	3	Asym. stretch	1331.15	gas	DL	5
			1379	Ne	IR	4
			1377.0s	Ar	IR	3,4
			1364vs Cs	Ar	IR	1,2

B_0 = 0.334 DL[5]

FDF^-

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
Π_u	2	Bend	880m Cs	Ar	IR	1,2
Σ_u^+	3	Asym. stretch	965s	Ar	IR	3,4
			969vs Cs	Ar	IR	1,2

References

[1]B. S. Ault, J. Phys. Chem. **82**, 844 (1978).
[2]B. S. Ault, J. Phys. Chem. **83**, 837 (1979).
[3]S. A. McDonald and L. Andrews, J. Chem. Phys. **70**, 3134 (1979).
[4]R. D. Hunt and L. Andrews, J. Chem. Phys. **87**, 6819 (1987).
[5]K. Kawaguchi and E. Hirota, J. Chem. Phys. **87**, 6838 (1987).

$FHCl^-$

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
Σ^+	3	"Asym." stretch	933 Cs	Ar	IR	1

$FDCl^-$

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
Σ^+	3	"Asym." stretch	668 Cs	Ar	IR	1

References

[1]B. S. Ault, J. Phys. Chem. **83**, 837 (1979).

$FHBr^-$

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
Σ^+	3	"Asym." stretch	849 Cs	Ar	IR	1

$FDBr^-$

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
Σ^+	3	"Asym." stretch	609 Cs	Ar	IR	1

References

[1]B. S. Ault, J. Phys. Chem. **83**, 837 (1979).

FHI^-

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
Σ^+	3	"Asym." stretch	763 Cs	Ar	IR	1

FDI^-

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
Σ^+	3	"Asym." stretch	548 Cs	Ar	IR	1

References

[1]B. S. Ault, J. Phys. Chem. **83**, 837 (1979).

$ClHCl^-$

An absorption maximum which appeared at 287 nm in argon–matrix studies[2] of the 122–nm photolysis of Ar:HCl or $Ar:H_2O:Cl_2$ samples and in argon–matrix studies[6] of the electron bombardment of Ar:HCl samples has been assigned to an electronic transition of $ClHCl^-$.

$\tilde{X}$ $D_{\infty h}$ Structure: DL[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
Σ_g^+	1	Sym. stretch	259.3[ab]	Ar	IR	1–3,7
			252.8[b]	Kr	IR	7
			248.8[b]	Xe	IR	7
Σ_u^+	3	Asym. stretch	722.90	gas	DL	5
			695.6s[a]	Ar	IR	1–3,7
			662.8	Kr	IR	7
			644.1	Xe	IR	7

$B_0 = 0.0974$ DL[5]

$ClDCl^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
Σ_g^+	1	Sym. stretch	267[ab]	Ar	IR	1–3
			255.3[b]	Kr	IR	7
Σ_u^+	3	Asym. stretch	463[a]	Ar	IR	1–3
			437.7	Kr	IR	7

[a] Attributed by Ref. 1 to the uncharged species. Reassigned to the anion by Ref. 2, and Ref. 3 demonstrated that the absorptions did not appear when the atoms were present but a supplementary high energy source suitable for inducing photoionization or electron transfer was not. The increase in the rate of isotopic exchange in the $^{37}Cl + H^{35}Cl$ reaction for vibrationally excited HCl[4] indicates that there is a potential barrier, rather than a minimum, for the ClHCl neutral species.

[b] $(\nu_1 + \nu_3) - \nu_3$.

References

[1]P. N. Noble and G. C. Pimentel, J. Chem. Phys. **49**, 3165 (1968).
[2]D. E. Milligan and M. E. Jacox, J. Chem. Phys. **53**, 2034 (1970).
[3]C. A. Wight, B. S. Ault, and L. Andrews, J. Chem. Phys. **65**, 1244 (1976).
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[5]K. Kawaguchi, J. Chem. Phys. **88**, 4186 (1988).
[6]J. Hacaloglu and L. Andrews, Chem. Phys. Lett. **160**, 274 (1989).
[7]M. Räsänen, J. Seetula, and H. Kunttu, J. Chem. Phys. **98**, 3914 (1993).

$ClHBr^-$

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
Σ^+	3	"Asym." stretch	742 Cs	Ar	IR	1

ClDBr⁻

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
Σ^+	3	"Asym." stretch	524 Cs	Ar	IR	1

References

[1]B. S. Ault and L. Andrews, J. Chem. Phys. **64**, 1986 (1976).

ClHI⁻

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
Σ^+	3	"Asym." stretch	644 Cs	Ar	IR	1

ClDI⁻

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
Σ^+	3	"Asym." stretch	456 Cs	Ar	IR	1

References

[1]C. M. Ellison and B. S. Ault, J. Phys. Chem. **83**, 832 (1979).

BrHBr⁻

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
Σ_g^+	1	Sym. stretch	164[ab]	Ar	IR	1,2
			158.5[b]	Kr	IR	3
			151.9[b]	Xe	IR	3
Σ_u^+	3	Asym. stretch	728s[a]	Ar	IR	1,2
			686.6	Kr	IR	3
			645.6	Xe	IR	3

BrDBr⁻

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
Σ_g^+	1	Sym. stretch	170[ab]	Ar	IR	1,2
			163.8[b]	Kr	IR	3
			157.9[b]	Xe	IR	3
Σ_u^+	3	Asym. stretch	498s[a]	Ar	IR	1,2
			465.5	Kr	IR	3
			434.6	Xe	IR	3

[a] Attributed in Ref. 1 to the uncharged species. Reassigned to the anion by Ref. 2. See $ClHCl^-$.
[b] $(\nu_1 + \nu_3) - \nu_3$.

References

[1]V. Bondybey, G. C. Pimentel, and P. N. Noble, J. Chem. Phys. **55**, 540 (1971).
[2]D. E. Milligan and M. E. Jacox, J. Chem. Phys. **55**, 2550 (1971).
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BrHI⁻

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
Σ^+	3	"Asym." stretch	666 Cs	Ar	IR	1

BrDI⁻

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
Σ^+	3	"Asym." stretch	470 Cs	Ar	IR	1

References

[1]C. M. Ellison and B. S. Ault, J. Phys. Chem. **83**, 832 (1979).

IHI⁻

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
Σ_g^+	1	Sym. stretch	121[ab]	Ar	IR	1,2
			116.7[b]	Kr	IR	3
			109.0[b]	Xe	IR	3
Σ_u^+	3	Asym. stretch	682m[a]	Ar	IR	1,2
			647.4	Kr	IR	3
			580.8	Xe	IR	3

IDI^-

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
Σ_g^+	1	Sym. stretch	124[ab]	Ar	IR	1,2
Σ_u^+	3	Asym. stretch	470m[a]	Ar	IR	1,2

[a] Attributed in Ref. 1 to the uncharged species. Reassigned by Ref. 2 to the anion. See $ClHCl^-$.
[b] $(\nu_1 + \nu_3) - \nu_3$.

References

[1]P. N. Noble, J. Chem. Phys. **56**, 2088 (1972).
[2]C. M. Ellison and B. S. Ault, J. Phys. Chem. **83**, 832 (1979).
[3]M. Räsänen, J. Seetula, and H. Kunttu, J. Chem. Phys. **98**, 3914 (1993).

HAr_2^+ [a]

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
Σ_u^+	3	Asym. stretch	905wm[b]	Ar	IR	1,2,4

DAr_2^+ [a]

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
Σ_u^+	3	Asym. stretch	644s[b]	Ar	IR	1–4

[a] May be complexed with two or four additional Ar atoms.[2]
[b] Assigned in Ref. 1 to vibration of uncharged H (or D) atoms trapped in the Ar lattice. Reassigned by Ref. 2 to the cation. Peak at 644 cm^{-1} was prominent in deuteron radiolysis experiments.[3] Ref. 4 demonstrated that the absorptions did not appear when H or D atoms were present but a supplementary high energy source suitable for inducing photoionization or electron transfer was not.

References

[1]V. E. Bondybey and G. C. Pimentel, J. Chem. Phys. **56**, 3832 (1972).
[2]D. E. Milligan and M. E. Jacox, J. Mol. Spectrosc. **46**, 460 (1973).
[3]L. Andrews, B. S. Ault, J. M. Grzybowski, and R. O. Allen, J. Chem. Phys. **62**, 2461 (1975).
[4]C. A. Wight, B. S. Ault, and L. Andrews, J. Chem. Phys. **65**, 1244 (1976).

HKr_2^+ [a]

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
Σ_u^+	3	Asym. stretch	852m[b]	Kr	IR	1–3

DKr_2^+ [a]

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
Σ_u^+	3	Asym. stretch	607m[b]	Kr	IR	1

[a] May be complexed with two or four additional Kr atoms.[2]
[b] Assigned in Ref. 1 to vibration of uncharged H (or D) atoms trapped in the Kr lattice. Reassigned by Ref. 2 to the cation. Ref. 3 demonstrated that the 852 cm^{-1} absorption did not appear when H atoms were present but a supplementary high energy source suitable for inducing photoionization or electron transfer was not.

References

[1]V. E. Bondybey and G. C. Pimentel, J. Chem. Phys. **56**, 3832 (1972).
[2]D. E. Milligan and M. E. Jacox, J. Mol. Spectrosc. **46**, 460 (1973).
[3]C. A. Wight, B. S. Ault, and L. Andrews, J. Chem. Phys. **65**, 1244 (1976).

HXe_2^+

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
Σ_g^+	1	Sym. stretch	111.9[a]	Xe	IR	1
Σ_u^+	3	Asym. stretch	729.9	Xe	IR	1

DXe_2^+

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
Σ_g^+	1	Sym. stretch	118.0[a]	Xe	IR	1
Σ_u^+	3	Asym. stretch	516.7	Xe	IR	1

[a] $(\nu_1 + \nu_3) - \nu_3$.

References

[1]H. Kunttu, J. Seetula, M. Räsänen, and V. A. Apkarian, J. Chem. Phys. **96**, 5629 (1992).

Ar_2H [a]

$\tilde{A}$
In an Ar matrix, unstructured emission with maximum at 60200 (166 nm)[1]
τ = 65 ns Ar EM[1]

Ar_2D

$\tilde{A}$
In an Ar matrix, unstructured emission with maximum at 60350 (166 nm)[1]
τ = 64 ns Ar EM[1]

[a] Excimer.

References

[1]M. Kraas and P. Gürtler, Chem. Phys. Lett. **174**, 396 (1990).

ArKrD [a]

$\tilde{A}$

In an Ar matrix, unstructured emission with maximum at 56150 (178 nm)[1]

τ = 37 ns Ar EM[1]

[a] Excimer.

References

[1]M. Kraas and P. Gürtler, Chem. Phys. Lett. **183**, 264 (1991).

ArXeH [a]

$\tilde{A}$

In an Ar matrix, unstructured emission with maximum at 46200 (216 nm)[1]

ArXeD

$\tilde{A}$

In an Ar matrix, unstructured emission with maximum at 45750 (218 nm)[1]

[a] Excimer.

References

[1]M. Kraas and P. Gürtler, Chem. Phys. Lett. **183**, 264 (1991).

Kr_2H [a]

$\tilde{A}$

T_0 = 64500 Kr AB[4]

In a Kr matrix, unstructured emission with maximum at 49600 (202 nm)[1-4]

τ = 48 ns Kr EM[2]

Kr_2D

$\tilde{A}$

T_0 = 64800 Kr AB[4]

In an Ar matrix, unstructured emission with maximum at 50750 (197 nm)[5]

In a Kr matrix, unstructured emission with maximum at 49700 (201 nm)[2,4]

τ = 58 ns Ar EM[5]
46 ns Kr EM[2]

[a] Excimer. Extensive delocalization of positive charge in Kr and Xe matrices.

References

[1]M. Creuzburg and F. Wittl, J. Mol. Struct. **222**, 127 (1990).
[2]M. Kraas and P. Gürtler, Chem. Phys. Lett. **174**, 396 (1990).
[3]F. Wittl, M. Creuzburg, and R. Schriever, J. Lumin. **48/49**, 611 (1991).
[4]H. Kunz, J. G. McCaffrey, M. Chergui, R. Schriever, Ö. Ünal, V. Stepanenko, and N. Schwentner, J. Chem. Phys. **95**, 1466 (1991).
[5]M. Kraas and P. Gürtler, Phys. Stat. Sol. (a) **130**, K229 (1992).

KrXeH [a]

$\tilde{A}$

T_0 = 50330(10) Kr AB[1-3]

In a Kr matrix, unstructured emission with maximum at 46500 (215 nm)[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
			742(10)	Kr	AB	1,3

τ = 18 ns Kr EM[1]

KrXeD

$\tilde{A}$

T_0 = 50170(10) Kr AB[1-3]

In a Kr matrix, unstructured emission with maximum at 46150 (217 nm)[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
			580(10)	Kr	AB	1,3

τ = 17 ns Kr EM[1]

[a] Excimer. Extensive delocalization of positive charge in Kr and Xe matrices.

References

[1]M. Kraas and P. Gürtler, Chem. Phys. Lett. **183**, 264 (1991).
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Xe_2H [a]

$\tilde{A}$

T_0 = 50240(20) Ar AB[4,7]
Kr AB[2,4]
50130(10) Xe AB[1,9]

In an Ar matrix, unstructured emission with maximum at 39800 (251 nm)[4,7]

In a Kr matrix, unstructured emission with maximum at 39600 (252 nm)[2,4,6]

In a Xe matrix, unstructured emission with maximum at 39700 (252 nm)[2,4,5,6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
			645(10)	Ar	AB	4,7
			600T	Kr	AB	4
			605(10)	Xe	AB	1

τ = 61 ns Ar EM[4]
54 ns Kr EM[4]
41 ns Xe EM[4]

Xe_2D

$\tilde{A}$

In a neon matrix, Xe_2D has a broad excitation profile with onset near 52400 and maximum near 58000.[3]

T_0 = 50070(10) Ar AB[7]
50055(10) Xe AB[1,9]

In a Ne matrix, unstructured emission with maximum at 40100 (249 nm)[3]
In an Ar matrix, unstructured emission with maximum at 39800 (251 nm)[7]
In a Kr matrix, unstructured emission with maximum at 39500 (253 nm)[8]
In a Xe matrix, unstructured emission with maximum at 39500 (253 nm)[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			428(10)	Ar	AB	7
			476(10)	Xe	AB	1

τ = 70 ns Ne EM[4]
61 ns Ar EM[8]
54 ns Kr EM[8]
39 ns Xe EM[4]

[a] Excimer. Extensive delocalization of positive charge in Kr and Xe matrices.

References

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6.3. Triatomic Nonhydrides

Li_3

$\tilde{C}$ D_{3h}[a]

T_0 = 21541 gas MPI[3] $\tilde{C}$–$\tilde{X}$ 450–472 nm
B = 0.57 MPI[4]

$\tilde{A}$ D_{3h}[a]

T_0 = 14583 gas MPI[2,3] $\tilde{A}$–$\tilde{X}$ 660–706 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	326	gas	MPI	2

Structure in the $\tilde{A}$ state is characterized[2] by a radial frequency ω_0 = 191 and linear and quadratic Jahn-Teller parameters k = 0.77 and g = 0.15.
B = 0.57 MPI[4]

$\tilde{X}$ D_{3h}[a] Structure: MPI[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	302	gas	MPI	3
			303	Xe	Ra	1

Barrier to pseudorotation = 26; pseudorotation frequency = 34 MPI[3]
B = 0.584 MPI[4]

[a] Subject to dynamic Jahn-Teller distortion.

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Na_3

$\tilde{D}$ $^2E''(^2A_2)$ $D_{3h}(C_{2v})$[a]

gas MPI[4,5,14]DPI[12]PE[14] $\tilde{D}$–$\tilde{X}$ 410–440 nm

$\tilde{C}$ $^2E''(^2A_2)$ $D_{3h}(C_{2v})$[a]

T_0 = 20813 gas MPI[2,4,6]DPI[8,12] $\tilde{C}$–$\tilde{X}$ 467–481 nm
Higher vibrational bands are predissociated.[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	135	gas	MPI,PF	8

Extensive vibronic structure has been tentatively assigned[8] to energy levels derived from excitation of ν_2 (e'), perturbed by dynamic Jahn-Teller interaction.
τ_0 = 7(3) ns gas MPI[7]

$\tilde{B}''$ $^2B_2$

T^b = 19200 gas DPI[12]

$\tilde{B}, \tilde{B}'$ $^2E'(^2A_1, ^2B_2)$ D_{3h}[a]

T_0 = 15996 gas MPI[1-6]DPI[12] $\tilde{B}$–$\tilde{X}$ 550–625 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	127	gas	MPI	1,3

$\tau_{\tilde{B}}$(16255) = 14(5) ns gas MPI[7]
$\tau_{\tilde{B}}$(17418) = 7(3) ns gas MPI[7]
Vibronic pseudorotation accompanied by fractional quantization occurs.[3]

$\tilde{A}$ $^2E''(^2A_2)$ $D_{3h}(C_{2v})$[a] Structure: MPI[15,16]

T_0 = 14894.769(4) gas MPI[1,2,4-6,11,13,15,16]DPI[12] $\tilde{A}$–$\tilde{X}$ 658–675 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	150	gas	MPI	11
	2	Bend	121	gas	MPI	4,6,11
	3	Asym. stretch	47	gas	MPI	4,6,11

Vibronic structure assigned in Ref. 11. First three bands are partially localized; pseudorotation barrier = 196.
τ_0 = 60(10) ns gas MPI[7]
A_0 = 0.166; B_0 = 0.085; C_0 = 0.056 MPI[15,16]

$\tilde{A}'\ ^2A_1$ D_{3h}
T^b = 13500 gas DPI[12]

$\tilde{X}\ ^2E'(^2B_2)$ $D_{3h}(C_{2v})^a$ Structure: MPI[15,16]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	139	gas	MPI, SEP	4,6 9,10
	2	Bend	49.5	gas	MPI, SEP	4,6 9,10
	3	Asym. stretch	87	gas	MPI, SEP	6,9,10

A_0 = 0.177; B_0 = 0.085; C_0 = 0.057 MPI[15,16]

[a] Distorted by Jahn-Teller interaction.
[b] Band maximum.

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Cu_3

$^2A_1'$ D_{3h}
T_0 = 18524 gas DPI[3,8]LF[5,6]AB[9] 522–567 nm
In an argon matrix, an absorption maximum at 18760 (533 nm) has been assigned[1] to Cu_3.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	146.4(5)	gas	DPI,LF AB	3,5,8 9
e'	2	Deformation	243	gas	DPI LF,AB	3,8 5,9

τ_0 = 35(5) ns gas MPI[3]LF[5]

$\tilde{X}\ ^2E'$ D_{3h}[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	269.5 354T	gas Ar	LF Ra	5,7 2,4

[a] Distorted by Jahn-Teller interaction.

References

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Cu_2Ag

$\tilde{A}$ C_{2v}
T_0 = 13188.3 gas MPI[1] $\tilde{A}$–$\tilde{X}$ 722–758 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CuCu stretch	253.6	gas	MPI	1
	2	CuAg s-stretch	172.6	gas	MPI	1
b_2	3	CuAg a-stretch	171.5H	gas	MPI	1

τ_{010} = 34.9(12.3) μs gas MPI[1]

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	CuAg a-stretch	201.0(6)	gas	MPI	1

References

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Cu_2Au

$\tilde{A}$ C_{2v}

T_0 = 17217.5 gas MPI[1] $\tilde{A}$–$\tilde{X}$ 572–587 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CuCu stretch	253.4(3)	gas	MPI	1
	2	CuAu s-stretch	148.6(4)	gas	MPI	1

τ_0 = 744(134) ns gas MPI[1]

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CuAu s-stretch	159.7(4)	gas	MPI	1

References

[1]G. A. Bishea, C. A. Arrington, J. M. Behm, and M. D. Morse, J. Chem. Phys. **95**, 8765 (1991).

CuAgAu

$\tilde{A}$ C_s

T_0 = 17470.8(3) gas MPI[1] $\tilde{A}$–$\tilde{X}$ 532–575 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CuAg stretch	234.6	gas	MPI	1
	2	CuAu stretch	168.6	gas	MPI	1
	3	AgAu stretch	130.9	gas	MPI	1

τ_{001} = 693(91) ns gas MPI[1]

$\tilde{X}$ $^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CuAg stretch	222.8(3)	gas	MPI	1
	2	CuAu stretch	153.3(2)	gas	MPI	1
	3	AgAu stretch	103.9(3)	gas	MPI	1

References

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Ag_3

In a krypton matrix study with mass selection,[6] an absorption maximum at 30200 (331 nm) behaves appropriately for assignment to Ag_3.

$^2E''$ D_{3h}[a]

T_0 = 26969.0 gas MPI[4,5]LF[7] $^2E''$–$\tilde{X}$ 365–385 nm

In a krypton matrix, an absorption maximum near 27500 (364 nm) and an emission maximum near 26200 (381 nm) may be contributed by this transition.[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	158.5	gas	MPI,LF	4,5,7
e'	2	Deformation	100	gas	MPI,LF	4,5,7

τ < 80 ns gas LF[7]

In a krypton matrix study with mass selection,[6] an absorption maximum at 24900 (402 nm) behaves appropriately for assignment to Ag_3.

In argon, krypton, and xenon matrices, an absorption maximum near 23700 (422 nm) has been attributed[2,3,6] to Ag_3.

In a krypton matrix study with mass selection,[6] absorption maxima at 21830 (458 nm) and 19500 (514 nm) and emission maxima at 17900 (560 nm) and 16000 (626 nm) behave appropriately for assignment to Ag_3.

$\tilde{X}$ $^2E'$ D_{3h}[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	184T	gas	LF	7
e'	2	Deformation	67	gas	LF	7
			60HT	Kr	Ra	1

[a] Distorted by Jahn-Teller interaction.

References

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Au_3

In an argon matrix study,[1] absorption maxima at 34200 (292 nm) and 21200 (471 nm) have been attributed to Au_3.

In a krypton matrix study with mass selection,[3] absorption maxima at 42900 (233 nm), 39200 (255 nm), 35500 (282 nm), 32500 (308 nm), 28600 (349 nm), 21900 (457 nm), and 19500 (513 nm) behave appropriately for assignment to Au_3.

$\tilde{a}\ ^4E'$ D_{3h}[a]

T_0 = 13354.15 gas MPI[2] $\tilde{a}$–$\tilde{X}$ 710–750 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	181.7	gas	MPI	2
e'	2	Deformation	56T	gas	MPI	2

τ_0 = 28(2) μs gas MPI[2]

$\tilde{X}\ ^2E'$ D_{3h}

[a] Distorted by Jahn–Teller interaction.

References

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Sc_3

$\tilde{X}\ ^2E'$? D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	248	Ar	Ra	1
e'	2	Bend	150T	Ar	Ra	1

References

[1]M. Moskovits, D. P. DiLella, and W. Limm, J. Chem. Phys. **80**, 626 (1984).

Mn_3

A broad absorption with maximum near 14750 (678 nm) has been assigned[1] to Mn_3 isolated in an argon matrix.

$\tilde{X}$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1		196	Ar	Ra	1
e'	2		124[a]	Ar	Ra	1

[a] Structure due to Jahn-Teller interaction observed.

References

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Ni_3

In an argon matrix, an absorption maximum at 420 nm has been attributed[1] to Ni_3.

$\tilde{A}$

gas LF[3] $\tilde{A}$–$\tilde{X}$ 455–470 nm

T_0 = 20820 Ar AB[1] $\tilde{A}$–$\tilde{X}$ 449–481 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	205(5)	gas	LF	3
			202	Ar	AB	1
	2	Bend	90(5)[a]	gas	LF	3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	230(5)	gas	LF,PE	3,4
			232	Ar	Ra	2
	2	Bend	100(5)T	gas	LF	3

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Pd_3

Structure in the photoelectron spectrum[1] of Pd_3 can be interpreted in terms of an electronic state with origin < 720(30) and with vibrational spacings of approximately 230. There may also be an electronic state near 1900, as well as one near 2570. A series of bands with a spacing of approximately 210 appears above the band at 2570.

References

[1]K. M. Ervin, J. Ho, and W. C. Lineberger, J. Chem. Phys. **89**, 4514 (1988).

Pt_3

The photoelectron spectrum of Pt_3^- suggests[1] that Pt_3 may possess an electronic state 1225(30) above the ground state. Structure may be contributed by a short vibrational progression with spacings of approximately 180 or by other low-lying electronic states.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Sym. stretch	225(30)[a]	gas	PE	1
		Bend	105(30)	gas	PE	1

[a] In an alternate assignment, this band is contributed by a low-lying electronic state.

References

[1]K. M. Ervin, J. Ho, and W. C. Lineberger, J. Chem. Phys. **89**, 4514 (1988).

Al_3

T_0[a] = 16610 gas MPI[1] 516–602 nm
Overlapping continuum with high-frequency edge at 19378(10). This continuum may be associated with unresolved high vibrational levels of another electronic state.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1		270.6	gas	MPI	1
	2		205	gas	MPI	1

Lifetimes (possibly radiative) vary[1] from 98 to 21 μs.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			132.6(8)	gas	MPI	1

[a] Possibly a 1_0^n band.

References

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MgNC

$\tilde{X}\ ^2\Sigma^+$ $C_{\infty v}$
B_0 = 0.199 MW[1]

References

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CaNC

$\tilde{C}\ ^2\Pi$ $C_{\infty v}$
Unstructured absorption gas LF[1] $\tilde{C}$–$\tilde{X}$ 385–418 nm
τ = 165(38) ns gas LF[1]

$\tilde{A}\ ^2\Pi$ $C_{\infty v}$
T_0 = 16229.54 gas LF[1,3–6]CL[2] $\tilde{A}$–$\tilde{X}$ 572–670 nm
τ(607 nm) = 40.81(1.5) ns gas LF[1]
A = 77.64 gas LF[6]
B_0 = 0.150 LF[6]

$\tilde{X}\ ^2\Sigma^+$ $C_{\infty v}$
B_0 = 0.135 gas LF[4,6]MW[7]

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SrNC [a]

$\tilde{C}\ ^2\Pi$ $C_{\infty v}$
Unassigned structure gas LF[1] $\tilde{C}$–$\tilde{X}$ 395–455 nm
τ = 104.4(6.3) ns gas LF[1]

$\tilde{A}, \tilde{B}\ ^2\Pi, ^2\Sigma^+$ $C_{\infty v}$
Unassigned structure gas LF[1,2] $\tilde{A}, \tilde{B}$–$\tilde{X}$ 645–725 nm
τ = 51.2(6.2) ns gas LF[1]
$A(\tilde{A})$ = 301 gas LF[2]

$\tilde{X}\ ^2\Sigma^+$ $C_{\infty v}$

[a] Originally assigned to the SrCN structure.

References

[1]L. Pasternack and P. J. Dagdigian, J. Chem. Phys. **65**, 1320 (1976).
[2]M. Douay and P. F. Bernath, Chem. Phys. Lett. **174**, 230 (1990).

BaCN

$\tilde{C}\ ^2\Pi$ $C_{\infty v}$
Unstructured absorption gas LF[1] $\tilde{C}$–$\tilde{X}$ ≅500–629 nm
τ = 229(13) ns gas LF[1]

$\tilde{X}\ ^2\Sigma^+$ $C_{\infty v}$

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cyc-BCC

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. BC stretch	1194.6	Ar	IR	1

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cyc-BBN

In the argon-matrix study,[2] the $\nu_1 + \nu_3$ combination band at 1998.3 and other combination bands between 3250 and 6150 are moderately intense, suggesting strong vibronic coupling to a low-lying excited electronic state.

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. BN stretch	1116[a]	Ar	IR	2
b_2	3	Asym. BN stretch	882.3s	Ar	IR	2
			910.4	N_2	IR	1
			890.3	N_2	IR	1

[a] $(\nu_1 + \nu_3) - \nu_3$.

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BNB

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	1736.5	Ar	IR	1

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FeCO

$\tilde{a}\ ^5\Sigma^-$ $C_{\infty v}$
T_0 = 1135(25) gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1990(15)	gas	PE	3
Π	2	Bend	180(60)	gas	PE	3
Σ^+	3	FeC stretch	460(15)	gas	PE	3

$\tilde{X}\ ^3\Sigma^-$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1950(10)	gas	IR,PE	2,3
			1898	Ar	IR	1
			1884	Kr	IR	1
Π	2	Bend	330(50)	gas	PE	3
Σ^+	3	FeC stretch	530(10)	gas	PE	3

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NUN

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1008.3[a]	Ar	IR	2
Σ_u^+	3	Asym. stretch	1051.0	Ar	IR	1,2

[a] Calculated from position of $^{14}NU^{15}N$ absorption.

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BBO

$\tilde{A}$ $C_{\infty v}$
T_0 = 16301 gas CL[1] $\tilde{A}$–$\tilde{X}$ 590–695 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	BB stretch	437	gas	CL	1

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	BB stretch	583	gas	CL	1

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BOB

$\tilde{X}$ C_{2v}?

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	3	Asym. stretch	1420.5	Ar	IR	1
			1415.7	Kr	IR	2

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Al_2O

Absorption bands observed at 210 and 212 nm in an argon matrix, between 202 and 217 nm in a krypton matrix, and between 207 and 225 nm in a xenon matrix when Al is vaporized from a Knudsen cell coated with Al_2O_3 have been attributed[9] to Al_2O.

$\tilde{B}\ ^1\Pi_u$ $D_{\infty h}$
T_0 = 37121(15) Ar AB[7] $\tilde{B}$–$\tilde{X}$ 263–270 nm
36444(15)[a] Kr AB[5–7,14]LF[7] $\tilde{B}$–$\tilde{X}$ 267–283 nm
gas LF[12] $\tilde{B}$–$\tilde{X}$ 248–262 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	451(15)	Ar	AB	7
			454(15)	Kr	AB	5-7
Π_u	2	Bend	156(15)	Ar	AB	7
			186(15)	Kr	AB	5-7

$\tau_1 \cong 100$ ns; $\tau_2 \cong 5\ \mu$s gas LF[12]
$B \cong 0.109$ LF[12]

$\tilde{A}$

T_0 = 23286(15) Kr AB[7] $\tilde{A}$–$\tilde{X}$ 415–430 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	482(15)	Kr	AB	7
	2	Bend	133(15)	Kr	AB	7

$\tilde{X}$ $^1\Sigma_g^+$ $D_{\infty h}$ Structure: LF[12]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	525	gas	LF	12
			472	Ar	Ra	10,11
			471(15)	Kr	LF	7
			475	N_2	Ra	11
Π_u	2	Bend	99	gas	LF	12
Σ_u^+	3	Asym. stretch	992	gas	LF	12
			992.8	Ar	IR	1-4,13
			989.4	Kr	IR	1,2
			991	N_2	IR	8,13

$B \cong 0.109$ LF[12]

[a] From absorption measurements.

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Ga_2O

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	822.3	Ar	IR	2,4-6
			809.4	N_2	IR	1,3-5

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InGaO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			793.1	Ar	IR	1
			781.9	N_2	IR	1,2

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In_2O

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	InO a-stretch	745.4	Ne	IR	2
			735.2	Ar	IR	2,4-6
			728.2	Kr	IR	2
			722.4	N_2	IR	1-5

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Tl_2O

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	3	Asym. stretch	643.6	Ar	IR	2
			634.6	Kr	IR	2
			625.3	N_2	IR	1-3

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C_3

$^1\Sigma_u^+$ $D_{\infty h}$

T_0 = 52826(30) Ar AB[15] 170–190 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1080(30)	Ar	AB	15
Π_u	2	Bend	300(30)H	Ar	AB	15
Σ_u^+	3	Asym. stretch	780(30)H[a]	Ar	AB	15

$\tilde{B}$

In 2-photon ionization studies of jet-cooled C_3, a complicated group of bands, all with rotational structure appropriate for a $\Sigma_u^+ - \Sigma_g^+$ vibronic transition arising from the $\tilde{X}$ state, has been observed between 266 and 302 nm.[20] Lifetimes of these bands range from 0.4 to 2.5 μs, and the B' value for the first intense band, at 33153(5), is 0.396(3). These same bands, as well as bands at somewhat lower energies (possibly below the ionization threshold) and some bands arising from a $\Sigma_u^+ - \Pi_g$ vibronic transition, have also been studied using LF measurements on cooled beams.[23] In an argon matrix,[30] absorptions attributable to the $\tilde{B} - \tilde{X}$ transition of C_3 are observed between 280 and 284 nm.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	390	Ar	AB	30

In an argon matrix,[30] bands attributable to C_3 have been observed between 367 and 373 nm.

$\tilde{A}\ ^1\Pi_u$ $D_{\infty h}$ Structure: UV[6]

T_0 =	24675.5	gas	EM[1,2,6]AB[3,6,9]LF[17,23]	$\tilde{A}-\tilde{X}$ 340–640 nm
	24640	Ne	AB[4,5,8]EM[5]LF[11]	$\tilde{A}-\tilde{X}$ 347–488 nm
	24370[b]	Ar	AB[4,5,7]LF[11]	$\tilde{A}-\tilde{X}$ 352–411 nm
	24350	Kr	AB[7]	
	23610	Xe	AB[4,7]	
	24635	N_2	AB[7]	

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1085.9	gas	AB	6
			1094(6)	Ne	AB	5
			1093(6)	Ar	AB	5,7
			1090	Kr	AB	7
			1120	Xe	AB	7
			1050	N_2	AB	7
Π_u	2	Bend	307.9[c]	gas	AB	6
Σ_u^+	3	Asym. stretch	840HT	Ne	AB	8

τ_0 = 200(10) ns gas LF[12,13]
In a neon or argon matrix,[11] efficient intersystem crossing into the $\tilde{a}\ ^3\Pi_u$ state occurs, and $\tau \leq 10$ ns.
B_0 = 0.430 UV[6]

$\tilde{b}\ ^3\Pi_g$ $D_{\infty h}$ Structure: DL,EM[29]

T_0 = 23570(210) gas DL[29]EM[29] $\tilde{b}-\tilde{a}$ 1530–1550 nm
A_0 = 13.919(44); B_0 = 0.424 DL[29]EM[29]

$\tilde{a}\ ^3\Pi_u$ $D_{\infty h}$ Structure: DL,EM[29]

T_0 =	17090(210)	gas	DL[29]EM[29]PE[31]	$\tilde{b}-\tilde{a}$ 1530–1550 nm
T_0 =	17080	Ne	EM[5]LF[11]	$\tilde{a}-\tilde{X}$ 585–631 nm
			IR[32]	$\tilde{b}-\tilde{a}$ 1250–1538 nm
	16930	Ar	EM[5]	
			IR[32]	$\tilde{b}-\tilde{a}$ 1253–1544 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1156.5[d]	Ne	IR	32
			1154.2[d]	Ar	IR	32
Σ_u^+	3	Asym. stretch	1454.1	Ne	IR	32
			1455.3	Ar	IR	32

$\tau \cong 0.02$ s Ne EM[5]
A_0 = 13.556; B_0 = 0.417 DL[29]EM[29]

$\tilde{X}\ ^1\Sigma_g^+$ $D_{\infty h}$ Structure: UV[6]

This state of C_3 is highly anharmonic. The term values of many excited vibrational energy levels have been determined in SEP[21,26,27] and LF[23] studies. Analysis of data from the SEP studies[28] using the semirigid bender model indicates that the molecule is linear in its ground state but that on excitation of ν_3 a potential barrier appears at the linear configuration.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1224.5	gas	AB,LF	9,17,23
			1226	Ne	EM	5
			1207[d]	Ar	IR	19
			1234[d]	N_2	IR	19
Π_u	2	Bend	63.41[e]	gas	UV,DL	6,22,23
					SEP,TF	24,25
			70[f]T	Ne,Ar	AB	5

$\tilde{X}\ ^1\Sigma_g^+$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	2040.02	gas	IR,DL	16,18
					LF	23
			2042	Ne	IR	4
			2038s	Ar	IR	4,10
			2031	N_2	IR	19

B_0 = 0.431 UV[6]IR[16]DL[18]TF[25]

[a] Alternate assignment gives 1320.
[b] In the LF studies,[11] a second site was observed with T_0 = 24408.
[c] ω. Large Renner splitting, with ϵ = 0.537.[6] Detailed comparisons of gas-phase with neon- and argon-matrix band positions are given in refs. 8 and 14. Ref. 14 also gives a more detailed analysis of electronic orbital angular momentum effects in the gas-phase molecule.
[d] $(\nu_1 + \nu_3) - \nu_3$.
[e] Most precise value with tunable far infrared laser spectrometer (TF).[25] $\cong$ 45 in $\tilde{X}(011)$.[22]
[f] Greatly broadened in a rare-gas matrix by interaction with lattice modes.[11]

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SiCC

$\tilde{A}\ ^1B_2$ C_{2v} Structure: PI^5AB^{11}
T_0 = 20065.505 gas $EM^1AB^{3,11}LF^{4,15}$ $\tilde{A}$–$\tilde{X}$ 402-507 nm
20142 Ne AB^2LF^4 $\tilde{A}$–$\tilde{X}$ 409-611 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CC stretch	1462	gas	EM,AB	1,3,4,
					LF	11,15
			1462	Ne	AB,LF	2,4
			1457	Ar	AB	9
	2	CSi s-stretch	455.04	gas	LF,EM	4,11,15
			462	Ne	AB,LF	2,4
			448	Ar	AB	9
b_2	3	CSi a-stretch	487	gas	LF	15

τ_0 = 370 ns gas LF^4
310 ns Ne LF^4
A_0 = 1.589; B_0 = 0.411; C_0 = 0.324 AB^{11}

$\tilde{X}\ ^1A_1$ C_{2v} Structure: $PI^5MW^{6,7}AB^{11}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CC stretch	1746.0(2.8)	gas	EM,LF	1,15
			1746s	Ne	IR,LF	2,4
			1741.3	Ar	IR	8,14
	2	CSi s-stretch	840.6(1.2)	gas	EM,LF	1,10,15
			836m	Ne	IR,LF	2,4
			824.3	Ar	IR	8,14
b_2	3	CSi a-stretch	196.37(4)	gas	MW,LF	13,15
			172H	Ne	LF	4
			160.4	Ar	IR	14

A_0 = 1.729; B_0 = 0.436; C_0 = 0.348 $MW^{6,7,12,13,16}AB^{11}$

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Si_2C

$\tilde{X}$ C_{2v} Structure: IR[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	839.5	Ar	IR	2
	2	Bend	166.4T[a]	Ar	IR	2
b_2	3	Asym. stretch	1188.4s	Ar	IR	1,2

[a] $(\nu_2 + \nu_3) - \nu_3$.

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Si_3

$\tilde{E}$
T_0 = 23635T gas EM[3] $\tilde{E}$–$\tilde{X}$ 418–448 nm
T_0 = 21460 Ne AB[1] $\tilde{E}$–$\tilde{X}$ 424–466 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	310(25)	gas	EM	3
			310T	Ne	AB	1

$\tilde{D}$
T_0 = 13470(80) gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	480T	gas	PE	2

$\tilde{C}$
T_0 = 8880(80) gas PE[2]

$\tilde{B}$
T_0 = 7180(80) gas PE[2]

$\tilde{A}$
T_0 = 3630(80) gas PE[2]EM[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	480(25)	gas	PE,EM	2,3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	370(25)	gas	PE,EM	2,3

References

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[2]T. N. Kitsopoulos, C. J. Chick, A. Weaver, and D. M. Neumark, J. Chem. Phys. **93**, 6108 (1990).
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CNC^+

$\tilde{X}\ ^1\Sigma_g^+$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	1974.07	gas	DL	1

B_0 = 0.461 DL[1]

References

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$FeCO^-$

Threshold for electron detachment from ground-state $FeCO^-$ = 9335(40) gas PE[1,2]

$\tilde{X}\ ^4\Sigma^-$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1980(100)T	gas	PE	1
Π	2	Bend	230(40)	gas	PE	2
Σ^+	3	FeC stretch	465(10)	gas	PE	2

References

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NBN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	3	Asym. stretch	1589.8	N_2	IR	1

References

[1]P. Hassanzadeh and L. Andrews, J. Phys. Chem. **96**, 9177 (1992).

BCO

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	2002.5	Ar	IR	1

References

[1]T. R. Burkholder and L. Andrews, J. Phys. Chem. **96**, 10195 (1992).

AlCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1867.7	Ar	IR	1,2

References

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C_3^-

Threshold for electron detachment from ground-state C_3^- = 15980(160) gas PE[1-3]

$\tilde{X}\ ^2\Sigma_g^+$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1075(100)	gas	PE	3

References

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Si_3^-

Threshold for electron detachment from ground-state Si_3^- = 18800(80) gas PE[1]

References

[1]T. N. Kitsopoulos, C. J. Chick, A. Weaver, and D. M. Neumark, J. Chem. Phys. **93**, 6108 (1990).

CCN

$\tilde{C}\ ^2\Sigma^+$ $C_{\infty v}$
T_0 = 26661.73 gas AB[1] $\tilde{C}$–$\tilde{X}$ 350–375 nm
Evidence for predissociation above 29100.[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Sym. stretch	1859.20	gas	AB	1
Π	2	Bend	465T	gas	AB	1

B_0 = 0.413 AB[1]

$\tilde{B}\ ^2\Sigma^-$ $C_{\infty v}$
T_0 = 22413.25 gas AB[1] $\tilde{B}$–$\tilde{X}$ 442–446 nm
22180 Ar AB[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	445T	gas	AB	1

B_0 = 0.405 AB[1]

$\tilde{A}\ ^2\Delta$ $C_{\infty v}$
T_0 = 21259.203 gas $AB^1LF^4EM^9$ $\tilde{A}$–$\tilde{X}$ 376–471 nm
21377 Ar LF^2AB^3 $\tilde{A}$–$\tilde{X}$ 373–550 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Stretch	1770.77	gas	AB	1
			1732(2)	Ar	LF	2
Π	2	Bend	475T	gas	AB	1
Σ^+	3	Stretch	1241.64	gas	AB	1
			1225(2)	Ar	LF	2

τ = 170 ns Ar LF^2
A_{eff} = −0.807 gas $AB^1LF^{4,6}$
B_0 = 0.414 $AB^1LF^{4,6}MODR^7$

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Stretch	1923.25	gas	LF,EM	5,8,9
					DL	10,11
			1717	Ar	LF	2
Π	2	Bend	324	gas	AB,LF	1,8
Σ^+	3	Stretch	1050.76	gas	LF,EM	5,8,9
			1066	Ar	LF	2

A_{eff} = 40.38, $\epsilon\omega_2$ = 132.8 gas $LF^8DL^{10,11}$
B_0 = 0.398 $AB^1LF^{4,6}DL^{10,11}$

References

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BNN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Stretch	958.1	N_2	IR	1

References

[1]P. Hassanzadeh and L. Andrews, J. Phys. Chem. **96**, 9177 (1992).

CNC

$\tilde{B}\ ^2\Sigma_u^-$ $D_{\infty h}$ Structure: AB^1

T_0 = 34802.33 gas AB^1 $\tilde{B}-\tilde{X}$ 283–288 nm
34602(20) Ar[a] AB^2 $\tilde{B}-\tilde{X}$ 276–292 nm
34305(20)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	398	gas	AB	1
			385(20)H	Ar	AB	2

B_0 = 0.443 AB^1

$\tilde{A}\ ^2\Delta_u$ $D_{\infty h}$ Structure: AB^1

T_0 = 30338.53 gas AB^1 $\tilde{A}-\tilde{X}$ 325–332 nm
30048(20) Ar AB^2 $\tilde{A}-\tilde{X}$ 324–333 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	440	gas	AB	1

A = 0.33 gas AB^1
B_0 = 0.450 AB^1

$\tilde{X}\ ^2\Pi_g$ $D_{\infty h}$ Structure: AB^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	321[b]	gas	AB	1
Σ_u^+	3	Asym. stretch	1453s	Ar	IR	2

A = 26.41; ϵ = 0.549 AB^1
B_0 = 0.454 AB^1

[a] Two prominent sites in argon matrix.
[b] Calculated position of lowest frequency component ($^2\Sigma_u^-$) is 144 cm^{-1}. Moderately intense absorption at 134 cm^{-1} in an argon matrix is tentatively assigned to this transition.

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CCO

In an argon matrix,[1] a broad, unstructured absorption is observed near 500 nm, and CCO photodissociates on exposure of the sample to visible light.

$\tilde{A}\ ^3\Pi$ $C_{\infty v}$ Structure: AB^3

T_0 = 11651.182 gas $AB^{2,3}LF^6DL^{10,11}$ $\tilde{A}-\tilde{X}$ 500–860 nm
11860 Ar AB^5 $\tilde{A}-\tilde{X}$ 600–850 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	2045.7	gas	AB	3
Π	2	Bend	607.8	gas	AB	3
Σ^+	3	CC stretch	1270T[a]	gas	AB	3

The fluorescence decay pattern[7] of CCO $\tilde{A}(101)$ and of higher vibronic levels is complex. There is a short-lived (ca. 15 μs) component and a long-lived (333 + 105/−64 μs) component which is, in turn, nonexponential, suggesting perturbation by the heretofore unobserved $\tilde{b}\ ^1\Sigma^+$ and $\tilde{a}\ ^1\Delta$ states, as well as by high ground-state vibrational levels.
A = −35.36; ϵ = −0.172 gas AB^3DL^{10}
B_0 = 0.407 AB^3DL^{10}

$\tilde{X}\ ^3\Sigma^-$ $C_{\infty v}$ Structure: AB^3

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1970.86	gas	LF,DL	6,9
			1969s	Ar	IR	1,4
			1978 N_2	Ar	IR	1
			1987	N_2	IR	1
Π	2	Bend	379.53	gas	AB,DL	3,11
			381m	Ar	IR	1
Σ^+	3	CC stretch	1063	gas	LF	6
			1064w	Ar	IR	1
			1074 N_2	Ar	IR	1
			1077	N_2	IR	1

B_0 = 0.385 AB^3MW^8

[a] In Fermi resonance with $2\nu_2$.

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SiCO

$\tilde{A}\ ^3\Pi$? $C_{\infty v}$
T_0 = 24056(10) Ar AB[1] $\tilde{A}-\tilde{X}$ 365–416 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1857(10)	Ar	AB	1
	3	SiC stretch	750(10)	Ar	AB	1

$\tilde{X}\ ^3\Sigma^-$?

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1899	Ar	IR	1

References

[1]R. R. Lembke, R. F. Ferrante, and W. Weltner, Jr., J. Am. Chem. Soc. **99**, 416 (1977).

CCS

$\tilde{X}$ $C_{\infty v}$ Structure: MW[2]
B_0 = 0.216 MW[1-3]

References

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NCN

$^1\Delta_u$ $D_{\infty h}$
gas AB[6] 250–290 nm

$\tilde{B}\ ^3\Sigma_u^-$ $D_{\infty h}$
$T_0 \leq$ 33512 gas AB[6] $\tilde{B}-\tilde{X}$ 258–300 nm
33100 Ar AB[2] $\tilde{B}-\tilde{X}$ 240–302 nm
33215 N_2 AB[2] $\tilde{B}-\tilde{X}$ 240–301 nm
In the gas phase, bands are diffuse. Threshold for photodecomposition into C + N_2 observed in argon and nitrogen matrices[2,4] near 280 nm.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1100(10)	gas	AB	6
			1050(10)	Ar,N_2	AB	2

$\tilde{b}\ ^1\Pi_u$ $D_{\infty h}$ Structure: AB[5]
T_0 = x + 30045.76 gas AB[5] $\tilde{b}-\tilde{a}$ 330–334 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1160T	gas	AB	6

$\epsilon\omega_2$ = −84.2 gas AB[5]
B_0 = 0.395 AB[5]

$\tilde{A}\ ^3\Pi_u$ $D_{\infty h}$ Structure: AB[1]
T_0 = 30383.74 gas AB[1] $\tilde{A}-\tilde{X}$ 326–329 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1254(5)	gas	LF	8
Π_u	2	Bend	460(50)	gas	AB	1

A = −37.56; $\epsilon\omega_2$ = −85.7[a] gas AB[1]
τ_0 = 183(6) ns gas LF[M]
B_0 = 0.396 AB[1]

$\tilde{a}\ ^1\Delta_g$ $D_{\infty h}$ Structure: AB[5]
T_0 = x gas AB[5] $\tilde{b}-\tilde{a}$ 330–334 nm
B_0 = 0.399 AB[5]

$\tilde{X}\ ^3\Sigma_g^-$ $D_{\infty h}$ Structure: AB[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1197[b]	Ar	IR	4
Π_u	2	Bend	370(50)	gas	AB	1
			423m	Ar	IR	2,4
Σ_u^+	3	Asym. stretch	1475vs	Ar	IR	2,4
			1478vs	N_2	IR	2-4

B_0 = 0.397 AB[1]

[a] An alternate assignment[7] gives $\epsilon\omega_2$ = −90.95.
[b] Frequency deduced from weak combination with ν_3 which appears at 2672.

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PCN

$\tilde{A}\ ^3\Pi$ [a]
T_0 = 33165 gas AB[1] $\tilde{A}-\tilde{X}$ 280–306 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1830T	gas	AB	1

$A \cong$ 104 gas AB[1]

$\tilde{X}\ ^3\Sigma^-$ [a]

[a] Tentative assignment, by analogy with NCN.

References

[1]N. Basco and K. K. Yee, Chem. Commun. 152 (1968).

AsCN

$\tilde{A}\ ^3\Pi$ •
$T_0 \cong 34900$ gas AB[1] $\tilde{A}-\tilde{X}$ 280–295 nm
$A \cong 550$ gas AB[1]

$\tilde{X}\ ^3\Sigma^-$ [a]

[a] Tentative assignment, by analogy with NCN.

References

[1] N. Basco and K. K. Yee, Chem. Commun. 153 (1968).

NCO^+

$^1\Pi$ [a]
$T_0 = 57280(160)$ gas PE[1]

$^3\Pi$ [a]
$T_0 = 56960(160)$ gas PE[1]

$^1\Pi$ [a]
$T_0 = 55910(160)$ gas PE[1]

$\tilde{A}\ ^3\Pi$ $C_{\infty v}$
$T_0 = 23960(160)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	"Sym." stretch	1320(30)	gas	PE	1

$\tilde{b}\ ^1\Sigma^+$ $C_{\infty v}$
$T_0 = 14520(160)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	"Sym." stretch	1150(30)	gas	PE	1

$\tilde{a}\ ^1\Delta$ $C_{\infty v}$
$T_0 = 9360(160)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Stretch	2020(30)	gas	PE	1
	3	Stretch	1110(30)	gas	PE	1

$\tilde{X}\ ^3\Sigma^-$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	"Sym." stretch	1000(30)	gas	PE	1

[a] Tentative assignment.

References

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CNN

An absorption which appears in a nitrogen matrix at 51070 when a high concentration of CNN is present has been tentatively attributed to this species.[10]

$\tilde{C}\ ^3\Pi$? $C_{\infty v}$
$T_0 = 48540(50)$ Ar AB[10] $\tilde{C}-\tilde{X}$ 206 nm
$49100(50)$ N_2 AB[10] $\tilde{C}-\tilde{X}$ 203.7 nm

$\tilde{B}\ ^3\Sigma^-$? $C_{\infty v}$
$T_0 \leq 39950$ Ar AB[10] $\tilde{B}-\tilde{X}$ 210–251 nm
39850 N_2 AB[10] $\tilde{B}-\tilde{X}$ 210–251 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		Stretch	1450(40)[a]	Ar,N_2	AB	10
		Stretch	990(40)	Ar,N_2	AB	10

$\tilde{A}\ ^3\Pi$ $C_{\infty v}$
$T_0 = 23850$[b] gas AB[6]LF[11] $\tilde{A}-\tilde{X}$ 395–420 nm
23750 Ne AB[5] $\tilde{A}-\tilde{X}$ 397–420 nm
23830
23597 Ar AB[2,3]LF[8,9] $\tilde{A}-\tilde{X}$ 401–424 nm
23865 N_2 AB[2,3] $\tilde{A}-\tilde{X}$ 396–419 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	"Sym." stretch	1325(10)	Ne	AB	5
			1322(2)	Ar	AB,LF	2,3,8,9
			1335(10)	N_2	AB	2,3
Π	2	Bend	525(2)	Ar	LF	8
Σ^+	3	"Asym." stretch	1807(2)	Ar	LF	8

$\tau_0 = 250(30)$ ns Ar LF[8,9]
$A = -26.5$[b] gas LF[11]
$A = 9$; $\epsilon = -0.07$ Ar LF[8]
$B_0 = 0.425(10)$[b] LF[11]

$\tilde{X}\ ^3\Sigma^-$ $C_{\infty v}$ Structure: ESR[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	"Sym." stretch	1235	Ne	EM	5
			1235	Ar	LF	8,12
			1241 N_2	Ar	IR	3
			1252	N_2	IR	3,4,7
Π	2	Bend	396	Ar	LF	8,12
			393 N_2	Ar	IR	3
			394	N_2	IR	4,7
Σ^+	3	"Asym." stretch	1419[c]	Ar	LF	12

$B_0 = 0.414(10)$[b] LF[11]

[a] Possibly 2440(40).[10]
[b] Approximate value, used in simulation.
[c] For many years, a prominent infrared absorption of CNN which appeared at 2847 in an argon matrix was assigned as the highest frequency fundamental, with approximate C≡N stretching character. Recently, a fluorescence signal corresponding to approximately half that value has been detected.[12] Associated CASSCF calculations indicate that the infrared absorption intensity of $2\nu_3$ of CNN should be greater than that of the fundamental.

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SiNN

$\tilde{B}\ ^3\Sigma^-$? $C_{\infty v}$
T_0 = 32162(10) Ar AB[1] $\tilde{B}$–$\tilde{X}$ 295–311 nm
31892(25) Kr AB[2] $\tilde{B}$–$\tilde{X}$ 297–314 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NN stretch	1672(10)	Ar	AB	1
			1671(25)	Kr	AB	2

$\tilde{A}\ ^3\Pi$? $C_{\infty v}$
$T_0 \leq$ 27170(20) Ar AB[1] $\tilde{A}$–$\tilde{X}$ 331–368 nm
Kr AB[2] $\tilde{A}$–$\tilde{X}$ 333–360 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	SiN stretch	450T	Ar	AB	1
			450T	Kr	AB	2

$\tilde{X}\ ^3\Sigma^-$? $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NN stretch	1731s	Ar	IR	1
	3	SiN stretch	485w	Ar	IR	1

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N_3^+

$\tilde{b}\ ^1\Sigma^+$
T_0 = 14520(160) gas PE[1]

$\tilde{a}\ ^1\Delta$
T_0 = 9120(160) gas PE[1]

$\tilde{X}\ ^3\Sigma^-$ $C_{\infty v}$ Structure: PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Sym. stretch	1170(30)	gas	PE	1
Σ^+	3	Asym. stretch	2565(30)[a]	gas	PE	1

[a] Alternate assignment of ν_3 = 1395 cm^{-1}, with the observed band separation of 2565 cm^{-1} corresponding to $\nu_1 + \nu_3$, would be consistent with assignments of ν_3 for such related species as NCN and CO_2^+ and cannot be excluded.

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$ZnCl_2^+$

$\tilde{F}\ ^2\Delta_g$ $D_{\infty h}$
T^a = 60630(90) gas PE[1]
A = 2310(100) gas PE[1]

$\tilde{E}\ ^2\Pi_g$ $D_{\infty h}$
T^a = 60170(80) gas PE[1]
A = 2190(80) gas PE[1]

$\tilde{D}\ ^2\Sigma_g^+$ $D_{\infty h}$
T^a = 58060(80) gas PE[1]

$\tilde{C}\ ^2\Sigma_g^+$ $D_{\infty h}$ Structure: PE[1]
T_0 = 17940(80) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	290(8)	gas	PE	1

$\tilde{B}\ ^2\Sigma_u^+$ $D_{\infty h}$
T^a = 10180(160) gas PE[1]

$\tilde{A}\ ^2\Pi_u$ $D_{\infty h}$
T^a = 4480(120) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	360T	gas	PE	1
Π_g	2	Bend	280T	gas	PE	1

A = 890(160) gas PE[1]

$\tilde{X}\ ^2\Pi_g$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_g	2	Bend	240(20)[b]	gas	PE	1

A = 630(80) gas PE[1]

[a] From vertical ionization potentials.
[b] 260(20) for $\tilde{X}\ ^2\Pi_{g,1/2}$.

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[1]L.-S. Wang, B. Niu, Y. T. Lee, and D. A. Shirley, J. Chem. Phys. **93**, 957 (1990).

$MnCl_2^+$

$\tilde{G}\ ^5\Sigma_g^+$ $D_{\infty h}$
T^a = 28080(160) gas PE[1]

$\tilde{F}\ ^5\Delta_g$ $D_{\infty h}$
T^a = 23640(160) gas PE[1]

$\tilde{E}\ ^7\Sigma_g^+$ $D_{\infty h}$
T^a = 20740(160) gas PE[1]

$\tilde{D}\ ^5\Pi_g$ $D_{\infty h}$
T^a = 11050(160) gas PE[1]

$\tilde{C}\ ^7\Sigma_u^+$ $D_{\infty h}$
T^a = 9280(160) gas PE[1]

$\tilde{B}\ ^7\Pi_u$ $D_{\infty h}$
T^a = 7500(160) gas PE[1]

$\tilde{A}\ ^7\Pi_g$ $D_{\infty h}$
T^a = 5240(160) gas PE[1]

$\tilde{X}\ ^5\Sigma_g^+$ $D_{\infty h}$

[a] From vertical ionization potentials.

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$NiCl_2^+$

$\tilde{H}\ ^2\Pi_g$ $D_{\infty h}$
T^a = 32350(160) gas PE[1]

$\tilde{G}\ ^4\Pi_g$ $D_{\infty h}$
T^a = 19850(160) gas PE[1]

$\tilde{F}\ ^4\Pi_u$ $D_{\infty h}$
T^a = 14200(160) gas PE[1]

$\tilde{E}\ ^4\Delta_u$ $D_{\infty h}$
T^a = 10970(160) gas PE[1]

$\tilde{D}\ ^4\Delta_g$ $D_{\infty h}$
T^a = 6780(160) gas PE[1]

$\tilde{C}\ ^4\Pi_g$ $D_{\infty h}$
T^a = 4200(160) gas PE[1]

$\tilde{B}\ ^4\Phi_g$ $D_{\infty h}$
T^a = 2580(160) gas PE[1]

$\tilde{A}\ ^4\Sigma_g^-$ $D_{\infty h}$
T^a = 1290(160) gas PE[1]

$\tilde{X}\ ^2\Pi_g$ $D_{\infty h}$

[a] From vertical ionization potentials.

References

[1]L.-S. Wang, B. Niu, Y. T. Lee, and D. A. Shirley, J. Chem. Phys. **93**, 957 (1990).

BO_2

$\tilde{B}\ ^2\Sigma_u^+$ $D_{\infty h}$ Structure: AB[1]
T_0 = 24508.0 gas AB[1] $\tilde{B}$–$\tilde{X}$ 405–410 nm
24481 Ar AB[2] $\tilde{B}$–$\tilde{X}$ 408–412 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	505	gas	AB	1
Σ_u^+	3	Asym. stretch	1410[a]	gas	AB	1

B_0 = 0.325 AB[1]

$\tilde{A}\ ^2\Pi_u$ $D_{\infty h}$ Structure: UV[1]
T_0 = 18291.597 gas UV[1]LF[3–5,14] $\tilde{A}$–$\tilde{X}$ 396–700 nm
17915[b] Ar AB[2] $\tilde{A}$–$\tilde{X}$ 423–558 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	994	gas	UV	1
Π_u	2	Bend	477.29	gas	UV,LF	1,14
Σ_u^+	3	Asym. stretch	2357H	gas	UV	1

τ_0 = 91(4) ns gas LF[6,9]
A systematic study of the dependence of τ on rotational and vibrational level has been given by Ref. 10.
A = −101.281; $\epsilon\omega_2$ = −13.896 gas UV[1]LF[14]
B_0 = 0.311 UV[1]LF[13,14]

$\tilde{X}\ ^2\Pi_g$ $D_{\infty h}$ Structure: UV[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1056.4	gas	UV,LF	1,3-5
Π_u	2	Bend	448.18[c]	gas	UV,LF	1,3-5,14
			446.6wm	Ar	IR	15
			398.2m	Ar	IR	15
			493.4	Kr	IR	15
			394.6	Kr	IR	15
Σ_u^+	3	Asym. stretch	1278.26	gas	DL,IR	8,12
			1299.3vs	Ar	IR	15
			1282.8s	Ar	IR	15
			1274.6s	Ar	IR	2,15
			1300.7vs	Kr	IR	15
			1285.5s	Kr	IR	15
			1292.2vs	Xe	IR	15
			1279.0	O_2	IR	15

A = −148.6; $\epsilon\omega_2$ = −86.91 gas UV[1]LF[3,7,14]
B_0 = 0.329 UV[1]LF[3,7,13,14]DL[8]IR[12]

[a] Estimated from isotopic shifts.
[b] Independent analysis of the matrix spectrum not given. Each argon-matrix absorption is shifted to lower frequency by approximately 400 cm^{-1} from the corresponding gas-phase R_1 branch band head.
[c] Band origin of $(010)\kappa^2\Sigma - (000)^2\Pi_{3/2}$ vibration-rotation transition observed[11] at 633.8049(9) using diode laser spectroscopy.

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BS_2

$\tilde{B}\ ^2\Sigma_u^+$ $D_{\infty h}$
T_0 = 24072(5) Ne AB^2 $\tilde{B}-\tilde{X}$ 395–412 nm
gas $AB^{1,3}$ $\tilde{B}-\tilde{X}$ 409–418 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	509	Ne	AB	2

$\tilde{A}\ ^2\Pi_u$ $D_{\infty h}$
T_0 = 13766(2) Ne AB^2 $\tilde{A}-\tilde{X}$ 514–721 nm
gas $AB^{1,3}$ $\tilde{A}-\tilde{X}$ 592–800 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	504(2)	Ne	AB	2
Π_u	2	Bend	311H	Ne	AB	2
Σ_u^+	3	Asym. stretch	1535H	Ne	AB	2

A = −263(2) Ne AB^2

$\tilde{X}\ ^2\Pi_g$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	510	Ne	AB	2
Π_u	2	Bend	120[a]T	Ne	AB	2
Σ_u^+	3	Asym. stretch	1014.6(5)s	Ne	IR	2

A = −440 gas $AB^{1,2}$

[a] Estimated from isotope shift in origin of $\tilde{A}-\tilde{X}$ transition.

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FBS^+

$\tilde{C}\ ^2\Sigma^+$ $C_{\infty v}$
T_0 = 70360(240) gas PE^1

$\tilde{B}\ ^2\Pi$ $C_{\infty v}$
T_0 = 50800(900) gas PE^1

$\tilde{A}\ ^2\Sigma^+$ $C_{\infty v}$
T_0 = 26687.9(8) gas PE^1EF^2 $\tilde{A}-\tilde{X}$ 350–425 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BS stretch	1718(2)	gas	PE,EF	1,2
	3	BF stretch	691(2)	gas	EF	2

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BS stretch	1721(2)	gas	EF	2
Π	2	Bend	339(2)	gas	EF	2
Σ^+	3	BF stretch	637(2)	gas	EF	2

A = −370(2) gas EF^2

References

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$ClBS^+$

$\tilde{C}\ ^2\Sigma^+$ $C_{\infty v}$
T^a = 50500(1000) gas PE^1

$\tilde{B}\ ^2\Pi_{3/2}$ $C_{\infty v}$
T_0 = 26019 gas EF^2 $\tilde{B}-\tilde{X}$ 405–516 nm

$\tilde{A}\ ^2\Sigma^+$ $C_{\infty v}$
T_0 = 24961.5(4) gas EF^2 $\tilde{A}-\tilde{X}$ 392–440 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BS stretch	1390.6(8)	gas	EF	2
	3	BCl stretch	516.0(8)	gas	EF	2

τ = 240(13) ns gas EF^2

$\tilde{X}\ ^2\Pi_{3/2}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BS stretch	1347.8(8)	gas	EF	2
	3	BCl stretch	508.9(8)	gas	EF	2

A = −383 gas EF^2

[a] From vertical ionization potential.

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cyc-AlO_2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	OO stretch	1097wT	Ar	IR,Ra	1,3
	2	AlO s-stretch	496.3	Ar	IR	1,2,4

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OAlO

$\tilde{A}\ ^2\Pi_u$ $D_{\infty h}$
T_0 = 17465 Ar LF[1] $\tilde{A}$–$\tilde{X}$ 495–620 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	790	Ar	LF	1
Π_u	2	Bend	70	Ar	LF	1
Σ_u^+	3	Asym. stretch	1015	Ar	LF	1

$\tilde{X}\ ^2\Pi_g$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	635	Ar	LF	1
Π_u	2	Bend	70	Ar	LF	1
Σ_u^+	3	Asym. stretch	1129.5	Ar	IR	2

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cyc-GaO_2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	OO stretch	1089.5vw	Ar	IR	1
			1092.7vw	N_2	IR	1
	2	GaO s-stretch	380.9s	Ar	IR	1,2
			381.5s	N_2	IR	1
b_2	3	GaO a-stretch	285.5m	Ar	IR	1
			289.3	N_2	IR	1

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OGaO

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	GaO a-stretch	912.7	Ar	IR	1

References

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cyc-InO_2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	OO stretch	1084.2w	Ar	IR	1,2
			1089.4w	N_2	IR	1
	2	InO s-stretch	332.0s	Ar	IR	1,2
			332.4s	N_2	IR	1
b_2	3	InO a-stretch	277.7T	Ar	IR	1

References

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OInO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	InO a-stretch	755.5	Ar	IR	1

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CCO^-

Threshold for electron detachment from ground-state CCO^- is 14910(220).[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1625(350)	gas	PE	1

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NCO

$\tilde{B}\ ^2\Pi$ $C_{\infty v}$

T_0 = 31751.1(5)	gas	$UV^2LF^{18}PD^{27}$	$\tilde{B}-\tilde{X}$	265–320 nm
31616(25)	Ne	UV^3	$\tilde{B}-\tilde{X}$	260–320 nm
31437(25)	Ar	UV^3	$\tilde{B}-\tilde{X}$	232–315 nm
31339(25)	N_2	UV^3	$\tilde{B}-\tilde{X}$	256–315 nm

All vibrational states are predissociated.[27]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Stretch	2303	gas	UV	2
			2295(50)	Ne	UV	3
			2303(50)	Ar	UV	3
	3	Stretch	1047	gas	UV	2
			1033(50)	Ne	UV	3
			1053(50)	Ar	UV	3
			1025(50)	N_2	UV	3

τ_0 = 63(3) ns gas LF^{13}
A = −76.6 gas LF^{18}
B_0 = 0.356 LF^{18}

$\tilde{A}\ ^2\Sigma^+$ $C_{\infty v}$ Structure: UV^{20}

T_0 = 22754.063	gas	$AB^1LF^{23}SEP^{26}$	$\tilde{A}-\tilde{X}$	360–512 nm
22800(10)	Ne	AB^3	$\tilde{A}-\tilde{X}$	398–440 nm
22712(2)	Ar	LF^8	$\tilde{A}-\tilde{X}$	390–530 nm
22956(10)	N_2	AB^3	$\tilde{A}-\tilde{X}$	395–440 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Stretch	2338.0	gas	UV	1
			2325(20)	Ne	UV	3
			2332(4)	Ar	UV,LF	3,8
			2321(20)	N_2	UV	3
Π	2	Bend	680.8	gas	UV	1
			673(20)	Ne	UV	3
Σ^+	3	Stretch	1289.3[a]	gas	UV	1
			1270(20)	Ne	UV	3
			1291(4)	Ar	UV,LF	3,8

τ_0 = 435(10) ns gas $LF^{9,13}$
350(30) ns gas $LF^{11,12}$
170 ns Ar LF^8
B_0 = 0.402 UV^1

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$ Structure: $UV^{1,7,20}MW^{4-6}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Sym. stretch	1272.79[b]	gas	LF,LMR	14,15,17
					SEP	19,23,26
			1275vw	Ar	IR,LF	3,8
Π	2	Bend	532.2(4)	gas	UV,LF	1,7,15
						23
			529.5[c]	Ar	LF	8
Σ^+	3	Asym. stretch	1921.35[d]	gas	LMR	10,14,15
					LF,DL	21,23
					SEP	25
			1923m	Ar	IR,LF	3,8
			1935	N_2	IR	3

A_0 = −96.7(1.5), $\epsilon\omega_2$ = −75.3(6) gas $LF^{23}SEP^{26}$
B_0 = 0.390 $UV^1MW^{16}LMR^{22}$

[a] In Fermi resonance with $2\nu_2$, at 1385.3.
[b] For $\tilde{X}\ ^2\Pi_{1/2}$, 1362.87 gas $LF^{14,15,19,23,24}SEP^{26}$
[c] Lowest frequency component ($^2\Sigma^+$) contributes a strong infrared absorption at 487.[3] Four components ($^2\Sigma^+$, $^2\Delta_{5/2}$, $^2\Delta_{3/2}$, $^2\Sigma^-$) observed at 484, 531, 626, and 672 in LF experiments.[8] Components of $(0n0)$, $n \geq 2$, have also been assigned in gas-phase studies.[19,23,26]
[d] For $\tilde{X}\ ^2\Pi_{1/2}$, 2017.7(5) gas $LF^{14,15,23,24}$

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NCS

$\tilde{B}\ ^2\Sigma^+$ $C_{\infty v}$
T_0 = 26987.8 gas EM[1]AB^{2}LF[4,6] $\tilde{B}$–$\tilde{X}$ 353–485 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	343(10)	gas	AB	2
Σ^+	3	CS stretch	921.5	gas	LF	4

τ_{001} = 225(5) ns gas LF[4]
B_0 = 0.197 AB^2

$\tilde{A}\ ^2\Pi$ $C_{\infty v}$
T_0 = 26054.56(1) gas EM[1]AB^{2}LF[4,6] $\tilde{A}$–$\tilde{X}$ 337–417 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CN stretch	1916.18(3)	gas	AB	2
Π	2	Bend	378(10)	gas	AB	2
Σ^+	3	CS stretch	755.28(3)	gas	AB	2

τ_0 = 160(5) ns gas LF[3,4]EF[5]
A = −91.58(1); $|\epsilon\omega_2|$ = 103(5) gas AB^{2}LF[4]
B_0 = 0.191 AB^{2}LF[6]

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$ Structure: AB^2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CN stretch	1942.2	gas	LF	4
Π	2	Bend	376.0(3)	gas	AB,LF SEP	2,4,6
Σ^+	3	CS stretch	761.9[a]	gas	SEP	6

A = −327.6(2); $\epsilon\omega_2$ = −60.06(44) gas AB^{2}LF[4,6]SEP[6]
B_0 = 0.204 AB^{2}LF[4,6]MW[7]

[a] In Fermi resonance with $2\nu_2$.

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PCO

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1912.8	Ar	IR	1

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CO_2^+

$\tilde{C}\ ^2\Sigma_g^+$ $D_{\infty h}$ Structure: MP[23]
T_0 = 45157(3) gas TPE[20]PE[22]MP[23] $\tilde{C}$–$\tilde{A}$ 585–640 nm
The band origin is perturbed by another state of $^2\Sigma_g^+$ symmetry at 45188 which has a rotational constant of 0.353.[23] This state may be an excited vibrational level of the $\tilde{A}$ or $\tilde{B}$ state.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1352(4)[a]	gas	PE	22
Π_u	2	Bend	614(4)	gas	TPE,PE	20,22
Σ_u^+	3	Asym. stretch	1567(4)	gas	PE	22

B_0 = 0.395 MP[23]

$\tilde{B}\ ^2\Sigma_u^+$ $D_{\infty h}$ Structure: EM[9]
T_0 = 34597.9 gas EM[1,9] $\tilde{B}$–$\tilde{X}$ 287–291 nm
Perturbations by the $\tilde{A}$ state are considered in Refs. 14-16.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1275(1)	gas	TPE,PE	20,22
Π_u	2	Bend	557(4)	gas	EM,PE	9,22
Σ_u^+	3	Asym. stretch	1840(5)	gas	TPE,PE	20,22

τ_0 = 140(7) ns gas T-PEFCO[10]PEFCO[13]LF[16]
B_0 = 0.378 EM[1]

$\tilde{A}\ ^2\Pi_u$ $D_{\infty h}$ Structure: EM[11]
T_0 = 28500.35 gas EM[2,11]LF[26] $\tilde{A}$–$\tilde{X}$ 290–490 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1126	gas	EM	2,5,11
					PE	22
Π	2	Bend	461	gas	EM,PE	11,22
Σ_u^+	3	Asym. stretch	2731	gas	EM	6

τ_0 = 102(8) ns gas EF[7]T-PEFCO[10]
124(6) ns gas PEFCO[13]HFD[17]
A = −95.51 gas EM[11]LF[26]
B_0 = 0.350 EM[2,11]LF[26]

$\tilde{X}\ ^2\Pi_g$ $D_{\infty h}$ Structure: EM[2-5,9,11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1244.3(3)	gas	EM,DL	4,5,8, 12,21

$\tilde{X}\ ^2\Pi_g$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	511.4(3)	gas	EM,DL	11,19,21
Σ_u^+	3	Asym. stretch	1423.08	gas	DL	18
			1421.7	Ne	IR	24

$A = -161.02(6)$[b]; $\epsilon\omega_2 = -98.8(3)$[b] gas EM[1,9,11]DL[19,21]
$B_0 = 0.380$ EM[1,3,9,11]

[a] Corrected for Fermi resonance.
[b] Reanalysis by Ref. 25 gives $A = -161.48(5)$ and $\epsilon\omega_2 = -100.4$.

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OCS^+

$\tilde{C}\ ^2\Sigma^+$ $C_{\infty v}$
$T_0 = 54640(30)$ gas PI[4]PE[10]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	2202(2)	gas	PE	10
Π	2	Bend	454(5)	gas	PE	10
Σ^+	3	CS stretch	926(5)	gas	PI,PE	4,10

$\tilde{B}\ ^2\Sigma^+$ $C_{\infty v}$
$T_0 = 39180(20)$ gas PI[4]PF[9]PE[10]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1850(8)	gas	PE	10
Π	2	Bend	515(3)	gas	PF,PE	9,10
Σ^+	3	CS stretch	829[a]	gas	PF	9

$\tilde{A}\ ^2\Pi_{3/2}$ $C_{\infty v}$
$T_0 = 31404.099(7)$ gas EF[1]LF[8]PF[9] $\tilde{A}$–$\tilde{X}$ 318–432 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	2036(6)	gas	PE	10
Π	2	Bend	336(20)H	gas	PE	10
Σ^+	3	CS stretch	803.8[b]	gas	PF	9

$\tau_0 = 93(9)$ ns[c] gas PEFCO[5]
τ_0 ($\omega = 3/2$) = 105(3) ns; τ_0 ($\omega = 1/2$) = 77(3) ns gas HFD[6]EF[7]
$A = -111.8$ gas EF[1]PF[9]
$B_0 = 0.187$ LF[8]

$\tilde{X}\ ^2\Pi_{3/2}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CS stretch	695.7[d]	gas	PF	9
Π	2	Bend	476(16)	gas	PE	10

$A = -367.2$ gas EF[1]PF[9]

[a] Ref. 10 gives value of 742(7).
[b] 816.9 for $\omega = 1/2$.[9]
[c] Absence of emission from states above the $\tilde{A}\ ^2\Pi$ band origin in photoionization experiments[2] suggested that the molecule is predissociated into CO + S^+ ($^4S^o$), as was later confirmed.[3] PEFCO studies[5] have yielded the branching ratio for photoexcitation vs. predissociation for the transition origin, permitting an estimate of 550(50) ns for the radiative lifetime.
[d] 699.7 for $\omega = 1/2$.[9]

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CS_2^+

$\tilde{C}\ ^2\Sigma_g^+$ $D_{\infty h}$ Structure: MP[15]
T_0 = 49064 gas PI[5]PF[13]MP[15] $\tilde{C}$–$\tilde{B}$ 658–724 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	652(2)	gas	PI,PE	5,9,11
					PF,AB	13-15
Π_u	2	Bend	348(9)	gas	PF,PE	13,14
Σ_u^+	3	Asym. stretch	1024(6)	gas	PE	14

τ_0 = 11(2) ps gas MP[15]
B_0 = 0.111 PF[13]MP[15]

$\tilde{B}\ ^2\Sigma_u^+$ $D_{\infty h}$ Structure: EM[1]
T_0 = 35238.01 gas EM[1] $\tilde{B}$–$\tilde{X}$ 277–307 nm
35270 Ne LF[7]
35226

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	602[b]	gas	EM	3
Π_u	2	Bend	351(5)	gas	PE	14
Σ_u^+	3	Asym. stretch	1320(5)H	gas	PE	14

τ_0 = 290(10) ns gas EF[2]PIFCO[4]PEFCO[8]UV[12]
There is also a long-lifetime component, with τ = 1.44(22) μs.[8,12]
B_0 = 0.108 EM[1]

$\tilde{A}\ ^2\Pi_u$ $D_{\infty h}$ Structure: EM[3]
T_0 = 20975 gas EM[3] $\tilde{A}$–$\tilde{X}$ 426–512 nm
21017 Ne LF[6,7] $\tilde{A}$–$\tilde{X}$ 400–638 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	610[a]T	gas	EM	3
			621	Ne	LF	6,7
Π_u	2	Bend	275HT	gas	EM	3
			280H	Ne	LF	6,7
Σ_u^+	3	Asym. stretch	1644H	Ne	LF	7

τ = 4.09(19) μs gas PIFCO[4]ID[10]UV[12]
2.3(1) μs Ne LF[6,7]
A = −176 gas EM[3]PE[14]
B_0 = 0.101 EM[3]

$\tilde{X}\ ^2\Pi_g$ $D_{\infty h}$ Structure: EM[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	617[a]	gas	EM,TPE	3,16
			618[a]	Ne	LF	6,7
Π_u	2	Bend	332[c]	gas	TPE	16
			349H	Ne	LF	6,7
Σ_u^+	3	Asym. stretch	1203H	gas	EM,PE	3,14
			1224H	Ne	LF	6,7

A = −440.39(3) gas EM[1,2]TPE[16]
B_0 = 0.109 EM[1]

[a] Strong Fermi resonance with $2\nu_2$; Ref. 7 has suggested a reversed assignment for ν_1 and $2\nu_2$ of the $\tilde{A}$ state.
[b] High resolution PE value 633(2).[14]
[c] Renner-Teller splitting is unresolved for $\tilde{X}\ ^2\Pi_{g,3/2}$. For $\tilde{X}\ ^2\Pi_{g,1/2}$, components at 320 ($\Delta_{u,3/2}$) and 341 (Σ_u^-) are observed in a gas-phase TPE study.[16]

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FCN^+

$\tilde{C}\ ^2\Sigma^+$ $C_{\infty v}$
T^a = 74700(1000) gas PE[1]

$\tilde{B}\ ^2\Pi$ $C_{\infty v}$
T^a = 48100(1000) gas PE[1]

$\tilde{A}\ ^2\Sigma^+$ $C_{\infty v}$
T_0 = 9200(500) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	CF stretch	1230(160)	gas	PE	1

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CN stretch	2100(160)	gas	PE	1

[a] From vertical ionization potential.

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$ClCN^+$

$\tilde{C}\ ^2\Sigma^+$ $C_{\infty v}$
T_0 = 54000(300) gas PE[1,2]

$\tilde{B}\ ^2\Pi_{3/2}$ $C_{\infty v}$
T_0 = 22515.54 gas EF[8]LF[10-12] $\tilde{B}-\tilde{X}$ 365–569 nm
22598(5) Ne AB[6] $\tilde{B}-\tilde{X}$ 380–442 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CN stretch	2128.5(7)	gas	LF	10
Π	2	Bend	303.1(7)	gas	LF	10
Σ^+	3	CCl stretch	531.90	gas	LF	10,11
			539(4)	Ne	AB	6

τ_1 = 205(40) ns gas EF[3]
280(56) ns gas PEFCO[5]
170(20) ns gas PIFCO[4,7]
τ_2 = 900(100) ns gas EF[3]
970(80) ns gas PIFCO[7]
Both lifetimes are dependent on extent of vibrational excitation[5].
A = −368(2) gas EF[8,9]LF[10]
B_0 = 0.177 LF[11]

$\tilde{A}\ ^2\Sigma^+$ $C_{\infty v}$
T_0 = 11690(1) gas EF[3,8] $\tilde{A}-\tilde{X}$ 843–881 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	CCl stretch	774(2)	gas	EF	8

τ = 4.4(1.0) μs gas EF[3]

$\tilde{X}\ ^2\Pi_{1/2}$ $C_{\infty v}$
T_0 = 276(2) gas EF[3,8,9] $\tilde{A}-\tilde{X}$ 843–881 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡N stretch	1914(2)	gas	EF	8
	3	CCl stretch	827(2)	gas	EF	8

$\tilde{X}\ ^2\Pi_{3/2}$ $C_{\infty v}$ Structure: UV,PE[3]LF[12]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡N stretch	1915(2)	gas	EF,LF	8-10
Π	2	Bend	376T	gas	LF	10
Σ^+	3	CCl stretch	827(2)	gas	EF,LF	8-10

B_0 = 0.205 LF[11]

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$BrCN^+$

$\tilde{C}\ ^2\Sigma^+$ $C_{\infty v}$
T_0 = 50200(200) gas PE[1,2]

$\tilde{B}\ ^2\Pi_{3/2}$ $C_{\infty v}$
T_0 = 18759.78(4) gas EF[7]LF[10,11] $\tilde{B}-\tilde{X}$ 445–620 nm
18586(14) Ne AB[5] $\tilde{B}-\tilde{X}$ 418–538 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡N stretch	1958(2)	gas	EF,LF	7,10
			1830(10)	Ne	AB	5
Π	2	Bend	395.7(2)H	gas	EF,LF	7,10
			377(10)	Ne	AB	5
Σ^+	3	CBr stretch	473.1(2)	gas	EF,LF	7,10
			478(10)	Ne	AB	5

τ_1 = 197(10) ns gas EF[3]PIFCO[6]T-PEFCO[8]
τ_2 = 713(40) ns gas PIFCO[6]T-PEFCO[8]
A = −880(40) gas EF[7]PE[9]
B_0 = 0.127 gas LF[10,11]

$\tilde{A}\ ^2\Sigma^+$ $C_{\infty v}$
T_0 = 13699(1) gas EF[7] $\tilde{A}-\tilde{X}$ 708–853 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CN stretch	1930(2)	gas	EF	7
Π	2	Bend	421(2)	gas	EF	7
Σ^+	3	CBr stretch	584(2)	gas	EF	7

τ = 2750(100) ns gas T-PEFCO[8]

$\tilde{X}\ ^2\Pi_{3/2}$ $C_{\infty v}$ Structure: LF[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡N stretch	1906(2)	gas	EF,LF	7,10
Π	2	Bend	287.2(2)H	gas	EF,LF	7,10
Σ^+	3	CBr stretch	649.4(5)	gas	EF,LF	7,10

A = −1477(2) gas EF[3]PIFCO[4]
B_0 = 0.142 gas LF[10,11]

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ICN^+

$\tilde{C}\ ^2\Sigma^+$ $C_{\infty v}$
T_0 = 46600(200) gas PE[1,2]

$\tilde{B}\ ^2\Pi_{3/2}$ $C_{\infty v}$
T_0 = 19630(160) gas EF[6] $\tilde{B}$–$\tilde{X}$ 568–644[a] nm
20023(16) Ne AB[4] $\tilde{B}$–$\tilde{X}$ 446–522 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CN stretch	2100(40)	gas	PE	7
Π	2	Bend	300(40)	gas	PE	7
Σ^+	3	CI stretch	473(2)[b]	gas	EF	6
			400(20)	Ne	AB	4

τ = 300(60) ns EF[3], 300(30) ns PIFCO[4] for overlapping $\tilde{A}$ and $\tilde{B}$ states. Triexponential fit of PIFCO data[5] gives $\tau_1 \cong 270$ ns and $\tau_2 \cong 2.3$ μs.
A = −890(160) gas EF[6]; −1130(40) gas PE[7]

$\tilde{A}\ ^2\Sigma^+$ $C_{\infty v}$
T_0 = 18262(1) gas EF[3,6] $\tilde{A}$–$\tilde{X}$ 537–758 nm
19135(15) Ne AB[4] $\tilde{A}$–$\tilde{X}$ 499 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	274(2)	gas	EF	6

τ = 1.2(2) μs EF[3]; ca. 900 ns from triexponential fit to PIFCO data.[5]

$\tilde{X}\ ^2\Pi_{1/2}$ $C_{\infty v}$
T_0 = 4343(2) gas EF[3,6] $\tilde{A}, \tilde{B}$–$\tilde{X}$ 537–758 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	253(2)	gas	EF	6
Σ^+	3	CI stretch	559(2)	gas	EF	6

$\tilde{X}\ ^2\Pi_{3/2}$ $C_{\infty v}$ Structure: UV,PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡N stretch	2082(2)	gas	EF	6
Π	2	Bend	239(2)	gas	EF	6
Σ^+	3	CI stretch	535(2)	gas	EF	6

[a] $\tilde{B}\ ^2\Pi_{1/2}$ – $\tilde{X}\ ^2\Pi_{1/2}$ transition observed.
[b] ω = 1/2.

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FCP^+

$\tilde{B}\ ^2\Pi$ $C_{\infty v}$
T_0 = 56960(320) gas PE[1]

$\tilde{A}\ ^2\Sigma^+$ $C_{\infty v}$
T_0 = 24077.7(6) gas PE[1]EF[2] $\tilde{A}$–$\tilde{X}$ 395–485 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CP stretch	1866(2)	gas	EF	2
	3	CF stretch	817(2)	gas	EF	2

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡P stretch	1729(2)	gas	PE,EF	1,2
Σ^+	3	CF stretch	765(1)	gas	PE,EF	1,2

A = −190.2(6) gas EF[2]

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$ClCP^+$

$\tilde{C}$ $C_{\infty v}$
T^a = 54100(500) gas PE[1]

$\tilde{B}$ $C_{\infty v}$
T^a = 29200(500) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	CCl stretch	500(50)	gas	PE	1

$\tilde{A}$ $C_{\infty v}$
T^a = 22900(500) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	CCl stretch	485(50)	gas	PE	1

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡P stretch	1350(50)T[b]	gas	PE	1

[a] From vertical ionization potential.
[b] Value taken from text of Ref. 1; Table 1 gives 1240(50).

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CNO

$\tilde{A}\ ^2\Sigma^+$ $C_{\infty v}$
T_0 = 12611.8 gas UV[2] $\tilde{A}$–$\tilde{X}$ 789–804 nm
12541 Ne UV[1] $\tilde{A}$–$\tilde{X}$ 581–797 nm
Threshold for photoisomerization to NCO at wavelength longer than 700 nm.[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CN stretch	2239	Ne	UV	1
Π	2	Bend	605	Ne	UV	1
Σ^+	3	NO stretch	1247	Ne	UV	1

B_0 = 0.398 UV[2]

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$
A = −110.6 UV[2]
B_0 = 0.38 UV[2]

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N_3

$\tilde{B}\ ^2\Sigma_u^+$ $D_{\infty h}$ Structure: AB^2
T_0[a] = 36738.750(2) gas $AB^{1,2}LF^{3,8}PD^7$ $\tilde{B}$–$\tilde{X}$ 260–273 nm
All bands above 37000 are diffuse. Fast beam photodissociation studies[7] show that predissociation into N (^{2}D) + N_2 ($X\ ^1\Sigma_g^+$) occurs throughout the 260–273 nm spectral region.

An absorption maximum was observed at 272 nm in mixed argon-nitrogen matrix studies.[6]
$\tau \geq 0.37, \leq 20$ ns gas $LF^{3,8}$
B_0 = 0.432 gas AB^2

$\tilde{X}\ ^2\Pi_g$ $D_{\infty h}$ Structure: AB^2IR^6

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1320T	gas	LF	3
			1287[b]	N_2[c]	IR	4
Π_u	2	Bend	457T	gas	LF	3
			472.7	N_2[c]	IR	4
Σ_u^+	3	Asym. stretch	1644.68	gas	LMR,IR	5,6
			1657.5	N_2[c]	IR	4

A_{eff} = −71.3; $\epsilon\omega_2$ = −94.38 gas AB^2IR^6
B_0 = 0.431 $AB^2LMR^5IR^6$

[a] Revised value resulting from reanalysis by Ref. 6.
[b] $(\nu_1 + \nu_3) - \nu_3$.
[c] Mixed with argon.

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P_3

T_0 = 23420(10) Ar AB^1 418–427 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	480(20)	Ar	AB	1

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Sb_3

$\tilde{a}\ ^4A_2''$ D_{3h}
$T^a \cong$ 11300 gas PE[1]

$\tilde{X}\ ^2E''$ D_{3h}
Jahn-Teller splitting occurs, with the $^2A_2$ and $^2B_1$ levels separated by ca. 1290 cm^{-1}. gas PE[1]

[a] Band maximum in photoelectron spectrum.

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Bi_3

$\tilde{a}\ ^4A_2''$ D_{3h}
T_0 = 7990(80) gas PE[1]
Bands separated by 1210(80) have been attributed[1] to the $E_{5/2}$ and $E_{3/2}$ components which result from strong spin-orbit interaction in the $\tilde{a}$ $^4A_2''$ state.

$\tilde{X}\ ^2E'$ D_{3h}
A = 2180(80) gas PE[1]

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N_2O^+

$\tilde{C}\ ^2\Sigma^+$ $C_{\infty v}$
T_0 = 58245(32) gas PE[1]PI[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Sym. stretch	1280(50)	gas	PE	1
	3	Asym. stretch	2300(50)	gas	PE	1

$\tilde{B}\ ^2\Pi$ $C_{\infty v}$
T_0 = 38440(100)[a] gas PE[1]PF[15] $\tilde{B}$–$\tilde{A}$ 538–866 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Sym. stretch	900[b]T	gas	PE	1

$\tilde{A}\ ^2\Sigma^+$ $C_{\infty v}$ Structure: EM[3]PF[16]
T_0 = 28162.33 gas EM[3,14]PF[6,10,11,16] $\tilde{A}$–$\tilde{X}$ 317–421 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Sym. stretch	1345.52	gas	EM,PF	3,10
Π	2	Bend	614.45	gas	EM	3,14
Σ^+	3	Asym. stretch	2451.7	gas	EM	3

τ = 230(10) ns gas EF[2,9]PIFCO[4]PEFCO[7]ID[8]EM[12]HFD[13]
B_0 = 0.433 EM[3,14]PF[10,11]

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$ Structure: EM[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Sym. stretch	1126.51	gas	EM	3
			1135.5	Ne	IR	17
Π	2	Bend	452.42	gas	EM,PF	3,11,14
Σ^+	3	Asym. stretch	1737.6	gas	EM	3
			1741.4wm	Ne	IR	17

A = −132.434, $\epsilon\omega_2$ = −90.2 gas EM[3,14]PF[11,16]
B_0 = 0.412 EM[3]PF[10,11,16]

[a] Calculated using first ionization potential of 12.886(2) eV, from Ref. 5.
[b] Somewhat irregular band spacings.

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NNS^+

$\tilde{B}\ ^2\Pi$[a] $C_{\infty v}$
T_0 ≅ 41500 gas PE[1]

$\tilde{A}\ ^2\Sigma$ $C_{\infty v}$
T_0 = 38810(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		NS stretch	820(50)	gas	PE	1

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		NS stretch	500T	gas	PE	1

A ≅ 400 gas PE[1]

[a] Tentative assignment.

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BeF_2

$\tilde{X}$ $D_{\infty h}$ Structure: MB[1]IR[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	330s	Ne	IR	2
			309s	Ar	IR	2
			302s	Kr	IR	2
Σ_u^+	3	Asym. stretch	1555.05	gas	IR	3
			1542vs	Ne	IR	2
			1528vs	Ar	IR	2
			1524vs	Kr	IR	2

B_0 = 0.235 IR[3]

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$BeCl_2$

$\tilde{X}$ $D_{\infty h}$ Structure: MB[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	238s	Ne	IR	3
Σ_u^+	3	Asym. stretch	1122s	Ne	IR	2,3
			1108s	Ar	IR	2
			1100s	Kr	IR	2

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$BeBr_2$

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	207s	Ne	IR	1
Σ_u^+	3	Asym. stretch	993s	Ne	IR	1
			985s	Ar	IR	1

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BeI_2

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	872s	Ne	IR	1
			877s	Ar	IR	1

References

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MgF_2

$\tilde{X}$ $D_{\infty h}$ Structure: MB[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	254wm	Ne	IR	2
			243wm	Ar	IR	2
			238wm	Kr	IR	2
Σ_u^+	3	Asym. stretch	862s	Ne	IR	2
			840s	Ar	IR	2
			834m	Kr	IR	2

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BO_2^-

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	587.8	Ar	IR	1
Σ_u^+	3	Asym. stretch	1931.0	Ar	IR	1
			1926.1	Kr	IR	1
			1915.6	Xe	IR	1
			1925.8	O_2	IR	1

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FBO

$\tilde{X}$ $C_{\infty v}$ Structure: MW,DL[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	B≡O stretch	2078.87	gas	DL	2
			2081	Ne	IR	1
			2071	Ar	IR	1
Π	2	Bend	502	Ne	IR	1
			493	Ar	IR	1

B_0 = 0.312 DL,MW[2]

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ClBO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	B≡O stretch	1958s	Ar	IR	1
	2	Bend	404s	Ar	IR	1
	3	BCl stretch	676.04	gas	DL	2
			673wm	Ar	IR	1

References

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[2]K. Kawaguchi, Y. Endo, and E. Hirota, J. Mol. Spectrosc. **93**, 381 (1982).

BrBO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	B=O stretch	1937vs	Ar	IR	1
	2	Bend	374s	Ar	IR	1
	3	BBr stretch	535w	Ar	IR	1

References

[1]A. Snelson, High Temp. Sci. **4**, 318 (1972).

FBS

$\tilde{X}$ $C_{\infty v}$ Structure: MW[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	370(50)	gas	MW	1

B_0 = 0.165 MW[1]

References

[1]T. A. Cooper, S. Firth, and H. W. Kroto, J. Chem. Soc., Faraday Trans. **87**, 1499 (1991).

ClBS

$\tilde{X}$ $C_{\infty v}$ Structure: MW[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	300(40)	gas	MW	1

B_0 = 0.093 MW[1]

References

[1]C. Kirby and H. W. Kroto, J. Mol. Spectrosc. **83**, 130 (1980).

BrBS

$\tilde{X}$ $C_{\infty v}$ Structure: MW[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	270(40)	gas	MW	1
Σ^+	2	BBr stretch	414(14)	gas	MW	1

B_0 = 0.061 MW[1]

References

[1]T. A. Cooper, S. Firth, and H. W. Kroto, J. Chem. Soc., Faraday Trans. **87**, 1 (1991).

FAlO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	AlO stretch	1148vs	Ar	IR	1
	3	AlF stretch	740s	Ar	IR	1

References

[1]H. Schnöckel, J. Mol. Struct. **50**, 267 (1978).

OAlCl

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	AlO stretch	1094vs	Ar	IR	1
	3	AlCl stretch	490m	Ar	IR	1

References

[1]H. Schnöckel, J. Mol. Struct. **50**, 267 (1978).

OGaF

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	GaO stretch	943	Ar	IR	1
	3	GaF stretch	690	Ar	IR	1

References

[1]H. Schnöckel and H. J. Gocke, J. Mol. Struct. **50**, 281 (1978).

NCO^-

Threshold for electron detachment from ground-state NCO^- = 29120(40) gas PE[2]

$\tilde{X}$ $C_{\infty v}$ Structure: PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	Asym. stretch	2124.31	gas	DL	1

B_0 = 0.384 DL[1]

References

[1]M. Gruebele, M. Polak, and R. J. Saykally, J. Chem. Phys. **86**, 6631 (1987).
[2]S. E. Bradforth, E. H. Kim, D. W. Arnold, and D. M. Neumark, J. Chem. Phys. **98**, 800 (1993).

NCS^-

Threshold for electron detachment from ground-state NCS^- = 28540(40) gas PE[2]

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	CN stretch	2065.93	gas	DL	1

B_0 = 0.197 DL[1]

References

[1]M. Polak, M. Gruebele, and R. J. Saykally, J. Chem. Phys. **87**, 3352 (1987).
[2]S. E. Bradforth, E. H. Kim, D. W. Arnold, and D. M. Neumark, J. Chem. Phys. **98**, 800 (1993).

FCO^+

$\tilde{X}\ ^1\Sigma^+$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	650(30)	gas	PE	1

B_0 = 0.359 MW[2]

References

[1]J. M. Dyke, N. Jonathan, A. Morris, and M. J. Winter, J. Chem. Soc., Faraday Trans. 2 **77**, 667 (1981).
[2]P. Botschwina, P. Sebald, M. Bogey, C. Demuynck, and J.-L. Destombes, J. Mol. Spectrosc. **153**, 255 (1992).

SiO_2

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	272.5	Ar	IR	3
Σ_u^+	3	Asym. stretch	1416.4	Ar	IR	1-3

References

[1]H. Schnöckel, Angew. Chem. **90**, 638 (1978); Angew. Chem. Int. Ed. Engl. **17**, 617 (1978).
[2]H. Schnöckel, Z. Anorg. Allg. Chem. **460**, 37 (1980).
[3]L. Andrews and M. McCluskey, J. Mol. Spectrosc. **154**, 223 (1992).

OSiS

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	SiO stretch	1265.4	Ar	IR	1
	3	SiS stretch	643.0	Ar	IR	1

References

[1]H. Schnöckel, Angew. Chem. **92**, 310 (1980); Angew. Chem. Int. Ed. Engl. **19**, 323 (1980).

SiS_2

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	SiS a-stretch	918.0	Ar	IR	1

References

[1]H. Schnöckel and R. Köppe, J. Am. Chem. Soc. **111**, 4583 (1989).

GeO_2

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	195.5	Ar	IR	2
Σ_u^+	3	GeO a-stretch	1052.3	Ar	IR	2,3
			1061.6	N_2	IR	1

References

[1]A. Bos, J. S. Ogden, and L. Orgee, J. Phys. Chem. **78**, 1763 (1974).
[2]L. Andrews and M. McCluskey, J. Mol. Spectrosc. **154**, 223 (1992).
[3]P. Hassanzadeh and L. Andrews, J. Phys. Chem. **96**, 6181 (1992).

OGeS

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	GeO stretch	984.3	Ar	IR	1

References

[1]P. Hassanzadeh and L. Andrews, J. Phys. Chem. **96**, 6181 (1992).

GeS_2

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	GeS a-stretch	653.4	Ar	IR	1,2

References

[1]R. Köppe and H. Schnöckel, J. Mol. Struct. **238**, 429 (1990).
[2]P. Hassanzadeh and L. Andrews, J. Phys. Chem. **96**, 6181 (1992).

FNN^+

$\tilde{X}$ $C_{\infty v}$
$B_0 = 0.372$ MW[1]

References

[1]P. Botschwina, P. Sebald, M. Bogey, C. Demuynck, and J.-L. Destombes, J. Mol. Spectrosc. **153**, 255 (1992).

N_3^-

Threshold for electron detachment from ground-state N_3^- is 21620(80).[1,5]

$\tilde{X}\ ^1\Sigma_g^+$ $D_{\infty h}$ Structure: DL[2,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	1986.47	gas	DL	2,3
			2003.5	N_2[a]	IR	4

$B_0 = 0.426$ DL[2,3]

[a] Mixed with argon.

References

[1]E. Ilenberger, P. B. Comita, J. I. Brauman, H. P. Fenzlatt, M. Heni, N. Heinrich, W. Koch, and G. Frenking, Ber. Bunsenges. Phys. Chem. **89**, 1026 (1985).
[2]M. Polak, M. Gruebele, and R. J. Saykally, J. Am. Chem. Soc. **109**, 2884 (1987).
[3]M. Polak, M. Gruebele, G. S. Peng, and R. J. Saykally, J. Chem. Phys. **89**, 110 (1988).
[4]R. Tian, J. C. Facelli, and J. Michl, J. Phys. Chem. **92**, 4073 (1988).
[5]R. E. Continetti, D. R. Cyr, R. B. Metz, and D. M. Neumark, Chem. Phys. Lett. **182**, 406 (1991).

NO_2^+

$^3B_2$ C_{2v}
T_0[a] = 74580(100) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1113(20)	gas	PE	1,2
	2	Bend	686(20)	gas	PE	1,2

$\tilde{d}\ ^3A_1$ C_{2v}
$T^a \cong 67600$ gas PE[2]

$\tilde{C}\ ^1B_1$ C_{2v}
T_0[a] = 60670(100) gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1017(20)	gas	PE	1,2

$\tilde{c}\ ^3B_1$ C_{2v}
T_0[a] = 60100(100) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1041(20)	gas	PE	1,2

$\tilde{B}\ ^1B_2$ C_{2v}
T_0[a] = 38940(100) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1025(20)	gas	PE	2
	2	Bend	573(20)	gas	PE	1,2

$\tilde{A}\ ^1A_2$ C_{2v}
T_0[a] = 35900(100) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	984(20)	gas	PE	1,2
	2	Bend	694(20)	gas	PE	1,2

$\tilde{b}\ ^3A_2$ C_{2v}
T_0[a] = 32110(100) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	662(20)	gas	PE	1,2

$\tilde{a}\ ^3B_2$ C_{2v}
T_0[a] = 26170(100) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	654(20)	gas	PE	1,2

$\tilde{X}\ ^1\Sigma_g^+$ $D_{\infty h}$ Structure: TPE[4,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1397	gas	TPE	5
			1362.4[b]	Ne	IR	6
Π	2	Bend	639	gas	TPE	5
Σ_u^+	3	Asym. stretch	2362	gas	TPE	5
			2348.2	Ne	IR	6

$B_0 = 0.417$ TPE[4]

[a] The band origins given here have been calculated using a first ionization potential of 9.62(1) eV for NO_2, as found in the photoionization study of Ref. 3.
[b] $(\nu_1 + \nu_3) - \nu_3$.

References

[1]C. R. Brundle, D. P. Neumann, W. C. Price, D. Evans, A. W. Potts, and D. G. Streets, J. Chem. Phys. **53**, 705 (1970).
[2]O. Edqvist, E. Lindholm, L. E. Selin, and I. Åsbrink, Phys. Scripta **1**, 127 (1970).
[3]P. C. Killgoar, Jr., G. E. Leroi, W. A. Chupka, and J. Berkowitz, J. Chem. Phys. **59**, 1370 (1973).
[4]G. P. Bryant, Y. Jiang, M. Martin, and E. R. Grant, J. Phys. Chem. **96**, 6875 (1992).
[5]G. Bryant, Y. Jiang, and E. Grant, Chem. Phys. Lett. **200**, 495 (1992).
[6]D. Forney, W. E. Thompson, and M. E. Jacox, J. Chem. Phys. **99**, 7393 (1993).

PNO

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NO stretch	1754.7	Ar	IR	1
	3	PN stretch	865.2	Ar	IR	1

References

[1]R. Ahlrichs, S. Schunck, and H. Schnöckel, Angew. Chem. **100**, 418 (1988); Angew. Chem. Int. Ed. Engl. **27**, 421 (1988).

P_2O

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		P=O stretch	1270.4	Ar	IR	1

References

[1]Z. Mielke, M. McCluskey, and L. Andrews, Chem. Phys. Lett. **165**, 146 (1990).

NNS

$\tilde{X}$ $C_{\infty v}$ Structure: IR^2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NN stretch	2047.59	gas	IR	2
			2040.2	Ar	IR	1,3,4
	3	NS stretch	752	Ar	IR	4

B_0 = 0.216 gas IR^2

References

[1]C. Wentrup, S. Fischer, A. Maquestiau, and R. Flammang, J. Org. Chem. **51**, 1908 (1986).
[2]R. D. Brown, P. S. Elmes, and D. McNaughton, J. Mol. Spectrosc. **140**, 390 (1990).
[3]P. Hassanzadeh and L. Andrews, J. Am. Chem. Soc. **114**, 83 (1992).
[4]P. Kambouris, T.-K. Ha, and C. Wentrup, J. Phys. Chem. **96**, 2065 (1992).

P_2S

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		"Asym." stretch	891.4	Ar	IR	1

References

[1]Z. Mielke, G. D. Brabson, and L. Andrews, J. Phys. Chem. **95**, 75 (1991).

FNC

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NC stretch	2123w	Ar	IR	1
Σ^+	3	NF stretch	928s	Ar	IR	1

References

[1]D. E. Milligan and M. E. Jacox, J. Chem. Phys. **47**, 278 (1967).

ClNC

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NC stretch	2074s	Ar	IR	1
Σ^+	3	NCl stretch	615?	Ar	IR	1

References

[1]D. E. Milligan and M. E. Jacox, J. Chem. Phys. **47**, 278 (1967).

BrNC

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NC stretch	2067s	Ar	IR	1

References

[1]D. E. Milligan and M. E. Jacox, J. Chem. Phys. **47**, 278 (1967).

Sb_3^-

Threshold for electron detachment from ground-state Sb_3^- = 14930(240) gas PE[1]

References

[1]M. L. Polak, G. Gerber, J. Ho, and W. C. Lineberger, J. Chem. Phys. **97**, 8990 (1992).

BF_2

$\tilde{B}\ ^2A_1$ C_{2v}
EF[1]EM[2,3] $\tilde{B}-\tilde{A},\tilde{X}$ 190–650 nm
$\tau \cong 11$ ns EF[1]EM[3]

$\tilde{A}\ ^2B_1$ C_{2v}
EF[1]EM[2,3] $\tilde{A}-\tilde{X}$ 220–650 nm
$\tau = 49$ ns EM[3]

$\tilde{X}\ ^2A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	525(30)	gas	EM	3
b_2	3	Asym. stretch	1389.9	Ar	IR	4
			1384.8	N_2	IR	4

References

[1]J. E. Hesser and K. Dressler, J. Chem. Phys. **47**, 3443 (1967).
[2]M. Suto, C. Ye, and L. C. Lee, Phys. Rev. A **42**, 424 (1990).
[3]J. C. Creasey, P. A. Hatherly, H. M. Jones, I. R. Lambert, and R. P. Tuckett, Mol. Phys. **78**, 837 (1993).
[4]P. Hassanzadeh and L. Andrews, J. Phys. Chem. **97**, 4910 (1993).

BCl_2

Emission which is observed between 200 and 260 nm on excitation of BCl_3 by radiation of wavelength shorter than 91 nm has been attributed[5] to BCl_2.

$\tilde{B}$

Emission which is observed between 200 and 500 nm on excitation of BCl_3 by radiation of wavelength between 100 and 124 nm (9.99–12.27 eV) has been attributed[8] to the $\tilde{B}-\tilde{X}$ transition of BCl_2. Other studies suggest two different emission systems, as summarized below.

Emission which is observed between 240 and 380 nm on excitation of BCl_3 by radiation of wavelength shorter than 118 nm[4,5] and on electron impact[6] has been attributed to BCl_2, as has been a similar chemiluminescence emission observed[1,2] on reaction of H atoms with BCl_3. The electron impact study[6] yielded a radiative lifetime of 1.65(20) μs and suggested that the lower state is the ground state of BCl_2.

Emission which is observed between 280 and 380 nm on excitation of BCl_3 by radiation of wavelength shorter than 124 nm[4,5] and on electron impact[6] has also been attributed to BCl_2.

$\tilde{A}$

Emission which is observed between 380 and 650 nm on excitation of BCl_3 by radiation of wavelength shorter than 138 nm[4,5,8] and on electron impact[6] has been attributed to the $\tilde{A}-\tilde{X}$ transition of BCl_2. The electron impact study indicated that the lower state is the ground state of BCl_2.

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	731w	Ar	IR	3
b_2	3	Asym. stretch	965.6vs	Ar	IR	3,7

References

[1]O. Dessaux, P. Goudmand, and G. Pannetier, Compt. Rend. Acad. Sci. Paris C **265**, 480 (1967).
[2]O. Dessaux, P. Goudmand, and G. Pannetier, Bull. Soc. Chim. Fr. **1969**, 447.
[3]J. H. Miller and L. Andrews, J. Am. Chem. Soc. **102**, 4900 (1980).
[4]M. Suto, C. Ye, J. C. Han, and L. C. Lee, J. Chem. Phys. **89**, 6653 (1988).
[5]L. C. Lee, J. C. Han, and M. Suto, J. Chem. Phys. **91**, 2036 (1989).
[6]I. Tokue, M. Kudo, M. Kusakabe, T. Honda, and Y. Ito, J. Chem. Phys. **96**, 8889 (1992).
[7]P. Hassanzadeh and L. Andrews, J. Phys. Chem. **97**, 4910 (1993).
[8]J. C. Creasey, P. A. Hatherly, I. R. Lambert, and R. P. Tuckett, Mol. Phys. **79**, 413 (1993).

BBr_2

In an argon matrix, an absorption maximum at 15900 (630 nm) has been attributed[2] to BBr_2.

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	551.0w	Ar	IR	2
b_2	3	Asym. stretch	833.4s	Ar	IR	1-3

References

[1]J. H. Miller and L. Andrews, J. Am. Chem. Soc. **102**, 4900 (1980).
[2]A. Moroz and R. L. Sweany, Inorg. Chem. **31**, 5236 (1992).
[3]P. Hassanzadeh and L. Andrews, J. Phys. Chem. **97**, 4910 (1993).

BI_2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	745.5 739.5	Ar	IR	1

References

[1]P. Hassanzadeh and L. Andrews, J. Phys. Chem. **97**, 4910 (1993).

$AlCl_2$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	460.0	Ar	IR	2
b_2	3	Asym. stretch	563.6	Ar	IR	1,2

References

[1]G. A. Olah, O. Farooq, S. M. F. Farnia, M. R. Bruce, F. L. Clouet, P. R. Morton, G. K. S. Prakash, R. C. Stevens, R. Bau, K. Lammertsma, S. Suzer, and L. Andrews, J. Am. Chem. Soc. **110**, 3231 (1988).

[2]E. D. Samsonova, S. B. Osin, and V. F. Pevel'kov, Zh. Neorgan. Khim. **33**, 2779 (1988); Russ. J. Inorg. Chem. **33**, 1598 (1988).

$GaCl_2$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	373.0	Ar	IR	1
b_2	3	Asym. stretch	415.1	Ar	IR	1

References

[1]E. D. Samsonova, S. B. Osin, and V. F. Pevel'kov, Zh. Neorgan. Khim. **33**, 2779 (1988); Russ. J. Inorg. Chem. **33**, 1598 (1988).

CO_2^-

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	1658.3	Ne	IR	1

References

[1]M. E. Jacox and W. E. Thompson, J. Chem. Phys. **91**, 1410 (1989).

FCO

$\tilde{C}$

T_0 ≤ 35741 gas AB[2,8] $\tilde{C}$–$\tilde{X}$ 220–280 nm
≤ 35587 Ar AB[3] $\tilde{C}$–$\tilde{X}$ 234–281 nm
≤ 35211 CO AB[1,3] $\tilde{C}$–$\tilde{X}$ 217–284 nm

In the gas phase,[2] bands are diffuse, and the onset of predissociation is estimated[7] to lie at a wavelength longer than 294 nm. In an argon matrix,[3] the threshold for photodissociation into F + CO was observed near 280 nm.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			650T	gas	AB	2,8
			650T	Ar	AB	3
			650T	CO	AB	1,3

$\tilde{B}$

T_0 ≥ 27586 gas CL[5]LF[6]AB[8] $\tilde{B}$–$\tilde{X}$ 280–455 nm
≤ 29586 Ar AB[3] $\tilde{B}$–$\tilde{X}$ 284–338 nm
≤ 29516 CO AB[1,3] $\tilde{B}$–$\tilde{X}$ 289–339 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	725T	gas	AB	8
			700T[a]	Ar	AB	3
			700T[a]	CO	AB	1,3

τ = 40(3) ns gas LF[6]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CO stretch	1861.64	gas	DL	4
			1857vs	Ar	IR	3
			1855vs	CO	IR	1
	2	Bend	627.5m	Ar	IR	3
			626m	CO	IR	1
	3	CF stretch	1026.13	gas	DL	4
			1023vs	Ar	IR	3
			1018s	CO	IR	1

A_0 = 6.38; B_0 = 0.382; C_0 = 0.360 DL[4]

[a] A second progression, offset by ca. 350, may be contributed by excitation of a CF-stretching mode near 1050; in the gas-phase chemiluminescence,[5] the major progression is in the ground-state bending mode, but structure associated with the CF-stretching mode is also observed.

References

[1]D. E. Milligan, M. E. Jacox, A. M. Bass, J. J. Comeford, and D. E. Mann, J. Chem. Phys. **42**, 3187 (1965).

[2]D. K. W. Wang and W. E. Jones, J. Photochem. **1**, 147 (1972).

[3]M. E. Jacox, J. Mol. Spectrosc. **80**, 257 (1980).

[4]K. Nagai, C. Yamada, Y. Endo, and E. Hirota, J. Mol. Spectrosc. **90**, 249 (1981).

[5]S. Toby and F. S. Toby, J. Phys. Chem. **85**, 4071 (1981).

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[7]G. Hancock and D. E. Heard, J. Photochem. Photobiol. A: Chem. **60**, 265 (1991).

[8]M. M. Maricq, J. J. Szente, G. A. Khitrov, and J. S. Francisco, Chem. Phys. Lett. **199**, 71 (1992).

ClCO

$\tilde{X}$ C_s Structure: IR[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CO stretch	1876.7vs	Ar	IR	1,2
			1880vs	CO	IR	1
	2	Bend	334.6	Ar	IR	2
	3	CCl stretch	570.1s	Ar	IR	1,2
			570s	CO	IR	1

References

[1]M. E. Jacox and D. E. Milligan, J. Chem. Phys. **43**, 866 (1965).
[2]H. Schnöckel, R. A. Eberlein, and H. S. Plitt, J. Chem. Phys. **97**, 4 (1992).

CF_2^+

$\tilde{F}\ ^2A_1$
T_0 = 101500(1000)[a] gas PE[1]

$\tilde{E}\ ^2B_2$
T_0 = 87000(1000)[a] gas PE[1]

$\tilde{D}\ ^2B_1$
T_0 = 75920(160)[a] gas PE[1]

$\tilde{C}\ ^2A_1$
T_0 = 62800(1000)[a] gas PE[1]

$\tilde{B}\ ^2A_2$
T_0 = 48200(1000)[a] gas PE[1]
Calculations[3] indicate that this state should dissociate into CF^+ + F.

$\tilde{A}\ ^2B_2$
T_0 = 40180(240)[a] gas PE[1]

$\tilde{X}\ ^2A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	650(40)	gas	PE	1
b_2	3	Asym. stretch	1588T	Ar	IR	2

[a] From vertical ionization potential.

References

[1]J. M. Dyke, L. Golob, N. Jonathan, A. Morris, and M. Okuda, J. Chem. Soc., Faraday Trans. 2 **70**, 1828 (1974).
[2]L. Andrews and B. W. Keelan, J. Am. Chem. Soc. **101**, 3500 (1979).
[3]D. A. Hrovat and W. T. Borden, J. Am. Chem. Soc. **107**, 8034 (1985).

CCl_2^+

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	1195.40	Ar	IR	1-3

References

[1]L. Andrews and B. W. Keelan, J. Am. Chem. Soc. **101**, 3500 (1979).
[2]B. W. Keelan and L. Andrews, J. Phys. Chem. **83**, 2488 (1979).
[3]B. J. Kelsall and L. Andrews, J. Mol. Spectrosc. **97**, 362 (1983).

$CClBr^+$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CCl stretch	1120.6	Ar	IR	1,2

References

[1]L. Andrews and B. W. Keelan, J. Am. Chem. Soc. **101**, 3500 (1979).
[2]B. J. Kelsall and L. Andrews, J. Mol. Spectrosc. **97**, 362 (1983).

CBr_2^+

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	1019.6	Ar	IR	1-3

References

[1]L. Andrews and B. W. Keelan, J. Am. Chem. Soc. **101**, 3500 (1979).
[2]B. W. Keelan and L. Andrews, J. Phys. Chem. **83**, 2488 (1979).
[3]B. J. Kelsall and L. Andrews, J. Mol. Spectrosc. **97**, 362 (1983).

SiF_2^+

$\tilde{E}\ ^2B_2$ C_{2v}
T_0 = 56600(1600) gas PE[2]

$\tilde{D}\ ^2B_1$ C_{2v}
T_0 = 50700(800)[a] gas PE[1,2]

$\tilde{C}\ ^2A_1$ C_{2v}
T_0 = 48600(1200)[a] gas PE[2]

$\tilde{B}\ ^2A_2$ C_{2v}
T_0 = 40500(1200)[a] gas PE[2]

$\tilde{A}\ ^2B_2$ C_{2v}
T_0 = 32400(1200) gas PE[1,2]

$\tilde{X}\ ^2A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	350(100)	gas	PE	2

[a] From vertical ionization potential.

References

[1]T. P. Fehlner and D. W. Turner, Inorg. Chem. **13**, 754 (1974).
[2]N. P. C. Westwood, Chem. Phys. Lett. **25**, 558 (1974).

$SiCl_2^+$

$\tilde{F}$ C_{2v}
T^a = 52850(1000) gas PE[1]

$\tilde{E}$ $^2B_2$ C_{2v}
T^a = 30260(1000) gas PE[1]

$\tilde{C},\tilde{D}$ $^2B_1,^2A_1$ C_{2v}
T^a = 23800(1000) gas PE[1]

$\tilde{A},\tilde{B}$ $^2B_2,^2A_2$ C_{2v}
T^a = 14120(400) gas PE[1]

$\tilde{X}$ $^2A_1$ C_{2v}

[a] From vertical ionization potentials.

References

[1]H. Bock, B. Solouki, and G. Maier, Angew. Chem. **97**, 205 (1985); Angew. Chem. Int. Ed. Engl. **24**, 205 (1985).

SiI_2^+

$\tilde{F}$ $^2A_1$ C_{2v}
T^a = 35500(160) gas PE[1]

$\tilde{E}$ $^2B_2$ C_{2v}
T^a = 20010(160) gas PE[1]

$\tilde{D}$ $^2A_1$ C_{2v}
T^a = 16140(160) gas PE[1]

$\tilde{C}$ $^2B_1$ C_{2v}
T^a = 12500(160) gas PE[1]

$\tilde{B}$ $^2A_2$ C_{2v}
T^a = 6780(160) gas PE[1]

$\tilde{A}$ $^2B_2$ C_{2v}
T^a = 3710(160) gas PE[1]

[a] From vertical ionization potentials.

References

[1]H. Bock, M. Kremer, M. Dolg, and H.-W. Preuss, Angew. Chem. **103**, 1200 (1991); Angew. Chem. Int. Ed. Engl. **30**, 1186 (1991).

GeF_2^+

$\tilde{F}$ $^2A_1$ C_{2v}
T_0 = 54220(480) gas PE[1]

$\tilde{E}$ $^2B_2$ C_{2v}
T_0 = 34050(1860) gas PE[1]

$\tilde{D}$ $^2B_1$ C_{2v}
T_0 = 31630(1860) gas PE[1]

$\tilde{C}$ $^2A_1$ C_{2v}
T_0 = 28800(640) gas PE[1]

$\tilde{A},\tilde{B}$ $^2B_2,^2A_2$ C_{2v}
T_0 = 19530(1860) gas PE[1]

$\tilde{X}$ $^2A_1$ C_{2v}

References

[1]G. Jonkers, S. M. van der Kerk, R. Mooyman, and C. A. de Lange, Chem. Phys. Lett. **90**, 252 (1982).

$GeCl_2^+$

$\tilde{F}$ $^2A_1$ C_{2v}
T_0 = 49860(560) gas PE[1]

$\tilde{E}$ $^2B_2$ C_{2v}
T_0 = 23080(480) gas PE[1]

$\tilde{D}$ $^2A_1$ C_{2v}
T_0 = 17270(640) gas PE[1]

$\tilde{C}$ $^2B_1$ C_{2v}
T_0 = 16380(640) gas PE[1]

$\tilde{B}$ $^2A_2$ C_{2v}
T_0 = 9280(560) gas PE[1]

$\tilde{A}$ $^2B_2$ C_{2v}
T_0 = 7180(560) gas PE[1]

$\tilde{X}$ $^2A_1$ C_{2v}

References

[1]G. Jonkers, S. M. van der Kerk, and C. A. de Lange, Chem. Phys. **70**, 69 (1982).

$GeBr_2^+$

$\tilde{F}$ $^2A_1$ C_{2v}
T_0 = 51640(640) gas PE[1]

$\tilde{E}$ $^2B_2$ C_{2v}
T_0 = 20900(480) gas PE[1]

$\tilde{D}$ $^2A_1$ C_{2v}
T_0 = 14520(640) gas PE[1]

$\tilde{C}$ $^2B_1$ C_{2v}
T_0 = 13310(640) gas PE[1]

$\tilde{B}$ $^2A_2$ C_{2v}
T_0 = 6780(480) gas PE[1]

$\tilde{A}$ $^2B_2$ C_{2v}
T_0 = 4200(560) gas PE[1]

$\tilde{X}$ $^2A_1$ C_{2v}

References

[1]G. Jonkers, S. M. van der Kerk, and C. A. de Lange, Chem. Phys. **70**, 69 (1982).

GeI_2^+

$\tilde{E}$ $^2B_2$ C_{2v}
T_0 = 20090(480) gas PE[1]

$\tilde{C},\tilde{D}$ $^2B_1,^2A_1$ C_{2v}
T_0 = 12430(480) gas PE[1]

$\tilde{B}\ ^2A_2$ C_{2v}
T_0 = 6050(480) gas PE[1]

$\tilde{A}\ ^2B_2$ C_{2v}
T_0 = 3390(480) gas PE[1]

$\tilde{X}\ ^2A_1$ C_{2v}

References

[1]G. Jonkers, S. M. van der Kerk, R. Mooyman, C. A. de Lange, and J. G. Snijders, Chem. Phys. Lett. **94**, 585 (1983).

PO_2

$^2B_1$? C_{2v}
T_0 = 30378(3) gas AB[1]LF[3] $^2B_1$–$\tilde{X}$ 268–600 nm
Ar AB[6] $^2B_1$–$\tilde{X}$ 292–301 nm

In LF studies,[3] there was an apparently continuous background signal, with a maximum between 400 and 500 nm. The similarity of the behavior of this band system to that of the visible bands of NO_2 suggests that the quasicontinuum may be contributed by high vibrational levels of the ground state.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	933	gas	AB	1
			942	Ar	AB	6
	2	Bend	396	gas	AB	1

$\tau \cong 500$ ns gas LF[3]
$\tau_{cont} \cong 4.5\ \mu$s gas LF[3]

$\tilde{X}\ ^2A_1$ C_{2v} Structure: AB[1]MW,LMR[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PO s-stretch	1117(20)	gas	MW,LMR LF	2,3
	2	Bend	387(20)	gas	MW,LMR LF	2,3
			386.4	Ar	IR	7
b_2	3	PO a-stretch	1278[a]	gas	MW,LMR	2
			1319.1	Ar	IR	4,5,7

A_0 = 3.486; B_0 = 0.287; C_0 = 0.264 MW,LMR[2]

[a] Average of values of 1059, 1371, and 1405 cm^{-1}, obtained from centrifugal distortion constants.

References

[1]R. D. Verma and C. F. McCarthy, Can. J. Phys. **61**, 1149 (1983).
[2]K. Kawaguchi, S. Saito, E. Hirota, and N. Ohashi, J. Chem. Phys. **82**, 4893 (1985).
[3]P. A. Hamilton, J. Chem. Phys. **86**, 33 (1987).
[4]L. Andrews and R. Withnall, J. Am. Chem. Soc. **110**, 5605 (1988).
[5]R. Withnall and L. Andrews, J. Phys. Chem. **92**, 4610 (1988).
[6]R. Withnall, M. McCluskey, and L. Andrews, J. Phys. Chem. **92**, 126 (1989).
[7]Z. Mielke, M. McCluskey, and L. Andrews, Chem. Phys. Lett. **165**, 146 (1990).

SNO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO stretch	1523s[a]	Ar	IR	1,2
	3	NS stretch	790m	Ar	IR	1,2

[a] In Fermi resonance with $2\nu_3$.

References

[1]P. O. Tchir and R. D. Spratley, Can. J. Chem. **53**, 2318 (1975).
[2]M. Hawkins and A. J. Downs, J. Phys. Chem. **88**, 3042 (1984).

FNO^+

T_0 = 41870(160) gas PE[1,2]

T^a = 14800(1000) gas PE[1,2]

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	590(25)	gas	PE	2

[a] From vertical ionization potential. Onset near 6780.

References

[1]D. C. Frost, S. T. Lee, C. A. McDowell, and N. P. C. Westwood, J. Electron Spectrosc. Relat. Phenom. **7**, 331 (1975).
[2]R. S. Alderdice and R. N. Dixon, J. Chem. Soc., Faraday Trans. **73**, 245 (1977).

$ClNO^+$

$\tilde{E}\ ^2A'$ C_s
T_0 = 61800(240) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO stretch	910[a]	gas	PE	2
	3	NCl stretch	520(30)	gas	PE	2

$\tilde{D}\ ^2A''$ C_s
T_0 = 46800(160) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO stretch	1250(30)	gas	PE	1,2
	3	NCl stretch	580T	gas	PE	2

$\tilde{C}\ ^2A'$ C_s
T_0 = 36550(160) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO stretch	1560(30)[b]	gas	PE	2
	3	NCl stretch	520(30)[b]	gas	PE	2

$\tilde{X}\ ^2A'$[c] C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	NCl stretch	540(30)	gas	PE	2

[a] Gradually increases to 1160.
[b] Average value.
[c] Overlapped by very low-lying transitions to the $\tilde{A}$ and $\tilde{B}$ states.[1-3] A band separation of approximately 1200 has been tentatively attributed to spin-orbit splitting.[3]

References

[1]D. C. Frost, S. T. Lee, C. A. McDowell, and N. P. C. Westwood, J. Electron Spectrosc. Relat. Phenom. **7**, 331 (1975).
[2]M. I. Abbas, J. M. Dyke, and A. Morris, J. Chem. Soc., Faraday Trans. 2 **72**, 814 (1976).
[3]R. S. Alderdice and R. N. Dixon, J. Chem. Soc., Faraday Trans. **73**, 245 (1977).

$BrNO^+$

$\tilde{F}$
T_0 = 63200(1000) gas PE[1]

$\tilde{E}$
T_0 = 53500(1000) gas PE[1]

$\tilde{D}$
T_0 = 45400(1000) gas PE[1]

$\tilde{C}$
T_0 = 36500(1000) gas PE[1]

$\tilde{X}\ ^2A'$ [a] C_s

[a] Overlapped by very low-lying transitions to the $\tilde{A}$ and $\tilde{B}$ states.[1,2] A band separation of approximately 3200 has been tentatively attributed to spin-orbit splitting.[2]

References

[1]D. C. Frost, S. T. Lee, C. A. McDowell, and N. P. C. Westwood, J. Electron Spectrosc. Relat. Phenom. **7**, 331 (1975).
[2]R. S. Alderdice and R. N. Dixon, J. Chem. Soc., Faraday Trans. **73**, 245 (1977).

NSO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		SO stretch	1195	Ar	IR	1

References

[1]P. O. Tchir and R. D. Spratley, Can. J. Chem. **53**, 2331 (1975).

NS_2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NS_2 s-stretch	660T	Ar	IR	1
b_2	3	NS_2 a-stretch	1225.2	Ar	IR	1

References

[1]P. Hassanzadeh and L. Andrews, J. Am. Chem. Soc. **114**, 83 (1992).

NSS

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	NS stretch	1017.1	Ar	IR	1
	3	SS stretch	594.6	Ar	IR	1

References

[1]P. Hassanzadeh and L. Andrews, J. Am. Chem. Soc. **114**, 83 (1992).

NSF^+

$\tilde{E}\ ^2A'$ C_s
T^a = 46000(800) gas PE[3]

$\tilde{D}\ ^2A''$ C_s
T^a = 40500(320) gas PE[1-3]

$\tilde{C}\ ^2A'$ C_s
T_0 = 27350(160) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NS stretch	895(30)	gas	PE	1-3

$\tilde{B}\ ^2A''$ C_s
T_0 = 18030(120) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NS stretch	1060(40)	gas	PE	1-3
	2	Bend	365(40)	gas	PE	1-3
	3	SF stretch	695(40)	gas	PE	1-3

$\tilde{A}\ ^2A'$ C_s
T_0 = 14860(120) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	460(50)	gas	PE	1-3
	3	SF stretch	820(40)	gas	PE	1-3

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	300(50)	gas	PE	3

[a] From vertical ionization potential.

References

[1]D. O. Cowan, R. Gleiter, O. Glemser, E. Heilbronner, and J. Scharblin, Helv. Chim. Acta **54**, 1559 (1971).
[2]R. N. Dixon, G. Duxbury, G. R. Fleming, and J. M. V. Hugo, Chem. Phys. Lett. **14**, 60 (1972).
[3]R. L. DeKock, D. R. Lloyd, A. Breeze, G. A. D. Collins, D. W. J. Cruickshank, and H. J. Lempka, Chem. Phys. Lett. **14**, 525 (1972).

$NSCl^+$

$\tilde{F}\ ^2A'$ C_s
T_0 = 47500(1000) gas PE[2]

$\tilde{E}\ ^2A''$ C_s
T^a = 35400(1000) gas PE[2]

$\tilde{D}\ ^2A'$ C_s
T_0 = 29610(240) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NS stretch	970(40)	gas	PE	2

$\tilde{C}\ ^2A'$ C_s
T_0 = 25170(240) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	250(30)	gas	PE	2

$\tilde{A},\tilde{B}\ ^2A',^2A''$ C_s
T_0 = 6210(240) gas PE[1,2]

$\tilde{X}\ ^2A'$ C_s

[a] From vertical ionization potential.

References

[1]D. O. Cowan, R. Gleiter, O. Glemser, and E. Heilbronner, Helv. Chim. Acta **55**, 2418 (1972).
[2]R. L. DeKock, M. A. Sheheth, D. R. Lloyd, and P. J. Roberts, J. Chem. Soc., Faraday Trans. 2 **72**, 807 (1976).

$NSBr^+$

$\tilde{D}\ ^2A'$ C_s
T^a = 24200(160) gas PE[1]

$\tilde{C}\ ^2A''$ C_s
T^a = 19520(160) gas PE[1]

$\tilde{B}\ ^2A'$ C_s
T^a = 5160(160) gas PE[1]

$\tilde{A}\ ^2A''$ C_s
T^a = 3230(160) gas PE[1]

[a] From vertical ionization potentials.

References

[1]A. W. Allaf, G. Y. Matti, R. J. Suffolk, and J. D. Watts, J. Electron Spectrosc. Relat. Phenom. **48**, 411 (1989).

NSI^+

$\tilde{E}\ ^2A'$ C_s
T^a = 35820(800) gas PE[1]

$\tilde{C},\tilde{D}\ ^2A',^2A''$ C_s
T^a = 23720(800) gas PE[1]

$\tilde{A},\tilde{B}\ ^2A'',^2A'$ C_s
T^a = 5490(800) gas PE[1]

[a] From vertical ionization potentials.

References

[1]A. W. Allaf, G. Y. Matti, R. J. Suffolk, and J. D. Watts, Chem. Phys. Lett. **155**, 32 (1989).

PS_2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	744.1	Ar	IR	1

References

[1]Z. Mielke, G. D. Brabson, and L. Andrews, J. Phys. Chem. **95**, 75 (1991).

O_3^+

$\tilde{E},\tilde{F}\ ^2A_1,^2B_2$ C_{2v}
T_0^b = 37680(160) gas PE[2,3,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1000(40)	gas	PE	5

$\tilde{D}\ ^2B_1$ C_{2v}
T_0[b] = 29530(160) gas PE[3,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	850(40)	gas	PE	5

$\tilde{C}\ ^2B_2$ C_{2v}
T^{ab} = 25580(160) gas PE[3,5]

$\tilde{B}\ ^2A_2$ C_{2v}
T^{ab} = 8960(160) gas PE[1-3,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	900T	gas	PE	2,5

$\tilde{A}\ ^2B_2$ C_{2v}
T^{ab} = 4600(160) gas PE[1-3,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1380(40)	gas	PE	2,5

$\tilde{X}\ ^2A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1050(80)	gas	PI	4
	2	Bend	640[c]T	gas	PE,PI	1-5

[a] From vertical ionization potential.
[b] The band origins given here have been calculated using a first ionization potential of 12.43 eV for O_3, as found by Refs. 3 and 5. If instead the value of 12.519(4) eV obtained in the photoionization study of Ref. 4 and in the photoelectron spectroscopy studies of Refs. 1 and 2 is chosen, the positions of the band origins are decreased by approximately 700.
[c] Average value.

References

[1]D. C. Frost, S. T. Lee, and C. A. McDowell, Chem. Phys. Lett. **24**, 149 (1974).
[2]C. R. Brundle, Chem. Phys. Lett. **26**, 25 (1974).
[3]J. M. Dyke, L. Golob, N. Jonathan, A. Morris, and M. Okuda, J. Chem. Soc., Faraday Trans. 2 **70**, 1828 (1974).
[4]M. J. Weiss, J. Berkowitz, and E. H. Appelman, J. Chem. Phys. **66**, 2049 (1977).
[5]S. Katsumada, H. Shiromaru, and T. Kimura, Bull. Chem. Soc. Japan **57**, 1784 (1984).

SO_2^+

$\tilde{F}\ ^2A_1$ C_{2v}
T_0 = 62200(500) gas PE[2]

$\tilde{E}\ ^2B_1$ C_{2v}
T_0 = 33550(50) gas PE[2,6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	706(4)	gas	PE	2,6

$\tilde{D}\ ^2A_1$ C_{2v}
T_0 = 32190(50) gas PE[1,2,6]PF[5] $\tilde{D}-\tilde{X}$ 300–317 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	912(1)	gas	PE,PF	1,2,5,6
	2	Bend	411(60)	gas	PF	5

$\tilde{C}\ ^2B_2$ C_{2v}
T_0 = 28670(50) gas PE[1,2,6]PF[5] $\tilde{C}-\tilde{B}$ 511–437 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	800(4)	gas	PE	6
	2	Bend	371(10)	gas	PF,PE	4-6

$\tilde{B}\ ^2B_2$ C_{2v}
T_0 = 7980(60) gas PE[1,6]PF[4,5] $\tilde{C}-\tilde{B}$ 437–511 nm[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	465(9)	gas	PE,PF	1,4-6
b_2	3	Asym. stretch	612(7)H	gas	PE	6

$\tau \cong 25\ \mu s$ gas PF[5]

$\tilde{A}\ ^2A_2$ C_{2v}
T_0 = 5156(65) gas PE[1,6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	981(60)	gas	PE	6
	2	Bend	353(7)	gas	PE	6
b_2	3	Asym. stretch	202(13)	gas	PE	6

$\tilde{X}\ ^2A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	404.2(5)	gas	PE	1,6

Barrier to linearity ca. 3400 PE[6]

[a] Attributed by Ref. 5 to the $\tilde{C}-\tilde{A}$ transition.

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SSO^+

$\tilde{F}\ ^2A'$ C_s
T^b = 64000(1000) gas PE[2,3]

$\tilde{E}\ ^2A'$ [a] C_s
T^b = 42100(320) gas PE[1-3]

$\tilde{D}\ ^2A''$ [a] C_s
T^b = 34200(320) gas PE[1-3]

$\tilde{C}\ ^2A'$ [a] C_s
T^b = 32600(320) gas PE[1-3]

$\tilde{B}\ ^2A''$ [a] C_s
T^b = 6132(40) gas PE[1-3,5]PI[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SO stretch	915(20)[c]	gas	PE,PI	1,5

$\tilde{A}\ ^2A'$ [a] C_s
T^b = 5665(40) gas PE[1-3,5]PI[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SO stretch	923(20)[c]	gas	PE,PI	1,5

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	SS stretch	480(20)	gas	PE,PI	1,4,5

[a] Tentative assignment.
[b] From vertical ionization potential. The first ionization potential is taken to be 10.58 eV.[4,5]
[c] An alternate assignment is given by Ref. 3.

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CF_2

$\tilde{B}$ [a]
$T_0 \cong 72740$ gas AB[10] $\tilde{B}-\tilde{X}$ 131–138 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	Bend	625	gas	AB	10

$\tilde{A}\ ^1B_1$ C_{2v} Structure: AB[10]
T_0 = 37226 gas EM[1]AB[2,3,5,10]LF[20] $\tilde{A}-\tilde{X}$ 220–380 nm
37219(2) Ne LF[17]
36878(2) Ar AB[4,6,16]EM[16]LF[17] $\tilde{A}-\tilde{X}$ 210–346 nm
37054(2) N_2 LF[17]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	496	gas	UV	1-3,5,10
			496(2)	Ne	LF	17
			496(2)	Ar	AB,LF	4,6,16,17
			496(2)	N_2	LF	17

τ_0 = 50(5) ns gas LF[20,21,28,30,33]EM[35,39]EF[37]
31 ns Ne LF[17]
27 ns Ar LF[17]
23 ns Kr LF[17]
A_0 = 4.577; B_0 = 0.334; C_0 = 0.311 AB[10]

$\tilde{a}\ ^3B_1$ C_{2v}
T_0 = 19828 gas CL[18,19,22,24,29]PE[34] $\tilde{a}-\tilde{X}$ 430–800 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	517	gas	CL	18,22, 24,29

$\tau \cong 1$ s gas CL[19]

$\tilde{X}\ ^1A_1$ C_{2v} Structure: MW[8]AB[9,10]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1225.08	gas	DL,IR	23,31,32
					PE	34,36
			1220	Ne	IR,LF	12,17
			1222vs	Ar	IR,LF	6,11,17
	2	Bend	667	gas	UV,PE	1,10,34
			668vw	Ar	IR,LF	6,11,17
b_2	3	Asym. stretch	1114.44	gas	IR,DL	7,13,27
						32,38
			1104	Ne	IR	12
			1102vs	Ar	IR	6,11

A_0 = 2.947; B_0 = 0.417; C_0 = 0.365 MW[8,15,26]AB[9,10]

[a] Tentative assignment. This band system was associated with the $\tilde{C}-\tilde{X}$ transition in Ref. 10. Subsequent studies[14,25] have dictated the reassignment to CF_3 of almost all of the bands between 136 and 160 nm which had tentatively been attributed[10] to CF_2.

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CFCl

$\tilde{A}\ ^1A''$ C_s Structure: LF[9,10]

T_0 = 25277.8 gas LF[6,7,9,10] $\tilde{A}-\tilde{X}$ 359–421 nm
24983 Ar AB[1]LF[2,3] $\tilde{A}-\tilde{X}$ 340–667 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CF stretch	1274T	gas	LF	7,9,10
	2	Bend	392	gas	LF	6,9,10
			392(1)	Ar	LF	3
	3	CCl stretch	722	gas	LF	9,10
			712(2)	Ar	LF	3

τ_0 = 620(30) ns gas LF[4,5,9]EM[8]
330(20) ns Ar LF[3]

A_{020} = 4.354; B_{020} = 0.185; C_{020} = 0.177 LF[9,10]

$\tilde{X}\ ^1A'$ C_s Structure: LF[9,10]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CF stretch	1156T	gas	LF	6,7,9,10
			1146vs	Ar	IR	1
	2	Bend	449	gas	LF	6,7,9,10
			442	Ar	LF	2,3
	3	CCl stretch	759	gas	LF	6,7,9,10
			742s	Ar	IR	1

A_0 = 2.349; B_0 = 0.214; C_0 = 0.196 LF[9,10]

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CFBr

$\tilde{A}\ ^1A''$ C_s

T_0 = 20906 gas LF[3,4] $\tilde{A}-\tilde{X}$ 420–471 nm
Ar LF[1] $\tilde{A}-\tilde{X}$ 442–535 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CF stretch	1140	gas	LF	4
	2	Bend	340	gas	LF	4
			240(40)	Ar	LF	1
	3	CBr stretch	645	gas	LF	4

τ = 1150(50) ns gas LF[3]

$\tilde{X}\ ^1A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CF stretch	1157vs	Ar	IR	2
	2	Bend	325T	gas	LF	3
			340(5)	Ar	LF	1
	3	CBr stretch	656s	Ar	IR	2

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CFI

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CF stretch	1133vs	Ar	IR	1
	3	CI stretch	573s	Ar	IR	1

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CCl_2

$\tilde{A}\ ^1B_1$ C_{2v} Structure: LF^{17}

T_0 = 17255.67(2) gas $CL^8LF^{7,9,10,15-18}EM^{11}$ $\tilde{A}$–$\tilde{X}$ 400–800 nm
17092 Ar $AB^{1,3}LF^{4-6}$ $\tilde{A}$–$\tilde{X}$ 440–827 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	634.3	gas	LF	10,15,17
			624	Ar	LF	6
	2	Bend	302.6	gas	LF	9,10,15 17
			304	Ar	AB,LF	1,3,6

τ = 3.81(30) μs gas LF^7;
τ_1 = 1.83(2) μs, τ_2 = 3.72(6) μs gas $EM^{11,13}$
τ = 3.6 μs Ar LF^6
A_0 = 3.640; B_0 = 0.106; C_0 = 0.103 LF^{17}

$\tilde{X}\ ^1A_1$ C_{2v} Structure: $MW^{14}LF^{17}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	730.0	gas	PE,LF	12,17
			721wm	Ar	IR,LF	1-3,5,6
	2	Bend	335.2	gas	PE,LF	12,17
			333	Ar	LF	4-6
b_2	3	Asym. stretch	748vs	Ar	IR	1-3

A_0 = 1.675; B_0 = 0.123; C_0 = 0.115 $MW^{14}LF^{16,17}$

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CClBr

$\tilde{A}$ C_s Structure: LF^5

T_0 = 16190 gas $LF^{5,6}$ $\tilde{A}$–$\tilde{X}$ 497–600 nm
16044 Ar $LF^{3,4}$ $\tilde{A}$–$\tilde{X}$ 540–776 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CCl stretch	684	Ar	LF	4
	2	Bend	246	gas	LF	5
			246	Ar	LF	4
	3	CBr stretch	532	gas	LF	5
			526	Ar	LF	4

τ = 5.6(6) μs Ar LF^4

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CCl stretch	744	Ar	IR	1,2
	2	Bend	262	gas	LF	6
			260	Ar	LF	3,4
	3	CBr stretch	618T	gas	LF	6
			611	Ar	IR	1,2

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CBr_2

$\tilde{A}\ ^1B_1$ C_{2v} Structure: LF[6]

T_0 = 15092.5(1.7) gas LF[5,6] $\tilde{A}-\tilde{X}$ 560–663 nm
14962 Ar LF[3,4] $\tilde{A}-\tilde{X}$ 600–857 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	474.8(1.2)	gas	LF	5,6
			468	Ar	LF	4
	2	Bend	185.5(4)	gas	LF	5,6
			186	Ar	LF	4

τ = 14.5(1.5) μs Ar LF[4]

$\tilde{X}\ ^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	598	gas	LF	6
			595w	Ar	IR	1,2
	2	Bend	196	Ar	LF	3,4
b_2	3	Asym. stretch	641s	Ar	IR	1,2

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SiF_2

$\tilde{b}\ ^3B_2$ [a] C_{2v}

T_0 = 62214 gas UV[11]MPI[15] $\tilde{b}-\tilde{X}$ 158–165 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	790T	gas	AB	11
	2	Bend	320T	gas	AB	11

$\tilde{A}\ ^1B_1$ C_{2v} Structure: AB[9]

T_0 = 44113.9 gas EM[1,2]AB[5,9]LF[14,16] $\tilde{A}-\tilde{X}$ 213–276 nm
≅ 43964 Ne AB[7] $\tilde{A}-\tilde{X}$ 216–225 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	250.1(3)	gas	AB,LF	5,9,16
			253T	Ne	AB	7

$\tau \leq$ 20 ns gas LF[16]
A_0 = 1.446; B_0 = 0.241; C_0 = 0.206 AB[9]

$\bar{a}\ ^3B_1$ C_{2v}

T_0 = 26310 gas EM[10] $\bar{a}-\tilde{X}$ 364–420 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	277	gas	EM	10

$\tilde{X}\ ^1A_1$ C_{2v} Structure: MW[3,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	855.01	gas	IR,LF	6,13,16
			851s	Ne	IR	8
			843s	Ar	IR	7,8
	2	Bend	345	gas	MW,UV	4,5
					LF	16
			343	Ar	IR	7
b_2	3	Asym. stretch	870.40	gas	IR	6,13
			864.6s	Ne	IR	8
			855vs	Ar	IR	7,8

A_0 = 1.021; B_0 = 0.294; C_0 = 0.228 MW[3,4]

[a] See Ref. 12.

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$SiCl_2$

$\tilde{A}\ ^1B_1$ C_{2v} Structure: LF[10]
T_0 = 30013.5(2) gas AB[4]EM[5-7]LF[8,10,13] $\tilde{A}$–$\tilde{X}$ 295–430 nm
In an argon matrix, unstructured absorption attributable to $SiCl_2$ has been observed[1] between 310 and 320 nm, with a maximum at approximately 315 nm.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	428.9	gas	LF	8,13
	2	Bend	149.8	gas	UV,LF	3,7,8,13

τ_{070} = 77(3) ns gas LF[8]
A_{060} = 0.909; B_{060} = 0.076; C_{060} = 0.069 LF[10]

$\tilde{a}\ ^3B_1$ C_{2v}
T_0 = 18943T gas EM[11,12] $\tilde{a}$–$\tilde{X}$ 500–650 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	159(2)	gas	EM	11,12

τ = 11(2) ms gas EM[12]

$\tilde{X}\ ^1A_1$ C_{2v} Structure: ED[4]MW[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	521.6	gas	LF	13
			518.7	Ne	IR	2
			512.5s	Ar	IR	1,2
	2	Bend	200.6	gas	EM,LF	7,8,11-13
			202.2	Ar	IR	2
b_2	3	Asym. stretch	509.4	Ne	IR	2
			502vs	Ar	IR	1,2

A_0 = 0.493; B_0 = 0.094; C_0 = 0.079 MW[9]LF[10]

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$SiBr_2$

$\tilde{A}\ ^1B_1$ C_{2v}
An unstructured absorption between 340 and 400 nm, with a maximum near 362 nm (27600) has been attributed[2] to the $\tilde{A}\ ^1B_1$–$\tilde{X}\ ^1A_1$ transition of $SiBr_2$, by analogy with the electronic spectra of related compounds.

$\tilde{X}\ ^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	402.6s	Ar	IR	1
b_2	3	Asym. stretch	399.5vs	Ar	IR	1

References

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GeF_2

The high-temperature vapor of GeF_2 shows unstructured absorption between 136 and 156 nm, with a maximum near 146.3 nm.[5]

$\tilde{A}\ ^1B_1$ C_{2v}
T_0 = 43843(10) gas AB[1] $\tilde{A}$–$\tilde{X}$ 222–243 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	164(3)	gas	AB	1

$\tilde{a}\ ^3B_1$ C_{2v}
T_0 = 30320(2) gas EM[6,8] $\tilde{a}$–$\tilde{X}$ 325–370 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	191	gas	EM	6,8

$\tilde{X}\ ^1A_1$ C_{2v} Structure: IR[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	663	gas	IR	2
			655	Ne	IR	2
			648	Ar	IR,Ra	2,7
			653	N_2	Ra	7
	2	Bend	263(2)	gas	AB,EM	1,6,8
b_2	3	Asym. stretch	692	gas	IR	2
			685	Ne	IR	2
			676	Ar	IR	2

A_0 = 0.513; B_0 = 0.262; C_0 = 0.173 MW[3,4]

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$GeCl_2$

$\tilde{A}\ ^1B_1$ C_{2v}
T_0 = 30622(2) gas AB[2]LF[11] $\tilde{A}$–$\tilde{X}$ 300–330 nm
Structured absorption[2] is superposed on a continuum with maximum near 32280, presumably due to predissociation of $GeCl_2$ into GeCl + Cl. In the LF excitation spectrum,[11] there is a marked increase in the line density beyond approximately 31630.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	354	gas	LF	11
	2	Bend	104	gas	AB,LF	2,11

τ = 89.7(6.8) ns gas EM[10]

$\tilde{a}\ ^3B_1$ C_{2v}
T_0 = 22315(2) gas CL[1]LF[11] $\tilde{a}$–$\tilde{X}$ 400–490 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	393	gas	LF	11
	2	Bend	118	gas	CL,LF	1,11

τ = 17.4(6) μs gas EM[10]

$\tilde{X}\ ^1A_1$ C_{2v} Structure: ED[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	399	gas	CL,Ra	1,4
			398.6	Ar	IR	3,5,7,9
			390	N_2	Ra	6
	2	Bend	160(4)	gas	CL,AB	1,2
					Ra	4
			163	N_2	Ra	6
b_2	3	Asym. stretch	373.5	Ar	IR	3,5,7,9
			362	N_2	Ra	6

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NO_2^-

Threshold for electron detachment from ground-state NO_2^- = 18340(40) gas PD[3]PE[4]

$\tilde{X}$ C_{2v} Structure: PE[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NO stretch	1284(30)	gas	PE	4
			1268.1[a]	Ne	IR	6
	2	Bend	776(30)	gas	PE	4
b_2	3	NO stretch	1241.5	Ne	IR	5,6
			1244	Ar	IR	1,2

[a] $(\nu_1 + \nu_3) - \nu_3$.

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[1]D. E. Milligan, M. E. Jacox, and W. A. Guillory, J. Chem. Phys. **52**, 3864 (1970).
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NS_2^-

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	NS_2 a-stretch	893.9	Ar	IR	1

References

[1]P. Hassanzadeh and L. Andrews, J. Am. Chem. Soc. **114**, 83 (1992).

INO

$\tilde{B}$

In the gas phase, a prominent, unstructured absorption between 223 and 310 nm, with maximum at 42000 (238 nm), has been attributed[2,5,6] to INO.

$\tilde{A}$

A relatively weak, unstructured gas–phase absorption between 390 and 470 nm, with maximum near 23800 (420 nm), has also been attributed[1,2,5,6] to INO.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO stretch	1785	gas	IR	7
			1809	Ar	IR	4
			1806	Kr	IR	3
	2	Bend	216	Ar	IR	4
	3	NI stretch	470	Ar	IR	4
			468	Kr	IR	3

References

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NF_2^+

$\tilde{A}$ $^1B_1$? C_{2v}
$T_0 \cong 38400^a$ gas PE[1,2]

$\tilde{a}$ $^3B_1$ C_{2v}
T_0 = 19610(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			520(20)	gas	PE	1,2

$\tilde{X}$ $^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NF stretch	1250(20)	gas	PE	1,2

[a] From vertical ionization potential.

References

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PO_2^-

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
b_2	3	PO a-stretch	1198.8	Ar	IR	1

References

[1]Z. Mielke, M. McCluskey, and L. Andrews, Chem. Phys. Lett. **165**, 146 (1990).

FPO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	1	PO stretch	1292.2	Ar	IR	1
	2	Bend	416.0	Ar	IR	1
	3	PF stretch	811.4	Ar	IR	1

References

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ClPO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	1	PO stretch	1258vs	Ar	IR	1-4
	2	Bend	308wm	Ar	IR	1
	3	PCl stretch	489vs	Ar	IR	1-3

References

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BrPO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	Refs.
a'	1	PO stretch	1253.0	Ar	IR	1,2
	2	Bend	253.7	Ar	IR	1
	3	PBr stretch	407.1	Ar	IR	1,2

References

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FPS

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	PF stretch	791.4	Ar	IR	1
	2	Bend	313.6	Ar	IR	1
	3	PS stretch	720.2	Ar	IR	1

References

[1]H. Schnöckel and S. Schunck, Z. Anorg. Allg. Chem. **552**, 163 (1987).

ClPS

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	PS stretch	716.1	Ar	IR,Ra	1
	2	Bend	229	Ar	Ra	1
	3	PCl stretch	462.4	Ar	IR	1

References

[1]H. Schnöckel and M. Lakenbrink, Z. Anorg. Allg. Chem. **507**, 70 (1983).

BrPS

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	PS stretch	712	Ar	IR	1
	2	Bend	185H	Ar	IR	1
	3	PBr stretch	372	Ar	IR	1

References

[1]H. Schnöckel and S. Schunck, Z. Anorg. Allg. Chem. **552**, 155 (1987).

PS_2^-

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	636.7	Ar	IR	1

References

[1]Z. Mielke, G. D. Brabson, and L. Andrews, J. Phys. Chem. **95**, 75 (1991).

ClAsO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	AsO stretch	984.4	Ar	IR	1
	3	AsCl stretch	378.7	Ar	IR	1

References

[1]H. Schnöckel, M. Lakenbrink, and Lin Zhengyan, J. Mol. Struct. **102**, 243 (1983).

PF_2^+

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PF stretch	1000(30)	gas	PE	1

References

[1]J. M. Dyke, N. Jonathan, and A. Morris, Int. Rev. Phys. Chem. **2**, 3 (1982).

FON

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	735vs	Ar	IR	1-3
			725	N_2	IR	1,2
	3	OF stretch	492vs	Ar	IR	1-3
			480	N_2	IR	1,2

References

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NSBr

$\tilde{X}$ $^1A_1'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	N=S stretch	1311	gas	IR	2
			1312.9m	Ar	IR	1
	2	Bend	226.2wm	Ar	IR	1
	3	SBr stretch	346.1s	Ar	IR	1

References

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NSI

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NS stretch	1295T	gas	IR	1

References

[1]A. W. Allaf, G. Y. Matti, R. J. Suffolk, and J. D. Watts, Chem. Phys. Lett. **155**, 32 (1989).

ClCS

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CS stretch	1189.3s	Ar	IR	1
	3	CCl stretch	632.1m	Ar	IR	1

References

[1]G. Schallmoser, B. E. Wurfel, A. Thoma, N. Caspary, and V. E. Bondybey, Chem. Phys. Lett. **201**, 528 (1993).

SSO

An absorption band system between 190 and 230 nm has been attributed[7] to SSO. However, an alternate assignment to the $\tilde{C}-\tilde{X}$ band system of SO_2 has been proposed.[15]

$\tilde{A}\ ^1A'$ C_s Structure: AB[11]
T_0 = 29689.6 gas AB[1,7,11]LF[12,13,16] $\tilde{A}-\tilde{X}$ 250–395 nm
29285(20) Xe AB[4] $\tilde{A}-\tilde{X}$ 280–342 nm
Predissociation limit between 31172 and 31307. AB[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SO stretch	1032	gas	AB,LF	11,13,16
	2	Bend	253	gas	AB,LF	11,13,16
	3	SS stretch	407	gas	AB,LF	7,11,13 16
			415(20)	Xe	AB	4

A_{020} = 1.016; B_{020} = 0.148; C_{020} = 0.129 AB[11]
τ = 10 ns gas LF[13]

$\tilde{a}\ ^3A'$ C_s
T_0 = 13943 gas AB[10,15]LF[13] $\tilde{a}-\tilde{X}$ 430–670 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SO stretch	1089	gas	AB	10,15
	2	Bend	332	gas	AB	10,15
	3	SS stretch	505	gas	AB	10,15

$\tilde{X}\ ^1A'$ C_s Structure: MW[2,6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SO stretch	1166.45	gas	IR,DL	1,3,14
			1156.2	Ar	IR,Ra	8,9
	2	Bend	380	gas	LF	16
			382	Ar	IR,Ra	8,9
	3	SS stretch	679.1	gas	IR,LF	1,3,13
			672.2	Ar	IR,Ra	8,9

A_0 = 1.398; B_0 = 0.169; C_0 = 0.150 MW[2,5,6]DL[14]

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S_3

T_0 = 23465(15) gas AB[1,2,5,8] 350–510 nm
23210 Ar AB[4,7,9] 355–435 nm
Kr AB[1,2] 310–420 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	420	gas	AB	2
			450T	Ar	AB	4,9
			420	Kr	AB	2
	2	Bend	340T	Ar	AB	9

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	590	gas	AB	2
			575	gas	Ra	5,6
			583	Ar	Ra,IR	3,7
	2	Bend	250	gas	Ra	5,6
b_2	3	Asym. stretch	656	gas	Ra	5
			680.0	Ar	IR	7,9
			676.2			
			674.5			

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Se_3

$\tilde{X}$ C_{2v}
T_0 = 17005 Ar LF^1AB^2 $\tilde{A}$–$\tilde{X}$ 480–842 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			290	Ar	AB	2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	311	Ar	Ra	1
			311	N_2	Ra	1
b_2	3	Asym. stretch	350	Ar	IR	2

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[1]H. Schnöckel, H.-J. Göcke, and R. Elsper, Z. Anorg. Allg. Chem. **494**, 78 (1982).
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Te_3

$\tilde{A}$ C_{2v}
Ar AB^2 $\tilde{A}$–$\tilde{X}$ 650–705 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	195(10)	Ar	AB	2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	203	N_2	Ra	1
b_2	3	Asym. stretch	232T	Ar	IR	2

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$OClO^+$

$\tilde{D}$ $^1A_2$ C_{2v}
T_0 = 62200(80) gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			485(40)	gas	PE	3

$\tilde{d}$ $^3A_2$ C_{2v}
T_0 = 59460(80) gas PE[1–3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ClO s-stretch	605(40)	gas	PE	3

$\tilde{B}$ $^1B_2$ C_{2v}
T_0 = 39530(80) gas PE[1–3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ClO s-stretch	765(40)	gas	PE	3

$\tilde{C}$ $^1A_2$ C_{2v}
T_0 = 25410(80) gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ClO s-stretch	725(40)	gas	PE	3

$\tilde{c}\ ^3A_2$ C_{2v}
T_0 = 24040(80) gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ClO s-stretch	810(40)	gas	PE	3

$\tilde{b}\ ^3B_2$ C_{2v}
T_0 = 20330(80) gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	485(40)	gas	PE	3

$\tilde{A}\ ^1B_1$ C_{2v}
T_0 = 16900(80) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ClO s-stretch	765(40)	gas	PE	3

$\tilde{a}\ ^3B_1$ C_{2v}
T_0 = 16540(80) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ClO s-stretch	765(40)	gas	PE	3

$\tilde{X}\ ^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ClO s-stretch	1015(40)	gas	PE	2,3
	2	Bend	520(40)	gas	PE	2,3

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CF_2^-

Threshold for electron detachment from ground-state CF_2^- = 1330(80) gas PE[1,2]

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF stretch	860(30)	gas	PE	1

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CCl_2^-

Threshold for electron detachment from ground-state CCl_2^- = 12840(80) gas PE[1,2]

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NF_2

$\tilde{A}\ ^2A_1$ C_{2v}
gas AB[1,4,5] $\tilde{A}$–$\tilde{X}$ 237–278 nm
Ar AB[9] $\tilde{A}$–$\tilde{X}$ 247–265 nm
In an argon matrix,[6,9] evidence has been obtained for predissociation into NF + F.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	390[a]	gas	AB	4,5
			408[a]	Ar	AB	9

$\tilde{X}\ ^2B_1$ C_{2v} Structure: IR[2]MW[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1074.99	gas	IR,DL LMR	2,10, 11,12
			1069m	Ar	IR	7,9
			1070	N_2	IR	2,3
	2	Bend	573w	N_2	IR	3
b_2	3	Asym. stretch	942.48	gas	IR,DL LMR	2,10, 13,14
			932vs	Ar	IR	7,9
			931	N_2	IR	2,3

A_0 = 2.351; B_0 = 0.396; C_0 = 0.338 MW[8]DL[12]

[a] Average value.

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NFCl

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NF stretch	917[a]	Ar	IR	1
	3	NCl stretch	720[a]	Ar	IR	1

[a] Similar values, not explicitly given, were obtained in krypton and xenon matrix experiments.

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NCl_2

$\tilde{A}$

gas AB[1-3] $\tilde{A}$–$\tilde{X}$ 275–314 nm

Photodissociation threshold near 310 nm.[1]
In an argon matrix, diffuse banded absorption was observed[6] in this same spectral region, with a maximum at 298 nm (33600).

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	557[a]	gas	AB	1
			560	Ar	AB	6

$\tilde{X}$ C_{2v} Structure: IR[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	679	Ar	IR	4-6

[a] Average value.

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NBr_2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	604	Ar	IR	1

References

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PF_2

$\tilde{a}\ ^4A_2$ C_{2v}

T_0 = 23998(6) gas EM[3] $\tilde{a}$–$\tilde{X}$ 400–520 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	505(2)	gas	EM	3
	2	Bend	219	gas	EM	3

$\tau \geq 1.9$ ms gas EM[3]

$\tilde{X}\ ^2B_1$ C_{2v} Structure: MW[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	841(4)	gas	EM	3
			852.1ms	Ar	IR	1
	2	Bend	366	gas	MW,EM	2,3
b_2	3	Asym. stretch	848(24)	gas	MW	2
			831.4s	Ar	IR	1

A_0 = 0.933; B_0 = 0.310; C_0 = 0.232 MW[2]

References

[1]J. K. Burdett, L. Hodges, V. Dunning, and J. H. Current, J. Phys. Chem. **74**, 4053 (1970).
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PCl_2

$\tilde{A}\ ^2A_1$ C_{2v}

In the gas phase, unstructured emission at wavelengths longer than 370 nm, with a maximum at approximately 460 nm, has been attributed[2] to PCl_2.
τ = 29(6) μs gas EM[2]

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	452	Ar	IR	1
b_2	3	Asym. stretch	525	Ar	IR	1

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PBr_2

$\tilde{A}\ ^2A_1$ C_{2v}

In the gas phase, unstructured emission at wavelengths longer than 510 nm, with a maximum at 527 nm, has been attributed[2] to PBr_2.
τ = 21(9) μs gas EM[2]

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	369	Ar	IR	1
b_2	3	Asym. stretch	410	Ar	IR	1

References

[1]L. Andrews and D. L. Frederick, J. Phys. Chem. **73**, 2774 (1969).
[2]M. J. Bramwell, S. E. Jaeger, and J. C. Whitehead, Chem. Phys. Lett. **196**, 547 (1992).

AsF_2

When gas-phase AsF_3 is subjected to 124 nm radiation, an emission band system, tentatively assigned to AsF_2, is observed between 330 and 610 nm, with a maximum near 450 nm.[1] The radiative lifetime of the species which contributes this band system is 25.5(1.8) μs.[2]

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O_3^-

$\tilde{C}\ ^2A_1$ C_{2v}
T_0 = 21420(40) gas PF[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	760(20)	gas	PF	8
	2	Bend	190(20)	gas	PF	8

Threshold for electron detachment from ground-state O_3^- = 16970(20) gas PE[7]PD[9]

$\tilde{A}\ ^2A_2$ C_{2v}
T_0 = 16508(16) gas PF[6,8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	815(10)	gas	PF	6,8
	2	Bend	275(10)	gas	PF	6,8

$\tilde{X}\ ^2B_1$ C_{2v} Structure: PD[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	975(10)	gas	PD,PF	6-8
			1016 Cs	Ar	Ra	3,5
			1011 Na	Ar	Ra	3,5
	2	Bend	590(10)	gas	PD,PF	7,8
			600w Cs	Ar	IR	4
b_2	3	Asym. stretch	796.3	Ne	IR	10
			789s Cs	Ar	IR	2,4
			802s			
			802s Na	Ar	IR	1,2,4

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FOO

An absorption maximum of gas-phase FOO has been reported[4] at 205 nm.

Unstructured absorption of FOO with a maximum near 420 nm has been observed in liquid CF_4.[2] In liquid O_2 and Ar:O_2 mixtures,[5] the corresponding absorption maximum lies near 445 nm. In all of these systems, photodissociation of FOO occurs in this spectral region. In an argon matrix, the onset of photodissociation has been observed[6] near 490 nm.

$\tilde{X}$ C_s Structure: DL[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OO stretch	1486.93	gas	IR	8,9
			1490vs	Ar	IR	1,6
			1500vs	N_2	IR	3
	2	Bend	376	N_2	IR	3
	3	OF stretch	579.32	gas	DL,IR	7,9
			584s	Ar	IR	1,6
			586s	N_2	IR	3

A_0 = 2.616; B_0 = 0.334; C_0 = 0.295 DL[7]IR[9]MW[10]LMR[11]

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ClOO

An unstructured gas-phase absorption[3,4,6,7] between 225 and 270 nm, with a maximum near 246 nm, has been assigned to ClOO.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OO stretch	1443[a]	gas	IR	4
			1441vs[b]	Ar	IR	2
			1438	N_2	IR	1
			1428			
	2	Bend	373m	Ar	IR	2
	3	ClO stretch	407s[b]	Ar	IR	2

[a] Absorption maximum; spectral slit width 13 cm^{-1}.
[b] Peaks at 1415 and 435 cm^{-1}, attributed in Ref. 2 to a structural isomer of ClOO, were attributed in Ref. 5 to the vibrationally unrelaxed molecule.

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BrOO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	1487	Ar	IR	1

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SO_2^-

Threshold for electron detachment from ground-state SO_2^- = 8930(65) gas PE[2,3]

$\tilde{X}$ $^2B_1$ C_{2v} Structure: PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	944(48)	gas	PE	3
			990.8	Ne	IR	4
			985m Cs	Ar	IR	1
			990 Na	Ar	IR	1
	2	Bend	435(100)	gas	PE	3
			495wm Cs	Ar	IR	1
			495 Na	Ar	IR	1
b_2	3	Asym. stretch	1086.2	Ne	IR	4
			1042s Cs	Ar	IR	1
			1041 Na	Ar	IR	1

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SSO^-

Threshold for electron detachment from ground-state SSO^- = 15140(65) gas PE[1]

$\tilde{X}$ $^2A''$ C_s Structure: PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	SS stretch	620(150)	gas	PE	1

References

[1]M. R. Nimlos and G. B. Ellison, J. Phys. Chem. **90**, 2574 (1986).

S_3^-

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			594.2T	Ar	IR	1

References

[1]G. D. Brabson, Z. Mielke, and L. Andrews, J. Phys. Chem. **95**, 79 (1991).

FSO

$\tilde{X}$ C_s Structure: MW[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	SO stretch	1215(33)	gas	MW	1
	2	Bend	396	gas	MW	1
	3	SF stretch	763(12)	gas	MW	1

References

[1]Y. Endo, S. Saito, and E. Hirota, J. Chem. Phys. **74**, 1568 (1981).

SSCl

T_0 = 21650 gas[a] AB[1,2,5] 378–481 nm
≤ 21925 Ar AB[3] 389–456 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	Stretch	480	gas	AB	5
			491(20)	Ar	AB	3
	3	Stretch	407	gas	AB	5

$\tilde{X}$ $^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SS stretch	659	gas	AB	5
			665	Ar	IR	4
	2	Bend	336	gas	AB	5
	3	SCl stretch	404	Ar	IR	4

[a] Diffuse band system. Ref. 3 also reported two very weak bands approximately 600 cm^{-1} below the principal progression which they attributed to ground-state vibrational excitation.

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SSBr

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SS stretch	558	Ar	IR	1
	3	SBr stretch	346	Ar	IR	1

References

[1]G. Vahl and M. Feuerhahn, J. Chem. Res., Synop., 237 (1979).

OF_2^+

$\tilde{E}$ C_{2v}
T^a = 51560(400) gas PE[1,2]

$\tilde{D}$ C_{2v}
T_0 = 38650 gas PE[1,2]

$\tilde{C}$ $^2A_2$ [b] C_{2v}
T^a = 26870(240) gas PE[1,2]

$\tilde{A},\tilde{B}$ $^2B_2, ^2A_1$ [b] C_{2v}
T_0 = 21220(240) gas PE[1,2]

$\tilde{X}$ $^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	OF s-stretch	1020(40)	gas	PE	1,2

[a] From vertical ionization potential. The first ionization potential is taken as 13.11(1) eV, from the photoionization study of Ref. 3.
[b] For assignment, see Ref. 4.

References

[1]A. B. Cornford, D. C. Frost, F. G. Herring, and C. A. McDowell, J. Chem. Phys. **55**, 2820 (1971).
[2]C. R. Brundle, M. B. Robin, N. A. Kuebler, and H. Basch, J. Am. Chem. Soc. **94**, 1451 (1972).
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Cl_2O^+

$\tilde{F}$ $^2B_1$ C_{2v}
T^b = 54380(320) gas PE[1]

$\tilde{E}$ $^2A_1$ C_{2v}
T^b = 46070(320) gas PE[1]

$\tilde{D}$ $^2B_2$ C_{2v}
T^b = 40020(320) gas PE[1]

$\tilde{C}$ $^2A_2$ [a] C_{2v}
T^b = 14930(320) gas PE[1]

$\tilde{B}$ $^2A_1$ [a] C_{2v}
T^b = 13800(320) gas PE[1]

$\tilde{A}$ $^2B_2$ [a] C_{2v}
T^b = 11540(320) gas PE[1]

$\tilde{X}$ $^2B_1$ [a] C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ClO s-stretch	670(40)	gas	PE	1
	2	Bend	300(40)	gas	PE	1

[a] For assignment, see Ref. 2.
[b] From vertical ionization potential.

References

[1]A. B. Cornford, D. C. Frost, F. G. Herring, and C. A. McDowell, J. Chem. Phys. **55**, 2820 (1971).
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SF_2^+

$\tilde{E}\ ^2A_1$ C_{2v}
T_0 = 74400(1000) gas PE[1]

$\tilde{D}\ ^2B_1$ C_{2v}
T_0 = 66300(1000) gas PE[1]

$\tilde{B},\tilde{C}\ ^2B_2,^2A_2$ C_{2v}
T_0 = 49400(1000) gas PE[1]

$\tilde{A}\ ^2A_1$ C_{2v}
T_0 = 42900(1000) gas PE[1]

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SF stretch	935(40)	gas	PE	1

References

[1]D. M. de Leeuw, R. Mooyman, and C. A. de Lange, Chem. Phys. **34**, 287 (1978).

SCl_2^+

$\tilde{F}\ ^2A_1$ C_{2v}
T^a = 51230(1100) gas PE[1,2]

$\tilde{E}\ ^2B_2$ C_{2v}
T^a = 42760(400) gas PE[1,2]

$\tilde{D}\ ^2B_1$ C_{2v}
T^a = 37110(400) gas PE[1,2]

$\tilde{B},\tilde{C}\ ^2A_1,^2A_2$ C_{2v}
T^a = 24290(400) gas PE[1,2]

$\tilde{A}\ ^2B_2$ C_{2v}
T^a = 22510(400) gas PE[1,2]

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SCl s-stretch	530(40)	gas	PE	1,2

[a] From vertical ionization potential. The first ionization potential was taken to equal 9.45(3) eV, from the appearance potential measurements of Ref. 3.

References

[1]B. Solouki, P. Rosmus, and H. Bock, Chem. Phys. Lett. **26**, 20 (1974).
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SBr_2^+

$\tilde{B}\ ^2A_2$ C_{2v}
$T_0 \cong$ 16000 gas PE[1]

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SBr stretch	400(50)	gas	PE	1

References

[1]D. M. de Leeuw, R. Mooyman, and C. A. de Lange, Chem. Phys. Lett. **61**, 191 (1979).

SeF_2^+

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	780(50)	gas	PE	1

References

[1]D. M. de Leeuw, R. Mooyman, and C. A. de Lange, Chem. Phys. **38**, 21 (1979).

$SeCl_2^+$

$\tilde{F}\ ^2B_2$ C_{2v}
T_0 = 44620(160) gas PE[1]

$\tilde{E}\ ^2A_1$ C_{2v}
T_0 = 37840(160) gas PE[1]

$\tilde{D}\ ^2B_1$ C_{2v}
T_0 = 31390(160) gas PE[1]

$\tilde{B},\tilde{C}\ ^2A_2,^2A_1$ C_{2v}
T_0 = 22430(160) gas PE[1]

$\tilde{A}\ ^2B_2$ C_{2v}
T_0 = 20170(160) gas PE[1]

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	450(50)	gas	PE	1

References

[1]D. M. de Leeuw, R. Mooyman, and C. A. de Lange, Chem. Phys. **38**, 21 (1979).

$SeBr_2^+$

$\tilde{F}\ ^2B_2$ C_{2v}
T_0 = 41470(160) gas PE[1]

$\tilde{E}\ ^2A_1$ C_{2v}
T_0 = 33890(160) gas PE[1]

$\tilde{D}\ ^2B_1$ C_{2v}
T_0 = 27350(160) gas PE[1]

$\tilde{C}\ ^2A_2$ C_{2v}
T_0 = 18800(160) gas PE[1]

$\tilde{B}\ ^2A_1$ C_{2v}
T_0 = 18070(160) gas PE[1]

$\tilde{A}\ ^2B_2$ C_{2v}
T_0 = 14850(160) gas PE[1]

$\tilde{X}\ ^2B_1$ C_{2v}

References

[1]D. M. de Leeuw, R. Mooyman, and C. A. de Lange, Chem. Phys. **38**, 21 (1979).

OClO

$\tilde{E}$
T_0 = 63774 gas AB[12,19] $\tilde{E}$–$\tilde{X}$ 148–157 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	1000T	gas	AB	12
	2	Bend	508	gas	AB	12,19

$\tilde{D}$
T_0 = 61430(20) gas AB[12,19,42] $\tilde{D}$–$\tilde{X}$ 155–163 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	1051(20)	gas	AB	12,19,42
	2	Bend	521(20)	gas	AB	12,19,42

$\tilde{C}\ ^2A_1$ C_{2v}
T_0 = 54689(20) gas AB[12,19,42] $\tilde{C}$–$\tilde{X}$ 176–183 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1020(20)	gas	AB	12,19,42

$^2A_1, ^2B_2$ C_{2v}
These two as yet undetected states are expected to lie close to the $\tilde{A}$ state and to interact strongly with it. One or both of them may contribute to the much-studied predissociation of the $\tilde{A}$ state.[21,24,29,35,40]

$\tilde{A}\ ^2A_2$ C_{2v}[a] Structure: AB[25]
T_0 = 21017.2 gas AB[1,2,5,14,25,31,32,34,35]LF[15,16]MPI[33,36]PF[41]
$\tilde{A}$–$\tilde{X}$ 260–780 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	711.5	gas	AB	5,14,34
	2	Bend	292.5	gas	AB	5,14,34
b_2	3	Asym. stretch	441.2	gas	AB	25,34

τ_1[b] = 56(20) ps gas AB[21,24]LF[29]
τ_2[c] = 336(27) ps gas LF[29]
A_0 = 1.057; B_0 = 0.311; C_0 = 0.240 AB[25]

$\tilde{X}\ ^2B_1$ C_{2v} Structure: MW[6,30]IR[26]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	945.59s	gas	IR,AB	3-5,14-16
					LF,LMR	20,23,26
					DL,LS	28,37,39
			947.6m	Ar	IR,Ra	13,17,18
			942	Kr	Ra	18
			940(2)	Xe	Ra	18
			950(2)	N_2	Ra	18
	2	Bend	447.70s	gas	IR,AB	4,5,14-16
					LF	22,25,38
						39
			451s	Ar	IR,LF	13,17,18
			448s			
			447	Kr	LF	18
b_2	3	Asym. stretch	1110.11vs	gas	IR	3,14,26
						38,39
			1106.0vs	Ar	IR	13,17
			1101.0vs			

A_0 = 1.737; B_0 = 0.332; C_0 = 0.278 MW[6–10,27]IR[37,38]

[a] Double minimum in potential for antisymmetric stretch,[11,25] with barrier height of 1153.[34]
[b] For $F_1(J = N + \frac{1}{2})$ spin states.
[c] For $F_2(J = N - \frac{1}{2})$ spin states.

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OBrO

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	852	Ar	IR	1

References

[1]D. E. Tevault, N. Walker, R. R. Smardzewski, and W. B. Fox, J. Phys. Chem. **82**, 2733 (1978).

OIO

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	765(25)	gas	PE	1
	2	Bend	192(35)	gas	PE	1

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[1]M. K. Gilles, M. L. Polak, and W. C. Lineberger, J. Chem. Phys. **96**, 8012 (1992).

BrOBr

In a nitrogen matrix, a strong absorption maximum at approximately 47000, a weaker shoulder near 31200, and a much weaker shoulder near 22100 have been attributed[3] to electronic transitions of BrOBr.

$\tilde{X}$ C_{2v} Structure: EXAFS[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	526.1s	Ar	IR	1,2
			528	N_2	IR	3
b_2	3	Asym. stretch	623.4w	Ar	IR	2
			626	N_2	IR	3

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SF_2

$\tilde{E}$ 4p Rydberg state C_{2v}
T_0 = 62015(30) gas MPI[10]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	931(59)	gas	MPI	10
	2	Bend	383(42)	gas	MPI	10

$\tilde{C}$
gas MPI[10] $\tilde{C}$–$\tilde{X}$ 165–175 nm

$\tilde{B}$ $^1B_1$ (4s) C_{2v}
T_0 = 54433(30) gas MPI[10]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	991(12)	gas	MPI	10
	2	Bend	361(24)	gas	MPI	10

$\tilde{A}$
T_0 = 18100(1000) gas CL[7,8,11] $\tilde{A}$–$\tilde{X}$ 550–850 nm
Chemiluminescence in the reaction of F_2 with CS_2, originally assigned[7,8] to FCS, has been reassigned[9] to SF_2.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	Bend	243(6)	gas	CL	11

$\tilde{X}$ C_{2v} Structure: MW[1,2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	838.53	gas	IR,CL	5,7-9,11
			834	Ne	IR	3
			832vs	Ar	IR	3,12
			825	N_2	IR	3
	2	Bend	355(2)	gas	MW,CL	2,7-9,11
			358	Ne	IR	3
			358m	Ar	IR	3
			358	N_2	IR	3
b_2	3	Asym. stretch	813.04	gas	IR,CL	5,11
			807.5	Ne	IR	3
			804vs	Ar	IR	3,12
			795	N_2	IR	6

$A_0 = 0.898$; $B_0 = 0.307$; $C_0 = 0.228$ MW[1,2]

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FSCl

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SF stretch	781vs	Ne	IR	1
			778vs	Ar	IR	1
	2	Bend	277vw	Ne	IR	1
			274vw	Ar	IR	1
	3	SCl stretch	552s[a]	Ne	IR	1
			543s[a]	Ar	IR	1

[a] In Fermi resonance with $2\nu_2$.

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SBr_2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	405	Ar	IR	1
b_2	3	Asym. stretch	418	Ar	IR	1

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SI_2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	368	Ar	IR	1
b_2	3	Asym. stretch	376	Ar	IR	1

References

[1]M. Feuerhahn and G. Vahl, Inorg. Nucl. Chem. Lett. **16**, 5 (1980).

$OClO^-$

Threshold for electron detachment from ground-state $OClO^-$ = 17270(65) gas PE[2]

$\tilde{X}\ ^1A_1$ C_{2v} Structure: PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	774(25)	gas	PE	2
			790 Cs	Ar	IR	1
	2	Bend	418 Cs	Ar	IR	1
b_2	3	Asym. stretch	823 Cs	Ar	IR	1

References

[1]D. E. Tevault, F. K. Chi, and L. Andrews, J. Mol. Spectrosc. **51**, 450 (1974).
[2]M. K. Gilles, M. L. Polak, and W. C. Lineberger, J. Chem. Phys. **96**, 8012 (1992).

OIO^-

Threshold for electron detachment from ground-state OIO^- ≈ 20790(65) gas PE[1]

$\tilde{X}\ ^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	675(25)	gas	PE	1

References

[1]M. K. Gilles, M. L. Polak, and W. C. Lineberger, J. Chem. Phys. **96**, 8012 (1992).

FClO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ClO stretch	1038s	Ar	IR	1
	2	Bend	315m	Ar	IR	1
	3	FCl stretch	593vs	Ar	IR	1

References

[1]L. Andrews, F. K. Chi, and A. Arkell, J. Am. Chem. Soc. **96**, 1997 (1974).

ClClO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ClO stretch	962	Ar	IR,Ra	3
			963	N_2	IR	1,2
	2	Bend	239	Ar	IR,Ra	3
	3	ClCl stretch	375	Ar	IR,Ra	3
			377	N_2	IR	1,2

References

[1]M. M. Rochkind and G. C. Pimentel, J. Chem. Phys. **46**, 4481 (1967).
[2]W. G. Alcock and G. C. Pimentel, J. Chem. Phys. **48**, 2373 (1968).
[3]F. K. Chi and L. Andrews, J. Phys. Chem. **77**, 3062 (1973).

BrBrO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	BrO stretch	804	Ar	IR	1
	3	BrBr stretch	236	Ar	IR	1

References

[1]D. E. Tevault, N. Walker, R. R. Smardzewski, and W. B. Fox, J. Phys. Chem. **82**, 2733 (1978).

OICl

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	IO stretch	779.1	Ar	IR	1
			772.2			
			778.2	Kr	IR	1
			775.1			
			778.2	N_2	IR	1
	3	ICl stretch	325.6	Ar	IR	1
			320.2			
			317.4	Kr	IR	1
			322.6	N_2	IR	1

References

[1]M. Hawkins, L. Andrews, A. J. Downs, and D. J. Drury, J. Am. Chem. Soc. **106**, 3076 (1984).

ClF_2

$\tilde{X}$ C_{2v} Structure: MO^3

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	500T	Ar	Ra	2
			536wT	N_2	IR	1
			500T	N_2	Ra	2
	2	Bend	242wT	N_2	IR	1
b_2	3	Asym. stretch	574s	Ar	IR	1,2
			578s	N_2	IR	1,2

References

[1]G. Mamantov, E. J. Vasini, M. C. Moulton, D. G. Vickroy, and T. Maekawa, J. Chem. Phys. **54**, 3419 (1971).
[2]E. S. Prochaska and L. Andrews, Inorg. Chem. **16**, 339 (1977).
[3]J. M. Galbraith, G. Vacek, and H. F. Schaefer III, J. Chem. Phys. **98**, 8051 (1993).

ClClF

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ClF stretch	559s	Ar	IR	1
	2	Bend	270w	Ar	IR	1
	3	ClCl stretch	464wm	Ar	IR	1

References

[1]E. S. Prochaska, L. Andrews, N. R. Smyrl, and G. Mamantov, Inorg. Chem. **17**, 970 (1978).

BrF_2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	569	Ar	IR	1

References

[1]E. S. Prochaska, L. Andrews, N. R. Smyrl, and G. Mamantov, Inorg. Chem. **17**, 970 (1978).

BrBrF

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	BrF stretch	507T	Ar	IR	1

References

[1]E. S. Prochaska, L. Andrews, N. R. Smyrl, and G. Mamantov, Inorg. Chem. **17**, 970 (1978).

IIF

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	IF stretch	499T	Ar	IR	1

References

[1]E. S. Prochaska, L. Andrews, N. R. Smyrl, and G. Mamantov, Inorg. Chem. **17**, 970 (1978).

KrF_2^+

$\tilde{D}\ ^2\Sigma_u$ $D_{\infty h}$
T^{ab} = 36600(1000) gas PE[1]

$\tilde{C}\ ^2\Pi_u$ $D_{\infty h}$
T_0^a = 30340(160) gas PE[1]

$\tilde{B}\ ^2\Pi_g$ $D_{\infty h}$
T_0^a = 9760(160) gas PE[1]

$\tilde{A}\ ^2\Sigma_g$ $D_{\infty h}$
T_0^a = 5970(160) gas PE[1]

$\tilde{X}\ ^2\Pi_u$ $D_{\infty h}$
A = −1050(160) gas PE[1]

[a] Calculated using the upper bound of 13.16 eV for the first adiabatic ionization potential. Value may be increased by as much as 800, corresponding to the lower bound of 13.06 eV for this ionization potential.[1]
[b] From vertical ionization potential.

References

[1]C. R. Brundle and G. R. Jones, J. Chem. Soc., Faraday Trans. 2 **68**, 959 (1972).

XeF_2^+

$\tilde{D}\ ^2\Sigma_u$ $D_{\infty h}$
T_0 = 35900(500) gas PE[1-3]

$\tilde{C}\ ^2\Pi_u$ $D_{\infty h}$
T_0^a = 23400(500) gas PE[1-3]
A = 3230(800) gas PE[1]

$\tilde{B}\ ^2\Pi_g$ $D_{\infty h}$
T_0 = 13310(500) gas PE[1-3]

$\tilde{A}\ ^2\Sigma_g$ $D_{\infty h}$
T_0 = 9920(500) gas PE[1-3]

$\tilde{X}\ ^2\Pi_{u,3/2}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	520(30)	gas	PE	1

A = 3790(160) gas PE[1,2]

[a] Onset of transition given.

References

[1]C. R. Brundle, M. B. Robin, and G. R. Jones, J. Chem. Phys. **52**, 3383 (1970).
[2]B. Brehm, M. Menzinger, and C. Zorn, Can. J. Chem. **48**, 3193 (1970).
[3]B. W. Yates, K. H. Tan, G. M. Bancroft, L. L. Coatsworth, J. S. Tse, and G. J. Schrobilgen, J. Chem. Phys. **84**, 3603 (1986).

F_3^-

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	461[a]	Ar	Ra	1,2
Σ_u^+	3	Asym. stretch	550[a]	Ar	IR	1,2

[a] K^+, Rb^+, or Cs^+ present.

References

[1]B. S. Ault and L. Andrews, J. Am. Chem. Soc. **98**, 1591 (1976).
[2]B. S. Ault and L. Andrews, Inorg. Chem. **16**, 2024 (1977).

$FClF^-$

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	566 Cs	Ar	IR	2
			565 Rb	Ar	IR	2
			571 K	Ar	IR	1
			589 Na	Ar	IR	2

References

[1]E. S. Prochaska, B. S. Ault, and L. Andrews, Inorg. Chem. **16**, 2021 (1977).
[2]B. S. Ault and L. Andrews, Inorg. Chem. **16**, 2024 (1977).

$FFCl^-$

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	FF stretch	365 Cs	Ar	IR	1,2
			371 Rb	Ar	IR	1,2
			391 K	Ar	IR	2

References

[1]B. S. Ault and L. Andrews, Inorg. Chem. **16**, 2024 (1977).
[2]J. H. Miller and L. Andrews, Inorg. Chem. **18**, 988 (1979).

$FBrF^-$

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	527 Cs	Ar	IR	1
			524 Rb	Ar	IR	1
			521 K	Ar	IR	1
			543 Na	Ar	IR	1

References

[1]J. H. Miller and L. Andrews, Inorg. Chem. **18**, 988 (1979).

$FFBr^-$

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	FF stretch	360 Cs	Ar	IR	1
			366 Rb	Ar	IR	1
			364 K	Ar	IR	1

References

[1]J. H. Miller and L. Andrews, Inorg. Chem. **18**, 988 (1979).

FIF^-

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	504 Cs	Ar	IR	1
			503 Rb	Ar	IR	1
			506 K	Ar	IR	1
			520 Na	Ar	IR	1

References

[1]J. H. Miller and L. Andrews, Inorg. Chem. **18**, 988 (1979).

FFI^-

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	FF stretch	354 Cs	Ar	IR	1
			356 Rb	Ar	IR	1
			357 K	Ar	IR	1

References

[1]J. H. Miller and L. Andrews, Inorg. Chem. **18**, 988 (1979).

$ClFCl^-$

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	474 Cs	Ar	IR	1
			480 Rb	Ar	IR	1
			486 K	Ar	IR	1
			511 Na	Ar	IR	1

References

[1]B. S. Ault and L. Andrews, Inorg. Chem. **16**, 2024 (1977).

$FClCl^-$

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+			412 Cs	Ar	IR,Ra	1
			409 Rb	Ar	IR	1

References

[1]B. S. Ault and L. Andrews, Inorg. Chem. **16**, 2024 (1977).

Cl_3^-

An absorption maximum which appears at 251 nm when CsCl is codeposited with Cl_2 in an argon matrix[3] and at 253 nm when an Ar:Cl_2 sample is subjected to electron bombardment during deposition[5] has been assigned to Cl_3^-.

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	225T Cs	Ar	Ra	2
			253 Rb	Ar	Ra	2
			258 K	Ar	Ra	2
			276 Na	Ar	Ra	2
Σ_u^+	3	Asym. stretch	327 Cs	Ar	IR,Ra	2
			340 Rb	Ar	IR,Ra	2
			345 K	Ar	IR,Ra	2
			375 Na	Ar	IR,Ra	2
			374[a]	Kr	IR	1

[a] Attributed in Ref. 1 to the uncharged species. Reassigned by Ref. 4 to the anion.

References

[1]L. Y. Nelson and G. C. Pimentel, J. Chem. Phys. **47**, 3671 (1967).
[2]B. S. Ault and L. Andrews, J. Chem. Phys. **64**, 4853 (1976).
[3]L. Andrews, J. Am. Chem. Soc. **98**, 2147 (1976).
[4]C. A. Wight, B. S. Ault, and L. Andrews, J. Chem. Phys. **65**, 1244 (1976).
[5]J. Hacaloglu and L. Andrews, Chem. Phys. Lett. **160**, 274 (1989).

$ClBrCl^-$

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	311 K	Ar	IR	1

References

[1]B. S. Ault and L. Andrews, J. Chem. Phys. **64**, 4853 (1976).

$ClClBr^-$

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	Stretch	273 K	Ar	IR	1

References

[1]B. S. Ault and L. Andrews, J. Chem. Phys. **64**, 4853 (1976).

$BrClBr^-$

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	282T K	Ar	IR	1

References

[1]B. S. Ault and L. Andrews, J. Chem. Phys. **64**, 4853 (1976).

$ClBrBr^-$

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	Stretch	229 K	Ar	IR	1

References

[1]B. S. Ault and L. Andrews, J. Chem. Phys. **64**, 4853 (1976).

Br_3^-

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	154T K	Ar	Ra	2
			197[a]	Kr	Ra	1
			190[a]	Xe	Ra	1
Σ_u^+	3	Asym. stretch	214 K	Ar	IR	2

[a] Assigned by Ref. 1 to the uncharged species. Arguments presented by Ref. 3 support reassignment to the anion.

References

[1]D. H. Boal and G. A. Ozin, J. Chem. Phys. **55**, 3598 (1971).
[2]B. S. Ault and L. Andrews, J. Chem. Phys. **64**, 4853 (1976).
[3]C. A. Wight, B. S. Ault, and L. Andrews, J. Chem. Phys. **65**, 1244 (1976).

I_3^-

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	113 Cs	Ar	Ra[a]	1

[a] Resonance Raman.

References

[1]L. Andrews, E. S. Prochaska, and A. Loewenschuss, Inorg. Chem. **19**, 463 (1980).

KrF_2

Continuous absorption in the gas phase between 210 and 320 nm, most intense at 210 nm.[5]

$\tilde{X}$ $D_{\infty h}$ Structure: IR[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	449	gas	Ra	2
			452	Kr	Ra	4
Π_u	2	Bend	233	gas	IR	2
			236m	Ar	IR	1
Σ_u^+	3	Asym. stretch	589.9(5)	gas	IR	2,3
			580s	Ar	IR	1

B_0 = 0.126 IR[3]

References

[1]J. J. Turner and G. C. Pimentel, Science **180**, 974 (1963).
[2]H. H. Claassen, G. L. Goodman, J. G. Malm, and F. Schreiner, J. Chem. Phys. **42**, 1229 (1965).
[3]C. Murchison, S. Reichman, D. Anderson, J. Overend, and F. Schreiner, J. Am. Chem. Soc. **90**, 5690 (1968).
[4]W. F. Howard, Jr., and L. Andrews, J. Am. Chem. Soc. **96**, 7864 (1974).
[5]G. N. Makeev, V. F. Sinyanskii, and B. M. Smirnov, Dokl. Akad. Nauk SSSR **222**, 151 (1975).

XeF_2

6p $^1\Sigma_g$ $D_{\infty h}$
T_0 = 87400 gas AB[11] $6p\,^1\Sigma_g$–$\tilde{X}$ 114 nm
A higher member of this Rydberg series has also been reported.[11]

5d $^1\Pi_{u,1/2}$ $D_{\infty h}$
T_0 = 86000 gas AB[3,4,11] $5d\,^1\Pi_{u,1/2}$–$\tilde{X}$ 116 nm
Higher members of this Rydberg series have also been reported.[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	484(24)	gas	AB	11
Π_u	2	Bend	200T	gas	AB	11

5d $^1\Pi_{u,3/2}$ $D_{\infty h}$
T_0 = 80800 gas AB[3,4,11] $5d\,^1\Pi_{u,3/2}$–$\tilde{X}$ 124 nm
Higher members of this Rydberg series have also been reported.[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	524(8)	gas	AB	11
Π_u	2	Bend	200T	gas	AB	11

6s $^1\Pi_{u,1/2}$ $D_{\infty h}$
T_0 = 73870 gas AB[3,4,8,11] $6s\,^1\Pi_{u,1/2}$–$\tilde{X}$ 135 nm
Higher members of this Rydberg series have also been reported.[3,4,11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	500(16)	gas	AB	11

6s $^1\Pi_{u,3/2}$ $D_{\infty h}$
T_0 = 69300 gas AB[3,4,8,11] $6s\,^1\Pi_{u,3/2}$–$\tilde{X}$ 144 nm
Higher members of this Rydberg series have also been reported.[3,4,11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	532(8)	gas	AB	11
Π_u	2	Bend	73(8)	gas	AB	11

$\tilde{B}$ $^1\Sigma_u$ $D_{\infty h}$
T^a = 63300 gas AB[3,4,11] $\tilde{B}$–$\tilde{X}$ 158 nm

$\tilde{A}$ $^1\Pi_g$ $D_{\infty h}$
T^a = 43500 gas AB[3,4,6,11] $\tilde{A}$–$\tilde{X}$ 230 nm

$\tilde{X}$ $^1\Sigma_g$ $D_{\infty h}$ Structure: IR[7,14]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	516.5(5)	gas	Ra	9,13
			512	Ar	Ra	10
			512	Xe	Ra	10
Π_u	2	Bend	213.2s	gas	IR	5,14
			215	Ar	IR	12
Σ_u^+	3	Asym. stretch	560.10s	gas	IR	1,5,7,14
			547	Ar	IR	2

B_0 = 0.113 IR[7,14]

[a] Absorption maximum.

References

[1]D. F. Smith, J. Chem. Phys. **38**, 270 (1963).
[2]J. J. Turner and G. C. Pimentel, in *Noble-Gas Compounds*, H. H. Hyman, Ed., University of Chicago Press, Chicago, Ill., 1963, p. 101.
[3]J. Jortner, E. G. Wilson, and W. A. Rice, in *Noble-Gas Compounds*, H. H. Hyman, Ed., University of Chicago Press, Chicago, Ill., 1963, p. 358.
[4]E. G. Wilson, J. Jortner, and S. A. Rice, J. Am. Chem. Soc. **85**, 813 (1963).
[5]P. A. Agron, G. M. Begun, H. A. Levy, A. A. Mason, C. G. Jones, and D. F. Smith, Science **139**, 842 (1963).
[6]E. S. Pysh, J. Jortner, and S. A. Rice, J. Chem. Phys. **40**, 2018 (1964).
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[10]W. F. Howard, Jr., and L. Andrews, J. Am. Chem. Soc. **96**, 7864 (1974).
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[12]B. S. Ault, L. Andrews, D. W. Green, and G. T. Reedy, J. Chem. Phys. **66**, 2786 (1977).
[13]N. J. Brassington and H. G. M. Edwards, J. Mol. Struct. **162**, 69 (1987).
[14]H. Bürger and S. Ma, J. Mol. Spectrosc. **157**, 536 (1993).

XeClF

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Stretch	316wm	Xe	IR	1
			315.5	Xe	Ra	1
	3	Stretch	481s	Xe	IR	1
			480	Xe	Ra	1

References

[1]W. F. Howard, Jr., and L. Andrews, J. Am. Chem. Soc. **96**, 7864 (1974).

$XeCl_2$

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	255	Xe	Ra	2-4
Σ_u^+	3	Asym. stretch	313	Xe	IR	1,3

References

[1]L. Y. Nelson and G. C. Pimentel, Inorg. Chem. **6**, 1758 (1967).
[2]D. Boal and G. A. Ozin, Spectrosc. Lett. **4**, 43 (1971).
[3]W. F. Howard, Jr., and L. Andrews, J. Am. Chem. Soc. **96**, 7864 (1974).
[4]I. R. Beattie, A. German, H. E. Blayden, and S. B. Brumbach, J. Chem. Soc., Dalton Trans. 1659 (1975).

Ne_2F

Unstructured gas-phase emission[1] between 117 and 125 nm has been attributed[2] to Ne_2F.

References

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Ar_2F

Unstructured gas-phase emission[1-3] between 250 and 340 nm, with maximum near 292 nm.
τ = 185(46) ns gas EM[4]

References

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ArKrF

Unstructured gas-phase emission[1,2] between 240 and 370 nm, with maximum near 305 nm.

References

[1]J. A. Mangano, J. H. Jacob, M. Rokni, and A. Hawryluk, Appl. Phys. Lett. **31**, 26 (1977).
[2]H. C. Brashears, Jr., D. W. Setser, and Y.-C. Yu, J. Chem. Phys. **74**, 10 (1981).

Kr_2F

9 $^2\Gamma$ C_{2v}

gas AB[6,8,9] $9^2\Gamma$–$4^2\Gamma$

Broad absorption, with maximum near 315 nm.

4 $^2\Gamma$ C_{2v}

Unstructured gas-phase emission[1-4] between 340 and 480 nm, with maximum near 410 nm.
τ = 200(28) ns gas LF[5]EF[7]

References

[1]J. A. Mangano, J. H. Jacob, M. Rokni, and A. Hawryluk, Appl. Phys. Lett. **31**, 26 (1977).
[2]N. G. Basov, V. A. Danilychev, V. A. Dolgikh, O. M. Kerimov, V. S. Lebedev, and A. G. Molchanov, Pis'ma Zh. Eksp. Teor. Fiz. **26**, 20 (1977); J. Exp. Theor. Phys. Lett. **26**, 16 (1977).
[3]R. O. Hunter, J. Oldenettel, C. Howton, and M. V. McCusker, J. Appl. Phys. **49**, 549 (1978).
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NeXeF

Unstructured gas-phase emission[1] between 370 and 550 nm.

References

[1]M. Rokni, J. H. Jacob, J. C. Hsia, and D. W. Trainor, Appl. Phys. Lett. **35**, 729 (1979).

ArXeF

Unstructured gas-phase emission[1,2] between 380 and 500 nm, with maximum near 460 nm.

References

[1]R. O. Hunter, J. Oldenettel, C. Hawton, and M. V. Cusker, J. Appl. Phys. **49**, 549 (1978).
[2]M. Rokni, J. H. Jacob, J. C. Hsia, and D. W. Trainor, Appl. Phys. Lett. **35**, 729 (1979).

KrXeF

Unstructured gas-phase emission[1] between 380 and 570 nm.

References

[1]N. G. Basov, V. A. Danilychev, V. A. Dolgikh, O. M. Kerimov, V. S. Lebedev, and A. G. Molchanov, Pis'ma Zh. Eksp. Teor. Fiz. **26**, 20 (1977); J. Exp. Theor. Phys. Lett. **26**, 16 (1977).

Xe_2F

4 $^2\Gamma$ C_{2v}

gas EM[1,2] $4^2\Gamma$–$1,2^2\Gamma$

Unstructured emission maximum at 16300 (614(5) nm), with bandwidth (FWHM) of 125(5) nm.

Xe EM[3] $4^2\Gamma$–$1,2^2\Gamma$

Unstructured emission maximum at 12900 (775 nm), with bandwidth (FWHM) of 2300 cm^{-1}.

τ = 152(+19, −10) ns gas EM[2]
190(10) ns Xe EM[3]

References

[1]W. Walter, R. Sauerbrey, F. K. Tittel, and W. L. Wilson, Appl. Phys. Lett. **41**, 387 (1982).
[2]R. Sauerbrey, W. Walter, F. K. Tittel, and W. L. Wilson, Jr., J. Chem. Phys. **78**, 735 (1983).
[3]M. E. Fajardo and V. A. Apkarian, J. Chem. Phys. **89**, 4102 (1988).

Ar_2Cl

Unstructured gas-phase emission maximum[1,2] at 245(5) nm, with bandwidth (FWHM) of 35 nm.
τ = 240(40) ns gas EF[2]

References

[1]D. C. Lorents, D. L. Huestis, M. V. McCusker, H. H. Nakano, and R. M. Hill, J. Chem. Phys. **68**, 4657 (1978).
[2]J. Liegel, H. Spiegel, R. Sauerbrey, and H. Langhoff, J. Chem. Phys. **79**, 247 (1983).

NeKrCl

Unstructured gas-phase emission[1,2] between 235 and 330 nm.

References

[1]I. N. Konovalov, V. F. Losev, V. V. Ryzhov, V. F. Tarasenko, and A. G. Tastremskii, Opt. Spektrosk. **47**, 239 (1979); Opt. Spectrosc. **47**, 137 (1979).
[2]V. S. Skakun and V. F. Tarasenko, Opt. Spektrosk. **58**, 293 (1985); Opt. Spectrosc. **58**, 175 (1985).

ArKrCl

Unstructured gas-phase emission[1] between 224 and 316 nm, with maximum near 270 nm.

References

[1]H. C. Brashears, Jr., D. W. Setser, and Y.-C. Yu, J. Chem. Phys. **74**, 10 (1981).

Kr_2Cl

Gas-phase excitation spectrum[4] shows a series of bands beginning at 44800 (5.55 eV) which have been assigned to Rydberg transitions of the excimer.

Unstructured gas-phase emission[1,2] between 290 and 380 nm, with maximum near 30800 (325 nm).
τ = 470(20) ns gas EF[3]

References

[1]D. C. Lorents, D. L. Huestis, M. V. McCusker, H. H. Nakano, and R. M. Hill, J. Chem. Phys. **68**, 4657 (1978).
[2]I. N. Konovalov, V. F. Losev, V. V. Ryzhov, V. F. Tarasenko, and A. G. Tastremskii, Opt. Spektrosk. **47**, 239 (1979); Opt. Spectrosc. **47**, 137 (1979).
[3]A. Luches, A. Perrone, and A. Giannattasio, Opt. Commun. **48**, 253 (1983).
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KrXeCl

Unstructured gas-phase emission[1] between 290 and 450 nm, with maximum near 370 nm.

References

[1]H. C. Brashears, Jr., D. W. Setser, and Y.-C. Yu, J. Chem. Phys. **74**, 10 (1981).

Xe_2Cl

9 $^2\Gamma$ C_{2v}

gas AB[4,6] $9^2\Gamma$–$4^2\Gamma$

Absorption maximum near 29800 (335 nm), absorption extending to wavelengths less than 193 nm.

8 $^2\Gamma$ C_{2v}

gas AB[6] $8^2\Gamma$–$4^2\Gamma$ ca. 435 nm

4 $^2\Gamma$ C_{2v}

gas EM[1–4,6] $4^2\Gamma$–$1,2^2\Gamma$

Unstructured emission maximum at 20600 (485 nm), with bandwidth (FWHM) of 4500 cm^{-1}.

Ne AB[8] $4^2\Gamma$–$1^2\Gamma$

Unstructured absorption maximum at 30400 (329 nm), with bandwidth (FWHM) of 1400 cm^{-1}.

Ne EM[8] $4^2\Gamma$–$1,2^2\Gamma$

Unstructured emission maximum at 17700 (564 nm), with bandwidth (FWHM) of approximately 2000 cm^{-1}.

Ar,Kr,Xe EM[5,7] $4^2\Gamma$–$1,2^2\Gamma$

Unstructured emission maximum at 17450 (573 nm), with bandwidth (FWHM) of 2000 cm^{-1}.

τ = 245(10) ns gas EM[4]
260(15) ns Ne EM[8]
250(10) ns Ar EM[5]
210(10) ns Kr EM[5]
225(5) ns Xe EM[5,7]

References

[1]J. A. Mangano, J. H. Jacob, M. Rokni, and A. Hawryluk, Appl. Phys. Lett. **31**, 26 (1977).
[2]D. C. Lorents, D. L. Huestis, M. V. McCusker, H. H. Nakano, and R. M. Hill, J. Chem. Phys. **68**, 4657 (1978).
[3]A. W. McKown and J. G. Eden, J. Chem. Phys. **81**, 2933 (1984).
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[7]M. E. Fajardo and V. A. Apkarian, J. Chem. Phys. **89**, 4102 (1988).
[8]R. Böhling, J. Langen, and U. Schurath, J. Mol. Struct. **222**, 171 (1990).

ArKrBr

Unstructured gas-phase emission[1] between 227 and 290 nm.

References

[1]V. S. Skakun and V. F. Tarasenko, Opt. Spektrosk. **58**, 293 (1985); Opt. Spectrosc. **58**, 175 (1985).

Kr_2Br

Unstructured gas-phase emission[1] between 265 and 370 nm.

References

[1]I. N. Konovalov, V. F. Losev, V. V. Ryzhov, V. F. Tarasenko, and A. G. Tastremskii, Opt. Spektrosk. **47**, 239 (1979); Opt. Spectrosc. **47**, 137 (1979).

NeXeBr

Unstructured gas-phase emission[1] between 255 and 350 nm.

References

[1]I. N. Konovalov and V. F. Tarasenko, Zh. Prikl. Spektrosk. **34**, 177 (1981).

ArXeBr

Unstructured gas-phase emission[1] between 270 and 380 nm.

References

[1]V. S. Skakun and V. F. Tarasenko, Opt. Spektrosk. **58**, 293 (1985); Opt. Spectrosc. **58**, 175 (1985).

KrXeBr

Unstructured gas-phase emission[1] between 285 and 375 nm, with maximum near 330 nm.

References

[1]H. C. Brashears, Jr., D. W. Setser, and Y.-C. Yu, J. Chem. Phys. **74**, 10 (1981).

Xe_2Br

$4\,^2\Gamma$ C_{2v}

gas EM[1,2] $4^2\Gamma$–$1,2^2\Gamma$

Unstructured emission between 380 and 460 nm, with maximum near 22700 (440 nm).

Xe EM[3] $4^2\Gamma$–$1,2^2\Gamma$

Unstructured emission maximum at 20800 (480 nm), with bandwidth (FWHM) of 2100 cm^{-1}.

τ = 245(30) ns gas EM[2]
185(10) ns Xe EM[3]

References

[1]I. N. Konovalov, V. F. Losev, V. V. Ryzhov, V. F. Tarasenko, and A. G. Tastremskii, Opt. Spektrosk. **47**, 239 (1979); Opt. Spectrosc. **47**, 137 (1979).
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KrXeI

Unstructured gas-phase emission[1] between 260 and 420 nm, with maximum near 290 nm.

References

[1]H. C. Brashears, Jr., D. W. Setser, and Y.-C. Yu, J. Chem. Phys. **74**, 10 (1981).

Xe_2I

$4\,^2\Gamma$ C_{2v}

gas EM[1,2] $4^2\Gamma$–$1,2^2\Gamma$

Unstructured emission maximum at 26700 (375 nm).

Xe EM[3] $4^2\Gamma$–$1,2^2\Gamma$

Unstructured emission maximum at 25600 (390 nm), with bandwidth (FWHM) of 2000 cm^{-1}.

τ = 1100(100) ns gas EM[2]
130(10) ns Xe EM[3]

References

[1]D. C. Lorents, D. L. Huestis, M. V. McCusker, H. H. Nakano, and R. M. Hill, J. Chem. Phys. **68**, 4657 (1978).
[2]A. Perrone, A. Luches, and A. Giannattasio, Opt. Commun. **53**, 95 (1985).
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6.4. Four–Atomic Trihydrides

CrH_3

X

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CrH stretch	1513.0	Ar	IR	1
			1510.3	Kr	IR	1

CrD_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CrD stretch	1106.4	Ar	IR	1
			1099.1	Kr	IR	1

References

[1]Z. L. Xiao, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **96**, 636 (1992).

MoH_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		MoH stretch	1680.0	Kr	IR	1

MoD_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		MoD stretch	1202.3	Kr	IR	1

References

[1]Z. L. Xiao, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **96**, 636 (1992).

BH_3

$\tilde{X}\ ^1A_1'$ D_{3h} Structure: IR[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	1140.88	gas	DL	2
			1125w	Ar	IR	1
e'	3	BH stretch	2601.57	gas	IR	3

B_0 = 7.874; $C_0 \cong$ 3.879 IR[3]

BD_3

$\tilde{X}\ ^1A_1'$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	845	Ar	IR	1
e'	3	BD stretch	2112T	Ar	IR	1

References

[1]A. Kaldor and R. F. Porter, J. Am. Chem. Soc. **93**, 2140 (1971).
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[3]K. Kawaguchi, J. Chem. Phys. **96**, 3411 (1992).

CH_3^+

$\tilde{A}\ ^1E'$ D_{3h}
T_0 = 50510(280) gas PE[2]

$\tilde{a}\ ^3E'$ D_{3h}
T_0 = 39700(280) gas PE[2]

$\tilde{X}\ ^1A_1'$ D_{3h} Structure: LD[3,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	1380(20)	gas	PE	1,2
e'	3	CH stretch	3108.38	gas	LD	3,4

B_0 = 9.362 LD[3,4]

CD_3^+

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	1070(30)	gas	PE	2

References

[1]T. Koenig, T. Balle, and W. Snell, J. Amer. Chem. Soc. **97**, 662 (1975); T. Koenig, T. Balle, and J. C. Chang, Spectrosc. Lett. **9**, 755 (1976).
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SiH_3^+

$\tilde{X}$ D_{3h} Structure: DL[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	838.067	gas	DL	1

B_0 = 5.215 DL[1]

References

[1]D. M. Smith, P. M. Martineau, and P. B. Davies, J. Chem. Phys. **96**, 1741 (1992).

GeH_3^+

$\tilde{X}$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	393(15)	gas	PI	1

References

[1]B. Ruscic, M. Schwarz, and J. Berkowitz, J. Chem. Phys. **92**, 1865 (1990).

BH_3^-

Threshold for electron detachment from ground-state BH_3^- = 310(120) gas PE[1]

BD_3^-

Threshold for electron detachment from ground-state BD_3 = 220(113) gas PE[1]

References

[1]C. T. Wickham-Jones, S. Moran, and G. B. Ellison, J. Chem. Phys. **90**, 795 (1989).

CH_3

4f $^2E'$ [a] D_{3h}
T_0 = 72508 gas MPI[12]
Higher member of Rydberg series observed at 74961. MPI[12]

4p $^2A_2''$ D_{3h}
T_0 = 69853.44(13) gas MPI[15]
B_0 = 9.90 gas MPI[15]

3d $^2A_1'$ D_{3h} Structure: AB^2
T_0 = 66805 gas $AB^{1,2}$ $3d^2A_1'$–$\tilde{X}$ 147–150 nm
Ar AB^3 $3d^2A_1'$–$\tilde{X}$ ca. 150.3 nm
First member of Rydberg series converging to 79392(5). Higher members observed at 72326, 74851, 76256, 77090, and 77643. AB^2
B_0 = 10.72(8) AB^2

3d $^2E''$ D_{3h} Structure: AB^2
T_0 = 66536 gas $AB^{1,2}MPI^{10}$ $3d^2E''$–$\tilde{X}$ 144–150 nm
Ar AB^3 $3d^2E''$–$\tilde{X}$ ca. 150.3 nm
Diffuse. First member of Rydberg series converging to 79392(5). Higher members observed at 72165, 74851, 76256, 77090, and 77643. AB^2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	1372H	gas	AB,MPI	2,10

3p $^2A_2''$ D_{3h} Structure: MPI[12]
T_0 = 59972 gas MPI[12]
Higher member of Rydberg series observed at 69837. MPI[12]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	CH stretch	2914	gas	MPI	12
a_2''	2	OPLA	1334	gas	MPI	12

3s $^2A_1'$ D_{3h} Structure: AB^2
T_0 = 46205 gas $AB^{1,2,7}Ra^{24}$ $3s^2A_1'$–$\tilde{X}$ 216 nm
Diffuse. First member of Rydberg series converging to 79392(5). Next member observed at 71042. AB^2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	CH stretch	2040T	gas	Ra	24

$\tilde{X}$ $^2A_2''$ D_{3h} Structure: $AB^2IR^{9,18}CAR^{23}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	CH stretch	3004.42(3)	gas	CAR,Ra	13,16,23
a_2''	2	OPLA	606.453	gas	IR,DL	5,9,21
			617vs	Ne	IR	4
			603[b]	Ar	IR	3,8
			611	N_2	IR	3
e'	3	CH stretch	3160.821	gas	LD	11
			3162wm	Ne	IR	4
			3150	Ar	IR	6
e'	4	Deformation	1396w	Ne	IR	4
			1398[c]	Ar	IR	8

B_0 = 9.578 AB^2DL^9; C_0 = 4.742 DL^9

CD_3

4f $^2E'$ [a] D_{3h}
T_0 = 72431 gas MPI[12]
Higher member of Rydberg series observed at 74885. MPI[12]

4p $^2A_2''$ D_{3h}
T_0 = 69777.40(4) gas MPI[15]
B_0 = 4.846(2) gas MPI[15]

3d $^2A_1'$ D_{3h} Structure: AB^2
T_0 = 66715 gas $AB^{1,2}$ $3d^2A_1'$–$\tilde{X}$ 145–150 nm
Ar AB^3 $3d^2A_1'$–$\tilde{X}$ ca. 150.3 nm
First member of Rydberg series converging to 79315(5). Higher members observed at 72296, 74781, 76181, 77023, 77562, and 77933. AB^2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	1040H	gas	AB	2

B_0 = 5.14 AB^2

3d $^2E''$ D_{3h} Structure: AB^2
T_0 = 66465 gas $AB^{1,2}MPI^{10}$ $3d^2E''$–$\tilde{X}$ 146–150 nm
Ar AB^3 $3d^2E''$–$\tilde{X}$ ca. 150.3 nm
Diffuse. First member of Rydberg series converging to 79315(5). Higher members observed at 72180, 74753, 76166, 77023, 77562, and 77933. AB^2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	1031H	gas	AB,MPI	2,10

3p $^2A_2''$ D_{3h} Structure: MPI^1
T_0 = 59886 gas $MPI^{12,17}$
Higher members of Rydberg series observed at 69789, 73645, and 75557. MPI^{12}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	CD stretch	2031[d]	gas	MPI	12,17
a_2''	2	OPLA	1032	gas	MPI	12,17

B_0 = 4.76(2); C_0 = 2.38 $MPI^{12,17}$

3s $^2A_1'$ D_{3h} Structure: AB^2
T_0 = 46629 gas $AB^{1,2,7}Ra^{24}$ $3s^2A_1''$–$\tilde{X}$ 204–225 nm
First member of Rydberg series converging to 79315(5). Higher members observed at 70910, 74246, 75869, and 76830. AB^2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	CD stretch	1684[d]	gas	AB	7
a_2''	2	OPLA	1094	gas	AB,Ra	7,24

B_0 = 4.42 AB^2

$\tilde{X}$ $^2A_2''$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	CD stretch	2157.5(2)	gas	Ra,CAR	19,20
a_2''	2	OPLA	457.81	gas	DL	14,18
			463s	Ne	IR	4
			453[b]	Ar	IR	3,8
			463	N_2	IR	3
e'	3	CD stretch	2381.09	gas	IR	22
			2381w	Ne	IR	4
			2369	Ar	IR	6
	4	Deformation	1026vw	Ne	IR	4
			1029	Ar	IR	6

B_0 = 4.802 AB^2DL^{14}

[a] Tentative assignment.
[b] Band center. Rotational structure assigned.[8]
[c] $^RR(0_0)$ transition.
[d] Approximate value; perturbed by Fermi resonance.

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SiH_3

$\tilde{M}$ $^2A_2''$ (6p) D_{3h}
T_0 = 60341 gas MPI^7

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	800(30)	gas	MPI	7

$\tilde{L}$ (5d) D_{3h}
T_0 = 59615(30)[c] gas MPI^8

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	839(26)	gas	MPI	8

$\tilde{J}'$ (4d) D_{3h}
T_0 = 57726(30) gas MPI^8

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	835(26)	gas	MPI	8

$\tilde{J}\ ^2A_2''$ (5p) D_{3h}
T_0 = 56929 gas MPI[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	821(4)	gas	MPI	7

$\tilde{I}'$ (4d) D_{3h}
T_0 = 56253(30) gas MPI[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	814(25)	gas	MPI	8

$\tilde{D}\ ^2A_1'$ (3d) D_{3h}
T_0 = 49787(30) gas MPI[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	810(31)	gas	MPI	8

$\tilde{E}\ ^2A_2''$ (4p) D_{3h}
T_0 = 48438 gas MPI[5,7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	796(7)	gas	MPI	5,7
e'	4	Deformation	870(5)H	gas	MPI	7

$\tilde{A}\ ^2A_1$ C_{3v}
gas AB[9] $\tilde{A}$–$\tilde{X}$ 205–250 nm

$\tilde{X}\ ^2A_1$ C_{3v} Structure: ESR[1,2]DL[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Umbrella	727.94[a]	gas	DL,MPI	3,6,7
			721.05[b]	gas	DL,MPI	3,6,7

Barrier to inversion = 1935 gas PE[4]MPI[7]
B_0 = 4.763 DL[3]

SiD_3

$\tilde{P}\ ^2A_2''$ (7p) D_{3h}
T_0 = 62002 gas MPI[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	615(3)	gas	MPI	7

$\tilde{N}\ ^2E'$ (5f) D_{3h}
T_0 = 61005 gas MPI[7,8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	619(7)	gas	MPI	7

$\tilde{M}\ ^2A_2''$ (6p) D_{3h}
T_0 = 60267 gas MPI[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	615(4)	gas	MPI	7

$\tilde{K}\ ^2E'$ (4f) D_{3h}
T_0 = 58417 gas MPI[7,8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	602(10)	gas	MPI	8

$\tilde{J}'$ (4d) D_{3h}
T_0 = 57840(30)[c] gas MPI[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	603(20)	gas	MPI	8

$\tilde{J}\ ^2A_2''$ (5p) D_{3h}
T_0 = 56874 gas MPI[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	608(3)	gas	MPI	7

$\tilde{I}'$ (4d) D_{3h}
T_0 = 56205(30) gas MPI[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	600(17)	gas	MPI	8

$\tilde{H}\ ^2E'$ (4p) D_{3h}
$T_0 \cong$ 50000 gas MPI[7,8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	602(5)	gas	MPI	7

$\tilde{D}\ ^2A_1'$ (3d) D_{3h}
T_0 = 49685(30)[c] gas MPI[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	600(28)	gas	MPI	8

$\tilde{E}\ ^2A_2''$ (4p) D_{3h}
T_0 = 48391 gas MPI[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	SiD_3 stretch	1576(3)	gas	MPI	7
a_2''	2	OPLA	589(3)	gas	MPI	7
e'	4	Deformation	635(6)H	gas	MPI	7

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Umbrella	545[a]	gas	MPI	7
			542[b]	gas	MPI	7

Barrier to inversion = 1925 gas MPI[7]

[a] $1^- - 0^+$ transition.
[b] $1^+ - 0^-$ transition.
[c] Extrapolated value.

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GeH_3

$5p\ ^2A_2''$ D_{3h}
T_0 = 47705(5) gas MPI[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	756(5)	gas	MPI	1

$\tilde{X}\ ^2A_1$ C_{3v}[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Umbrella	663(10)	gas	MPI	1

[a] Estimated inversion barrier is 1530.

References

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NH_3^+

$\tilde{A}\ ^2E$ D_{3h}
T_0 = 36590(100) gas PE[3,4]
Broad, partially resolved vibrational structure has been discussed[3] in terms of the expected Jahn–Teller distortion. Continuous background absorption may be associated with the formation of NH_2^+, for which the threshold is ca. 44700,[1,3] or NH^+.

$\tilde{X}\ ^2A_2''$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	NH stretch	2740T	gas	PE	3
a_2''	2	OPLA	903.39	gas	PE,DL	3,6
e'	3	NH stretch	3388.65	gas	LD	5
	4	Bend	1507.1	gas	TPE	7,8

B_0 = 10.644; C_0 = 5.247 LD[5]DL[6]

ND_3^+

$\tilde{X}\ ^2A_2''$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	725(25)	gas	PE	2

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PH_3^+

$\tilde{A}\ ^2E$

$T_0 \leq 21800(120)$ gas PE[1]

As for NH_3^+, this band shows complicated, poorly resolved vibrational structure, expected to be associated with Jahn–Teller distortion of the molecule.

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	Umbrella	694(80)[a]	gas	PE	1

Inversion barrier ≅ 1290[1]

[a] Higher levels are above the inversion barrier, and have typical spacings near 500.[1] There is also some evidence for a weak $\nu_1 + 2\nu_2$ progression in the photoelectron spectrum.

References

[1]R. Maripuu, I. Reineck, H. Ågren, Wu Nian-Zu, Ji Ming Rong, H. Veenhuizen, S. H. Al-Shamma, L. Karlsson, and K. Siegbahn, Mol. Phys. **48**, 1255 (1983).

AsH_3^+

$\tilde{A}\ ^2E$

$T_0 = 18000(300)$ gas PE[1]

As for NH_3^+, this band shows complicated, poorly resolved vibrational structure, expected to be associated with Jahn–Teller distortion of the molecule.

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA[a]	452(25)	gas	PE,PI	1,2

[a] Low inversion barrier. Observed vibrational structure is above this barrier.

References

[1]A. W. Potts and W. C. Price, Proc. Roy. Soc. (London) **A326**, 181 (1972).
[2]J. Berkowitz, J. Chem. Phys. **89**, 7065 (1988).

SbH_3^+

$\tilde{A}\ ^2E$

$T_0 = 15170(240)$ gas PE[1]

As for NH_3^+, this band shows complicated, poorly resolved vibrational structure, expected to be associated with Jahn–Teller distortion of the molecule.

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA[a]	387(25)	gas	PE	1

[a] Low inversion barrier. Observed vibrational structure is above this barrier.

References

[1]A. W. Potts and W. C. Price, Proc. Roy. Soc. (London) **A326**, 181 (1972).

CH_3^-

Threshold for electron detachment from ground-state CH_3^- is 645(240).[1]

$\tilde{X}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Umbrella	460(40)	gas	PE	1

References

[1]G. B. Ellison, P. C. Engelking, and W. C. Lineberger, J. Amer. Chem. Soc. **100**, 2556 (1978).

SiH_3^-

Threshold for electron detachment from ground-state SiH_3^- = 11340(110) gas PE[1]

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Umbrella	880(120)	gas	PE	1

Barrier to inversion = 9000(2000) gas PE[1]

SiD_3^-

Threshold for electron detachment from ground-state SiD_3^- = 11180(180) gas PE[1]

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Umbrella	580(160)	gas	PE	1

References

[1]M. R. Nimlos and G. B. Ellison, J. Am. Chem. Soc. **108**, 6522 (1986).

H_3O^+

$\tilde{X}$ C_{3v} Structure: CC[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Umbrella	954.40[a]	gas	DL	2,3,5,7
			525.82[b]	gas	DL	5–7

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	OH stretch	3535.56[c,d]	gas	CC	1,4,10,15
			3518.95[c,e]	gas	CC	1,4,10,14 15
	4	Deformation	1625.95[d]	gas	DL	11
			1638.53[e]	gas	DL	11

$B(0^+)$ = 11.254; (C–B)(0^+) = −4.91(6) IR,MW[9,12,15]

D_3O^+

$\tilde{X}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Umbrella	645.13[a]	gas	DL	8
			438.39[b]	gas	DL	8
e	3	OD stretch	2629.65[d]	gas	LD	13
			2624.24[e]	gas	LD	13

$B(0^+)$ = 5.675 DL[8]LD[13]

[a] $1^- - 0^+$ transition.
[b] $1^+ - 0^-$ transition. For H_3O^+, $0 - 0^+$ = 55.35 cm^{-1},[6,12] and for D_3O^+, 15.39 cm^{-1}.[8]
[c] $\nu - C'\zeta + 7/4\eta_K$.
[d] $1^+ - 0^+$ transition.
[e] $1^- - 0^-$ transition.

References

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H_3S^+

$\tilde{X}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SH stretch	2521.05	gas	LD	3
	2	Umbrella	1033.31	gas	DL	2
e	3	SH stretch	2525.74	gas	LD	1,3

B_0 = 4.895; C_0 = 4.228 LD[1,3]DL[2]

References

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6.5. Four–Atomic Dihydrides

Ca_2H_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1237.4	Kr	IR	1

Ca_2D_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			892.2	Kr	IR	1

References

[1]Z. L. Xiao, R. H. Hauge, and J. L. Margrave, High Temp. Sci. **31**, 59 (1991).

Zn_2H_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ZnH stretch	1850.1	Ar	IR	1
		Bend	612.5	Ar	IR	1
		Bend	600.8	Ar	IR	1

Zn_2D_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ZnD stretch	1343.4	Ar	IR	1

References

[1]Z. L. Xiao, R. H. Hauge, and J. L. Margrave, High Temp. Sci. **31**, 59 (1991).

Cu_2H_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1341.7	Ar	IR	1
			938.7	Ar	IR	1
			528.0	Ar	IR	1

Cu_2D_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			975.3	Ar	IR	1
			687.7	Ar	IR	1

References

[1]R. H. Hauge, Z. H. Kafafi, and J. L. Margrave, in *Physics and Chemistry of Small Clusters*, P. Jena, B. K. Rao, and S. N. Khanna, Eds., p. 787 (Plenum, New York, 1987).

$ZnCH_2$

Photolysis threshold near 360 nm. In an argon matrix,[1] rearranges to HZnCH.

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s-stretch	2958.5	Ar	IR	1
			2956.1			
	2	CH_2 scissors	1341.5	Ar	IR	1
			1339.1			
	3	ZnC stretch	513.7	Ar	IR	1
			512.0			
b_1	4	OPLA	524.8	Ar	IR	1
b_2	5	CH_2 a-stretch	3047.2	Ar	IR	1
	6	CH_2 rock	543.8	Ar	IR	1

$ZnCD_2$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_2 s-stretch	2165.7	Ar	IR	1
	2	CD_2 scissors	1009.8	Ar	IR	1
	3	ZnC stretch	472.2	Ar	IR	1
b_1	4	OPLA	419.0	Ar	IR	1
b_2	6	CD_2 rock	412.2	Ar	IR	1

References

[1]S.-C. Chang, R. H. Hauge, Z. H. Kafafi, J. L. Margrave, and W. E. Billups, J. Chem. Soc., Chem. Commun. 1682 (1987).

HZnCH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ZnH stretch	1924.4ms	Ar	IR	1
		ZnC stretch	647.5wm	Ar	IR	1
		HZnC bend	469.3s	Ar	IR	1

DZnCD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ZnD stretch	1386.8m	Ar	IR	1
		ZnC stretch	627.2wm	Ar	IR	1
		DZnC bend	344.7s	Ar	IR	1

References

[1]S.-C. Chang, R. H. Hauge, Z. H. Kafafi, J. L. Margrave, and W. E. Billups, J. Chem. Soc., Chem. Commun. 1682 (1987).

$FeCH_2$

Photolysis threshold near 360 nm. In an argon matrix,[2] rearranges to HFeCH.

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s-stretch	2941.6m	Ar	IR	1,2
	3	FeC stretch	623.9vs	Ar	IR	1,2
b_1	4	OPLA	700.3s	Ar	IR	1,2
			697.4			
b_2	5	CH_2 a-stretch	3011.5	Ar	IR	2
	6	CH_2 rock	452.0	Ar	IR	2

$FeCD_2$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_2 s-stretch	2134.3	Ar	IR	2
	3	FeC stretch	575.2	Ar	IR	2
b_1	4	OPLA	552.7 550.9	Ar	IR	2
b_2	5	CD_2 a-stretch	2201.0	Ar	IR	2
	6	CD_2 rock	347.6	Ar	IR	2

References

[1]S.-C. Chang, Z. H. Kafafi, R. H. Hauge, W. E. Billups, and J. L. Margrave, J. Am. Chem. Soc. **107**, 1447 (1985).
[2]S.-C. Chang, R. H. Hauge, Z. H. Kafafi, J. L. Margrave, and W. E. Billups, J. Am. Chem. Soc. **110**, 7975 (1988).

HFeCH

Photolysis threshold near 400 nm. In an argon matrix,[1] rearranges to $FeCH_2$.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		FeH stretch	1681.6	Ar	IR	1
		FeC stretch	674.2	Ar	IR	1
		FeCH bend	632.1	Ar	IR	1

DFeCD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		FeD stretch	1209.2	Ar	IR	1
		FeC stretch	648.3	Ar	IR	1
		FeCD bend	503.7	Ar	IR	1

References

[1]S.-C. Chang, R. H. Hauge, Z. H. Kafafi, J. L. Margrave, and W. E. Billups, J. Am. Chem. Soc. **110**, 7975 (1988).

$CuCH_2$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s-stretch	2960.7	Ar	IR	1
	2	CH_2 scissors	1344.9	Ar	IR	1
	3	CuC stretch	614.0	Ar	IR	1
b_1	4	OPLA	526.0	Ar	IR	1
b_2	5	CH_2 a-stretch	3034.7	Ar	IR	1

$CuCD_2$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_2 scissors	1013.7	Ar	IR	1
	3	CuC stretch	570.4	Ar	IR	1
b_1	4	OPLA	409.1	Ar	IR	1

References

[1]S.-C. Chang, Z. H. Kafafi, R. H. Hauge, W. E. Billups, and J. L. Margrave, J. Am. Chem. Soc. **109**, 4508 (1987).

$CaNH_2$

$\tilde{C}\ ^2A_1$ C_{2v} Structure: LF^2
$T_0{}^a = 17375.129(5)$ gas CL^1LF^2 $\tilde{C}$-$\tilde{X}$ 575 nm
$B^a = 0.306$; $C^a = 0.298$ LF^2

$\tilde{B}\ ^2B_1$ C_{2v}
$T_0 = 15886$ gas CL^1LF^{3-5} $\tilde{B}$-$\tilde{X}$ 620–650 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CaN stretch	545.8(5)	gas	LF	4

$A = 14.6(2)$; $\frac{1}{2}(B + C) = 0.304$ LF^5

$\tilde{A}\ ^2B_2$ C_{2v}
$T_0 = 15464$ gas CL^1LF^{3-5} $\tilde{A}$-$\tilde{X}$ 620–650 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CaN stretch	549.5(1.0)	gas	LF	3,4

$A = 11.4$; $\frac{1}{2}(B + C) = 0.304$ LF^5

$\tilde{X}\ ^2A_1$ C_{2v} Structure: LF^2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CaN stretch	524(10)	gas	LF	3

$A = 13.0$; $B^a = 0.301$; $C^a = 0.293$ $LF^{2,5}$

[a] From analysis of $K_{-1} = 1$ subband of $\tilde{C}$-$\tilde{X}$ transition.

References

[1]R. F. Wormsbecher, M. Trkula, C. Martner, R. E. Penn, and D. O. Harris, J. Mol. Spectrosc. **97**, 29 (1983).
[2]R. F. Wormsbecher, R. E. Penn, and D. O. Harris, J. Mol. Spectrosc. **97**, 65 (1983).
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[4]C. J. Whitham, B. Soep, J.-P. Visticot, and A. Keller, J. Chem. Phys. **93**, 991 (1990).
[5]C. J. Whitham and Ch. Jungen, J. Chem. Phys. **93**, 1001 (1990).

$SrNH_2$

$\tilde{C}\ ^2A_1$ C_{2v}
T_0 = 15862(10) gas CL[1]LF[2] $\tilde{C}$–$\tilde{X}$ 632 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	SrN stretch	458(10)	gas	LF	2

$\tilde{B}\ ^2B_1$ C_{2v}
T_0 = 14724(10) gas CL[1]LF[2] $\tilde{B}$–$\tilde{X}$ 670–725 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	SrN stretch	450T	gas	LF	2

$\tilde{A}\ ^2B_2$ C_{2v}
T_0 = 14274(10) gas CL[1]LF[2] $\tilde{A}$–$\tilde{X}$ 670–725 nm

$\tilde{X}\ ^2A_1$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	SrN stretch	459(10)	gas	LF	2

References

[1]R. F. Wormsbecher, M. Trkula, C. Martner, R. E. Penn, and D. O. Harris, J. Mol. Spectrosc. **97**, 29 (1983).
[2]A. M. R. P. Bopegedera, C. R. Brazier, and P. F. Bernath, J. Phys. Chem. **91**, 2779 (1987).

$BaNH_2$

$\tilde{D},\tilde{E}\ ^2B_1, ^2B_2$ [a] gas CL[1] $\tilde{D},\tilde{E}$–$\tilde{X}$ ca. 530 nm

$\tilde{C}\ ^2A_1$ [a] gas CL[1] $\tilde{C}$–$\tilde{X}$ ca. 765 nm

$\tilde{A},\tilde{B}\ ^2B_1, ^2B_2$ [a] gas CL[1] $\tilde{A},\tilde{B}$–$\tilde{X}$ 835–950 nm

$\tilde{X}\ ^2A_1$ [a]

[a] Symmetries proposed by analogy to BaF.

References

[1]R. F. Wormsbecher, M. Trkula, C. Martner, R. E. Penn, and D. O. Harris, J. Mol. Spectrosc. **97**, 29 (1983).

$CuNH_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NH stretch	3369.3	Ar	IR	1
		NH_2 deform.	1528.0	Ar	IR	1
		CuN stretch	748.2	Ar	IR	1

$CuND_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ND stretch	2471.7	Ar	IR	1
		ND_2 deform.	1147.9	Ar	IR	1

References

[1]D. W. Ball, R. H. Hauge, and J. L. Margrave, Inorg. Chem. **28**, 1599 (1989).

$HCCH^+$

$\tilde{C}\ ^2\Sigma^+$ $D_{\infty h}$
T_0 = 92460(80) gas PE[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	2	CC stretch	1370T	gas	PE	6

$\tilde{B}\ ^2\Sigma_u^+$ $D_{\infty h}$
T_0 = 56380(80) gas PE[1,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	CC stretch	2500(20)	gas	PE	1,3
	2	CH s–stretch	1815(20)	gas	PE	1,3

τ < 14 fs gas PE[3]

$\tilde{A}\ ^2A_g$ [a] C_{2h}
T_0 = 39486(80) gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	CH s–stretch	2530(20)	gas	PE	3
	2	CC stretch	1730(20)	gas	PE	3
	3	Bend	492(12)	gas	PE	3
b_u	6	Bend	605(12)	gas	PE	3

Decays in less than one period of bending vibration, possibly into the vinylidene structure.[3]

$\tilde{X}\ ^2\Pi_u$ $D_{\infty h}$ Structure: LD[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	2	CC stretch	1829(3)	gas	PE	1,3
Σ_u^+	3	CH a–stretch	3135.98	gas	LD	5,9
			3137.6	Ne	IR	8
			3105.5	Ar	IR	4,8
Π_g	4	Deform.	572(20)T[b]	gas	PE	7
Π_u	5	Deform.	837(12)[b]	gas	PE	3

A = −30.1(1.5) gas LD[5]
B_0 = 1.105 LD[5,9]

$DCCD^+$

$\tilde{B}\ ^2\Sigma_u^+$ $D_{\infty h}$
T_0 = 56655(80) gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	CC stretch	2275(20)	gas	PE	1,3
	2	CD s-stretch	1475(20)	gas	PE	1,3

$\tilde{A}\ ^2A_g$ C_{2h}
T_0 = 39906(80) gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	CD s-stretch	2280(20)	gas	PE	3
	2	CC stretch	1450(20)	gas	PE	3
	3	Bend	339(12)	gas	PE	3
b_u	6	Bend	516(12)	gas	PE	3

$\tilde{X}\ ^2\Pi_u$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	CD s-stretch	2572(16)	gas	PE	3
	2	CC stretch	1651(4)	gas	PE	1,3
Σ_u^+	3	CD a-stretch	2329.1	Ne	IR	8
			2311T	Ar	IR	4,8
Π_u	5	Bend	702(12)[b]	gas	PE	3

[a] Threshold for formation of $HCC^+ \leq 48000\ cm^{-1}$.[2,3]
[b] Vibrational separations of 509(20) and 634(20) in the photoelectron spectrum of HCCH ($\tilde{A}\ ^1A_u$) have been tentatively attributed[7] to the two K = 0 Renner components of ν_4 (Π_g) of $HCCH^+$, necessitating the reassignment to ν_5 (Π_u) of the peaks previously assigned[3] to ν_4 of $HCCH^+$ and $DCCD^+$.

References

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HMgOH

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	MgH stretch	1591.8	Ar	IR	1
		MgO stretch	742.3	Ar	IR	1

DMgOD

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	MgD stretch	1162.8	Ar	IR	1
		MgO stretch	715.3	Ar	IR	1

References

[1]J. W. Kauffman, R. H. Hauge, and J. L. Margrave, High Temp. Sci. **18**, 97 (1984).

HCaOH

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	OH stretch	3697	Ar	IR	1
	2	CaH stretch	1232.8	Ar	IR	1
	3	CaO stretch	574.8	Ar	IR	1

DCaOD

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	CaD stretch	887.3	Ar	IR	1
	3	CaO stretch	576.5	Ar	IR	1

References

[1]J. W. Kauffman, R. H. Hauge, and J. L. Margrave, High Temp. Sci. **18**, 97 (1984).

HSrOH

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	SrH stretch	1143.2	Ar	IR	1
	3	SrO stretch	498.2	Ar	IR	1

DSrOD

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	SrD stretch	818.0	Ar	IR	1
	3	SrO stretch	487.4	Ar	IR	1

References

[1]J. W. Kauffman, R. H. Hauge, and J. L. Margrave, High Temp. Sci. **18**, 97 (1984).

HBaOH

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	BaH stretch	1059.4	Ar	IR	1
	3	BaO stretch	458.9	Ar	IR	1

DBaOD

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	BaD stretch	757.2	Ar	IR	1
	3	BaO stretch	447.7	Ar	IR	1

References

[1]J. W. Kauffman, R. H. Hauge, and J. L. Margrave, High Temp. Sci. **18**, 97 (1984).

HScOH

In an argon matrix,[1] photolyzes with 300–400 nm radiation, producing H_2 + ScO.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ScH stretch	1485.1	Ar	IR	1
		ScO stretch	715.8	Ar	IR	1

DScOD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ScD stretch	1070.0	Ar	IR	1
		ScO stretch	698.2	Ar	IR	1

References

[1]J. W. Kauffman, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **89**, 3547 (1985).

HTiOH

In an argon matrix,[1] photolyzes with 400–500 nm radiation, producing H_2 + TiO.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		TiH stretch	1538.9	Ar	IR	1
		TiO stretch	699.7	Ar	IR	1

DTiOD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		TiD stretch	1107.7	Ar	IR	1
		TiO stretch	697.3	Ar	IR	1

References

[1]J. W. Kauffman, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **89**, 3547 (1985).

HVOH

In an argon matrix,[1] photolyzes with radiation having a short wavelength cutoff of 400 nm.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		VH stretch	1583.0	Ar	IR	1
		VO stretch	703.3	Ar	IR	1
		Bend	414.5	Ar	IR	1

DVOD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		VD stretch	1140.3	Ar	IR	1
		VO stretch	696.6	Ar	IR	1

References

[1]J. W. Kauffman, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **89**, 3547 (1985).

HCrOH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CrH stretch	1639.9	Ar	IR	1
		CrO stretch	674.1	Ar	IR	1
		Bend	433.8	Ar	IR	1

DCrOD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CrD stretch	1184.5	Ar	IR	1
		CrO stretch	654.0	Ar	IR	1

References

[1]J. W. Kauffman, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **89**, 3541 (1985).

HMnOH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	MnH stretch	1663.4	Ar	IR	1
		MnO stretch	648.1	Ar	IR	1

DMnOD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	MnD stretch	1197.1	Ar	IR	1
		MnO stretch	628.5	Ar	IR	1

References

[1]J. W. Kauffman, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **89**, 3541 (1985).

HFeOH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	FeH stretch	1731.9	Ar	IR	1
		FeO stretch	682.4	Ar	IR	1
		Bend	457.6	Ar	IR	1

DFeOD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	FeD stretch	1245.3	Ar	IR	1
		FeO stretch	660.5	Ar	IR	1

References

[1]J. W. Kauffman, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **89**, 3541 (1985).

HCoOH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CoH stretch	1790.4	Ar	IR	1
		CoO stretch	667.4	Ar	IR	1

DCoOD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CoD stretch	1291.2	Ar	IR	1
		CoO stretch	641.9	Ar	IR	1

References

[1]J. W. Kauffman, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **89**, 3541 (1985).

HNiOH

Photodissociates, losing H, on 280–360 nm irradiation.[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3698.6	Ar	IR	1
			3688.4	Kr	IR	1
		NiH stretch	1901.0	Ar	IR	1
			1837.3			
			1893.0	Kr	IR	1
			1830.8			
		NiO stretch	707.0	Ar	IR	1
			690.6			
			699.1	Kr	IR	1
			685.8			

DNiOD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OD stretch	2726.4	Ar	IR	1
		NiD stretch	1336.2	Ar	IR	1
			1323.9			
		NiO stretch	681.2	Ar	IR	1
			664.8			

References

[1]M. Park, R. H. Hauge, and J. L. Margrave, High Temp. Sci. **25**, 1 (1988).

HCuOH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CuH stretch	1910.8	Ar	IR	1
		CuO stretch	615.6	Ar	IR	1
		CuOH bend	668.6	Ar	IR	1

DCuOD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CuD stretch	1380.8	Ar	IR	1
		CuO stretch	613.8	Ar	IR	1
		CuOD bend	496.0	Ar	IR	1

References

[1]J. W. Kauffman, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **89**, 3541 (1985).

HBNH

$\tilde{X}$ $C_{\infty v}$ Structure: MO[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NH stretch	3700m	Ar	IR	3
	3	BN stretch	1786.19	gas	DL	4
			1785m	Ar	IR	3
Π	4	Bend	460m	Ar	IR	3

B_0 = 1.099 DL[4]

DBND

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	ND stretch	2836	Ar	IR	3
	2	BD stretch	2730	Ar	IR	3
	3	BN stretch	1734	Ar	IR	3
Π	4	Bend	360	Ar	IR	3

References

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[2]D. R. Armstrong and D. T. Clark, Theor. Chim. Acta **24**, 307 (1972).
[3]E. R. Lory and R. F. Porter, J. Am. Chem. Soc. **95**, 1766 (1973).
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$H_2C{=}C{:}$

A transient absorption at 63873 and a structured transient absorption having its strongest member at 72795, formed in the vacuum ultraviolet flash photolysis of HCCH,[1] CH_2CO,[1] or C_2H_3Cl,[4] have been assigned[2] to transitions arising from the $\tilde{a}\ ^3B_2$ state of $H_2C{=}C{:}$.

$\tilde{b}\ ^3A_2$ C_{2v}
T_0 = 22200(160) gas PE[6]

$\tilde{a}\ ^3B_2$ C_{2v}
T_0 = 16660(50) gas PE[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s–stretch	2930(10)	gas	PE	6
	2	C=C stretch	1530(70)	gas	PE	6
	3	CH_2 scissors	1375(10)	gas	PE	6

$\tilde{X}\ ^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s–stretch	3025(30)	gas	PE	6
	2	C=C stretch	1635(10)	gas	PE	3,6
	3	CH_2 scissors	1165(10)	gas	PE	3,6

$D_2C{=}C{:}$

A transient absorption at 64102 and a structured transient absorption having its strongest member at 72978, formed in the vacuum ultraviolet flash photolysis of DCCD,[1], CD_2CO,[1] or C_2D_3Cl,[5] have been assigned[2] to transitions arising from the $\bar{a}\ ^3B_2$ state of $D_2C{=}C{:}$.

$\bar{a}\ ^3B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_2 s–stretch	2160(10)	gas	PE	6
	2	C=C stretch	1495(10)	gas	PE	6
	3	CD_2 scissors	1010(10)	gas	PE	6

$\bar{X}\ ^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_2 s–stretch	2190(30)	gas	PE	6
	2	C=C stretch	1590(20)	gas	PE	3,6
	3	CD_2 scissors	865(10)	gas	PE	3,6

References

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[2]A. H. Laufer, Chem. Phys. Lett. **94**, 240 (1983).
[3]S. M. Burnett, A. E. Stevens, C. S. Feigerle, and W. C. Lineberger, Chem. Phys. Lett. **100**, 124 (1983).
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[6]K. M. Ervin, J. Ho, and W. C. Lineberger, J. Chem. Phys. **91**, 5974 (1989).

H_2CSi

$^1B_2$ C_{2v}
T_0 = 29312.883(4) gas AB[1] $^1B_2$–$\bar{X}$ 310–340 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_2 scissors	1101.96	gas	AB	1
	3	CSi stretch	702.00	gas	AB	1

A_0 = 8.537; B_0 = 0.509; C_0 = 0.479 AB[1]

$\bar{X}\ ^1A_1$ C_{2v}
A_0 = 10.193; B_0 = 0.553; C_0 = 0.521 AB[1]

D_2CSi

$^1B_2$ C_{2v}
T_0 = 29272 gas AB[1] $^1B_2$–$\bar{X}$ 310–340 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_2 scissors	829	gas	AB	1
	3	CSi stretch	691	gas	AB	1

References

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br–Si_2H_2

$\bar{X}$ C_{2v} Structure: MW[1]
A_0 = 5.244; B_0 = 0.243; C_0 = 0.240 MW[1]

References

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Si(H)SiH

$\bar{X}$ C_s Structure: MW[1]
A_0 = 8.744; B_0 = 0.246; C_0 = 0.239 MW[1]

Si(D)SiD

$\bar{X}$ C_s
A_0 = 4.571; B_0 = 0.227; C_0 = 0.216 MW[1]

References

[1]M. Cordonnier, M. Bogey, C. Demuynck, and J.-L. Destombes, J. Chem. Phys. **97**, 7984 (1992).

$HCNH^+$

$\bar{X}$ $C_{\infty v}$ Structure: LD[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NH stretch	3482.84	gas	LD	1,2
	2	CH stretch	3187.86	gas	LD	1,2
	3	CN stretch	2155.70	gas	DL	7,8
Π	4	HCN bend	801.59	gas	DL	5
	5	HNC bend	645.92	gas	DL	6

B_0 = 1.236 LD[1,2]MW[3]

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HAlOH

Photolysis of HAlOH isolated in a Kr matrix with radiation having a 330 nm short wavelength cutoff leads to the formation of AlOH and, in the deuterium-substituted system, of some AlO.[2,3]

In a Kr matrix, very broad absorption between 400 and 630 nm, with maximum near 450 nm.[2,3]

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3743	Ar	IR	1
		HAl stretch	1743.3	Ar	IR	1
		AlO stretch	817.9	Ar	IR	1
		HAlO bend	605.4	Ar	IR	1

DAlOD

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		DAl stretch	1280.9	Ar	IR	1
		AlO stretch	797.2	Ar	IR	1
		DAlO bend	473.6	Ar	IR	1

References

[1]R. H. Hauge, J. W. Kauffman, and J. L. Margrave, J. Am. Chem. Soc. **102**, 6005 (1980).

[2]M. A. Douglas, R. H. Hauge, and J. L. Margrave, *Metal Bonding and Interactions in High Temperature Systems*, J. L. Gole and W. C. Stwalley, Eds., ACS Symposium Ser. 179 (American Chemical Society, Washington, D. C., 1982), pp. 347–354.

[3]M. A. Douglas, R. H. Hauge, and J. L. Margrave, J. Chem. Soc., Faraday Trans. 1 **79**, 1533 (1983).

HGaOH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3675	Ar	IR	1
		HGa stretch	1669.8	Ar	IR	1
		HGaO bend	784.9	Ar	IR	1
		GaO stretch	646.4	Ar	IR	1
		GaOH bend	520.5	Ar	IR	1

DGaOD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OD stretch	2708	Ar	IR	1
		DGa stretch	1213.8	Ar	IR	1
		GaO stretch	644.6	Ar	IR	1
		DGaO bend	582.9	Ar	IR	1

References

[1]R. H. Hauge, J. W. Kauffman, and J. L. Margrave, J. Am. Chem. Soc. **102**, 6005 (1980).

HInOH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3663	Ar	IR	1
		HIn stretch	1486.3	Ar	IR	1
		HInO bend	713.4	Ar	IR	1
		InO stretch	548.0	Ar	IR	1

DInOD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		DIn stretch	1080.1	Ar	IR	1
		InO stretch	550.9	Ar	IR	1

References

[1]R. H. Hauge, J. W. Kauffman, and J. L. Margrave, J. Am. Chem. Soc. **102**, 6005 (1980).

$H_2C{=}C{:}^-$

Threshold for electron detachment from ground-state $H_2C{=}C{:}^-$ = 3950(50) gas PE[1]

$\tilde{X}\ ^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CC stretch	1485(30)	gas	PE	1
	3	CH_2 scissors	1305(10)	gas	PE	1

$D_2C{=}C{:}^-$

Threshold for electron detachment from ground-state $D_2C{=}C{:}^-$ = 3970(50) gas PE[1]

$\tilde{X}\ ^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CD_2 scissors	960(20)	gas	PE	1

References

[1]K. M. Ervin, J. Ho, and W. C. Lineberger, J. Chem. Phys. **91**, 5974 (1989).

H_2CN

$\tilde{C}\ ^2B_1$ [a] C_{2v}

T_0 = 35620 gas $AB^{2,3,5}$ $\tilde{C}$–$\tilde{X}$ 280–285 nm
35436(25) Ar AB^6 $\tilde{C}$–$\tilde{X}$ 270–285 nm

Gas-phase absorption is diffuse.[5] Photolysis is observed in an argon matrix.[6]

$\tilde{B}\ ^2A_1$ [a] C_{2v}

T_0 = 35075[a] gas $AB^{2,3,5}$ $\tilde{B}$–$\tilde{X}$ 280–285 nm
34990(25) Ar AB^6 $\tilde{B}$–$\tilde{X}$ 270–285 nm

All gas-phase bands are diffuse.[5] Photolysis is observed in an argon matrix.[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s-stretch	2774(50)T	Ar	AB	6
	2	CN stretch	1883(50)	Ar	AB	6
	3	CH_2 scissors	1413(50)	Ar	AB	6

$\tilde{X}\ ^2B_2$ C_{2v} Structure: ESR[1,4]MW[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s-stretch	2820T	gas	PE	7
	2	CN stretch	1725.4vw	Ar	IR	6
	3	CH_2 scissors	1337T	gas	PE	7
			1336.6m	Ar	IR	6
b_1	4	OPLA	954.1wm	Ar	IR	6
b_2	5	CH_2 a-stretch	3103.2m	Ar	IR	6
	6	CH_2 rock	912.8w	Ar	IR	6

A_0 = 9.484; B_0 = 1.306; C_0 = 1.142 MW[8]

D_2CN

$\tilde{C}\ ^2B_1$ [a] C_{2v}

T_0 = 35481[a] gas $AB^{2,5}$ $\tilde{C}$–$\tilde{X}$ 271–285 nm

$\tilde{B}\ ^2A_1$ [a] C_{2v}

T_0 = 35036[a] gas $AB^{2,5}$ $\tilde{B}$–$\tilde{X}$ 271–285 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CN stretch	1894T	gas	AB	2,5
	3	CD_2 scissors	1079T	gas	AB	2,5

$\tilde{X}\ ^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_2 s-stretch	2080T	gas	PE	7
	3	CD_2 scissors	990T	gas	PE	7
			1073.4	Ar	IR	6
b_1	4	OPLA	776	Ar	IR	6
b_2	5	CD_2 a-stretch	2427.5T	Ar	IR	6

[a] Tentative assignment.

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[1]E. L. Cochran, F. J. Adrian, and V. A. Bowers, J. Chem. Phys. **36**, 1938 (1962).
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H_2CO^+

$\tilde{C}\ ^2B_2$ C_{2v}

T_0 = 43172(11) gas PE[1,4,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1895T	gas	PE	4,5
			1412T	gas	PE	1,4,5

$\tilde{B}\ ^2A_1$ C_{2v}

T_0 = 39928(6) gas PE[1,4,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CO stretch	1304(4)	gas	PE	1,4,5

$\tilde{A}\ ^2B_1$ C_{2v}

T_0 = 25929(5) gas PE[1,4,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1488(4)	gas	PE	4,5
			1250(4)	gas	PE	1,4,5
b_1	4	OPLA	263(4)	gas	PE	4,5

$\tilde{X}\ ^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	2580(4)	gas	PE	1,4,5
	2	CO stretch	1675(4)	gas	PE	4,5
	3	CH_2 scissors	1210(4)	gas	PE	1,4,5
b_1	4	OPLA	777(4)	gas	PE	4,5

D_2CO^+

$\tilde{C}\ ^2B_2$ C_{2v}
T_0 = 44600(160) gas PE[4,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1604T	gas	PE	4,5
			943T	gas	PE	1,4,5
			819T	gas	PE	4,5

$\tilde{B}\ ^2A_1$ C_{2v}
T_0 = 39816(5) gas PE[1,4,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CO stretch	1311(4)	gas	PE	1,4,5
	3	CD_2 scissors	957(4)	gas	PE	1,4,5

$\tilde{A}\ ^2B_1$ C_{2v}
T_0 = 25756(7) gas PE[1,4,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		1282(4)	gas	PE	1,4,5
	3		1064(4)	gas	PE	4,5
b_1	4	OPLA	777(4)	gas	PE	5

τ_0 = 64(22) μs gas PEPICO[3]

$\tilde{X}\ ^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD stretch	1948(4)	gas	PE	1,4,5
	2	CO stretch	1657(4)	gas	PE	4,5
	3	CD_2 scissors	920(4)	gas	PE	1,4,5
b_1	4	OPLA	648(4)	gas	PE	4,5

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[4]B. Niu, D. A. Shirley, Y. Bai, and E. Daymo, Chem. Phys. Lett. **201**, 212 (1993).
[5]B. Niu, D. A. Shirley, and Y. Bai, J. Chem. Phys. **98**, 4377 (1993).

H_2CS^+

$\tilde{D}\ ^2A_1$ C_{2v}
T^a = 84900 gas PE[2]

$\tilde{C}\ ^2B_2$ C_{2v}
T^a = 46960(160) gas PE[2]

$\tilde{B}\ ^2A_1$ C_{2v}
T^a = 36060(160) gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			930(100)	gas	PE	2

$\tilde{A}\ ^2B_1$ C_{2v}
T^a = 19200(160) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			840(100)	gas	PE,PI	1-3

$\tilde{X}\ ^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CS stretch	990(130)	gas	PE,PI	1-3

[a] Calculated from vertical ionization potential.

References

[1]H. W. Kroto and R. J. Suffolk, Chem. Phys. Lett. **15**, 545 (1972).
[2]B. Solouki, P. Rosmus, and H. Bock, J. Am. Chem. Soc. **98**, 6054 (1976).
[3]B. Ruscic and J. Berkowitz, J. Chem. Phys. **98**, 2568 (1993).

H_2CSe^+

$\tilde{C}\ ^2B_2$ C_{2v}
T^a = 49620(320) gas PE[1]

$\tilde{B}\ ^2A_1$ C_{2v}
T^a = 34700(320) gas PE[1]

$\tilde{A}\ ^2B_1$ C_{2v}
T^a = 17350(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CSe stretch	750T	gas	PE	1

$\tilde{X}\ ^2B_2$ C_{2v}

[a] From vertical ionization potentials.

References

[1]H. Bock, S. Aygen, P. Rosmus, B. Solouki, and E. Weissflog, Chem. Ber. **117**, 187 (1984).

t-$N_2H_2^+$

$\tilde{C}\ ^2A_g$ C_{2h}
T_0 = 53250(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	3	NNH bend	940(30)	gas	PE	1

$\tilde{B}\ ^2B_u$ C_{2h}
T_0 = 41310(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	3	NNH bend	1170(30)	gas	PE	1

$\tilde{A}\ ^2A_u$ C_{2h}
T_0 = 36390(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2	NN stretch	1110(30)	gas	PE	1

$\tilde{X}\ ^2A_g$ C_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2	NN stretch	1850T	gas	PE	1
	3	NNH bend	1180(30)	gas	PE	1

t-$N_2D_2^+$

$\tilde{B}\ ^2B_u$ C_{2h}
T_0 = 40990(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	3	NND bend	960(30)	gas	PE	1

$\tilde{A}\ ^2A_u$ C_{2h}
T_0 = 36310(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2	NN stretch	1110(30)	gas	PE	1

$\tilde{X}\ ^2A_g$ C_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	3	NND bend	1020(30)	gas	PE	1

References

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H_2BF

$\tilde{X}$ C_{2v} Structure: MW[1]
A_0 = 7.51; B_0 = 1.069; C_0 = 0.932 MW[1]

D_2BF

$\tilde{X}$ C_{2v}
A_0 = 3.753(3); B_0 = 0.888; C_0 = 0.715 MW[1]

References

[1]H. Takeo, M. Sugie, and C. Matsumura, J. Mol. Spectrosc. **158**, 201 (1993).

H_2BCl

$\tilde{X}$ C_{2v} Structure: MW[1]
A_0 = 7.61; B_0 = 0.525; C_0 = 0.490 MW[1]

D_2BCl

$\tilde{X}$ C_{2v}
A_0 = 3.83(2); B_0 = 0.440; C_0 = 0.393 MW[1]

References

[1]Y. Kawashima, H. Takeo, M. Sugie, C. Matsumura, and E. Hirota, J. Chem. Phys. **99**, 820 (1993).

H_2BBr

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	BH_2 s-stretch	2643.5	Ar	IR	1
	2	BH_2 scissors	1185.5	Ar	IR	1
	3	BBr stretch	679.0	Ar	IR	1
b_2	5	BH_2 a-stretch	2548.5	Ar	IR	1

D_2BBr

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	BD_2 s-stretch	2005.2	Ar	IR	1
	2	BD_2 scissors	906.5	Ar	IR	1
	3	BBr stretch	625.5	Ar	IR	1
b_2	5	BD_2 a-stretch	1870.0	Ar	IR	1

References

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GaH_2Cl

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	GaH_2 s-stretch	1964.6m	Ar	IR	1
	2	GaH_2 scissors	731.4vs	Ar	IR	1
	3	GaCl stretch	406.9wm	Ar	IR	1
b_1	4	OPLA	620.0ms	Ar	IR	1
b_2	5	GaH_2 a-stretch	1978.1s	Ar	IR	1
	6	GaH_2 rock	510.1wm	Ar	IR	1

GaD_2Cl

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	GaD_2 s-stretch	1408.3	Ar	IR	1
	2	GaD_2 scissors	523.6	Ar	IR	1
	3	GaCl stretch	406.4	Ar	IR	1
b_1	4	OPLA	448.9	Ar	IR	1
b_2	5	GaD_2 a-stretch	1430.4	Ar	IR	1
	6	GaD_2 rock	371.2	Ar	IR	1

References

[1]R. Köppe and H. Schnöckel, J. Chem. Soc., Dalton Trans. 3393 (1992).

H_2CN^-

Threshold for electron detachment from ground-state H_2CN^- = 4120(65) gas PE[1]

$\tilde{X}\ ^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CH_2 scissors	1400T	gas	PE	1

D_2CN^-

Threshold for electron detachment from ground-state D_2CN^- = 4020(90) gas PE[1]

$\tilde{X}\ ^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CD_2 scissors	1034T	gas	PE	1

References

[1]D. C. Cowles, M. J. Travers, J. L. Frueh, and G. B. Ellison, J. Chem. Phys. **94**, 3517 (1991); J. Chem. Phys. **95**, 3864 (1991).

H_2CS

$\tilde{E}$ $3p_z\ ^1B_2$ C_{2v}
T_0 = 55096 gas AB[8,19] $\tilde{E}$–$\tilde{X}$ 181.5 nm

$\tilde{D}$ $3p_y\ ^1A_1$ C_{2v}
T_0 = 53134 gas AB[8,19] $\tilde{D}$–$\tilde{X}$ 188.2 nm

$\tilde{C}$ $3s\ ^1B_2$ C_{2v} Structure: AB[19]
T_0 = 47110.821(9) gas AB[1,8,15,19] $\tilde{C}$–$\tilde{X}$ 212.1 nm
A_0 = 8.557; B_0 = 0.603; C_0 = 0.562 AB[19]

$\tilde{B}\ ^1A_1$ [a] C_{2v}
T_0 = 45197 gas AB[8,18] $\tilde{B}$–$\tilde{X}$ 185–215 nm
All but the first absorption band show evidence for predissociation.[18]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CS stretch	476	gas	AB	18
b_1	4	OPLA	363H	gas	AB	18

$\tilde{A}\ ^1A_2$ C_{2v} Structure: $AB^{10,21}LF^{28}$
T_0 = 16394.628(4) gas $AB^{7,9,10}LF^{24,28}$ $\tilde{A}$–$\tilde{X}$ 440–610 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	3033.4[b]	gas	AB,LF	9,28
	2	CH_2 scissors	1334.5[b]	gas	LF	28
	3	CS stretch	819.7	gas	AB,LF	7,9,28
b_1	4	OPLA	371.1	gas	AB,LF	9,28
b_2	5	CH stretch	3054.9[b]	gas	LF	28
	6	CH_2 rock	785.2	gas	LF	28

A_0 = 9.434; B_0 = 0.538; C_0 = 0.509 $AB^{10}LF^{24,28}$
τ_0 = 140(3) μs gas $LF^{22,25}$

$\bar{a}\ ^3A_2$ C_{2v} Structure: $AB^{11,21}LF^{29}$
T_0 = 14507.38 gas $AB^{7,11}LF^{20,24,29}CL^{26,30}$ $\bar{a}$–$\tilde{X}$ 610–800 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_2 scissors	1318.6	gas	AB,LF	11,29
	3	CS stretch	861.6	gas	AB,LF	11,23
b_1	4	OPLA	308(30)	gas	LF,CL	20,21, 26,30
b_2	6	CH_2 rock	762.3	gas	LF	23

A_0 = 9.383; B_0 = 0.552; C_0 = 0.521 $AB^{11}LF^{24}$
τ > 1.5 ms gas $LF^{22,25}$

$\tilde{X}\ ^1A_1$ C_{2v} Structure: $MW^{2,4,5}IR^{3,14}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	2971.03	gas	IR	3,14
			2970w	Ar	IR	6,17
			2973w	N_2	IR	6
	2	CH_2 scissors	1455.50	gas	LF,IR	13,31
			1447	Ar	IR	17
	3	CS stretch	1059.20	gas	LS,IR	12,14
			1063w	Ar	IR	6,17
			1062w	N_2	IR	6

$\tilde{X}\ ^1A_1$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_1	4	OPLA	990.19	gas	LS,IR	12,14
			993s	Ar	IR	6,17
			995s	N_2	IR	6
b_2	5	CH stretch	3024.61	gas	IR	3,14
	6	CH_2 rock	991.01	gas	LS,IR	12,14
			988m	Ar	IR	6,17

A_0 = 9.729; B_0 = 0.590; C_0 = 0.555 $MW^{2,4,5}AB^{10}IR^{31}$

D_2CS

$\tilde{C}$ 3s $^1B_2$ C_{2v}
T_0 = 47325.563(4) gas $AB^{8,19}$ $\tilde{C}$–$\tilde{X}$ 211.2 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD stretch	1783	gas	AB	8,19
	2	CD_2 scissors	746	gas	AB	19

A_0 = 4.350; B_0 = 0.510; C_0 = 0.456 AB^{19}

$\tilde{B}\ ^1A_1$ [a] C_{2v}
$T_0 \cong$ 45200 gas AB^{18} $\tilde{B}$–$\tilde{X}$ 185–215 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CS stretch	467	gas	AB	18
b_1	4	OPLA	263H	gas	AB	18

$\tilde{A}\ ^1A_2$ C_{2v}
T_0 = 16483.502(8) gas $AB^{7,9,10}$ $\tilde{A}$–$\tilde{X}$ 440–610 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD stretch	2139(2)	gas	AB	9
	2	CD_2 scissors	1013(2)	gas	AB	9
	3	CS stretch	771.3(5)	gas	AB	7,9
b_1	4	OPLA	275.33	gas	AB	9
b_2	5	CD stretch	2324.85	gas	AB	9
	6	CD_2 rock	599(2)	gas	AB	9

A_0 = 4.736; B_0 = 0.458; C_0 = 0.417 AB^{10}
τ_0 = 182 μs gas LF^{25}

$\tilde{a}\ ^3A_2$ C_{2v} Structure: AB^{21}
T_0 = 14613.54 gas $AB^{7,11}CL^{26,30}$ $\tilde{a}$–$\tilde{X}$ 610–815 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_2 scissors	1012	gas	AB,CL	11,30
	3	CS stretch	798	gas	AB,CL	7,11,30
b_1	4	OPLA	219.4(5.0)	gas	AB,CL	21,26,30
b_2	6	CD_2 rock	572.6(5.0)	gas	CL	30

A_0 = 4.716; B_0 = 0.469; C_0 = 0.426 AB^{11}

$\tilde{X}\ ^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD stretch	2158.5	gas	IR	14
			2155m	Ar	IR	17
	2	CD_2 scissors	1171.8	gas	IR	14
			1167m	N_2	IR	17
	3	CS stretch	936.13	gas	IR,LS	14,16
			941vw	Ar	IR	6,17
			939wm	N_2	IR	6
b_1	4	OPLA	781.2	gas	IR	14
			783m	Ar	IR	6,17
			784s	N_2	IR	6
b_2	6	CD_2 rock	757.4	gas	IR	14

A_0 = 4.883; B_0 = 0.497; C_0 = 0.450 $MW^2AB^{10}LF^{27}$

[a] Barrier to inversion ≅ 50.[18]
[b] From fit to combination bands.

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H_2CSe

$\tilde{A}\ ^1A_2$ C_{2v} Structure: LF[7]
$T_0 \cong 13555$ gas LF[5,6]CL[8] $\tilde{A}$-$\tilde{X}$ 685–833 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	C=Se stretch	662	gas	LF	6
b_1	4	OPLA	355T	gas	LF	6

$A^a = 9.015$; $B^a = 0.377$; $C^a = 0.360$ LF[7]

$\tilde{a}\ ^3A_2$ C_{2v}
$T_0 = 12171.0$ gas $AB^1CL^{3,8}LF^{5,6}$ $\tilde{a}$-$\tilde{X}$ 658–865 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_2 scissors	1312	gas	LF	5,6
	3	C=Se stretch	704	gas	AB,CL LF	1,3,5,6,8
b_1	4	OPLA	297[b]	gas	AB,LF	1,5,6
b_2	6	HCSe bend	812H	gas	LF	5,6

$\tilde{X}\ ^1A_1$ C_{2v} Structure: MW[2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_2 scissors	1460(30)	gas	CL	8
	3	C=Se stretch	860(10)	gas	CL	8
b_1	4	OPLA	906(10)	gas	CL	8
b_2	6	HCSe bend	914(20)	gas	CL	8

$A_0 = 9.690$; $B_0 = 0.414$; $C_0 = 0.396$ $MW^{2,4}LF^7$

D_2CSe

$\tilde{A}\ ^1A_2$ C_s
$T_0 = 13631.4$ gas LF[6] $\tilde{A}$-$\tilde{X}$ 671–734 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	C=Se stretch	619	gas	LF	6

$A_0 = 4.711$; $B_0 = 0.316$; $C_0 = 0.296$ LF[7]

$\tilde{a}\ ^3A_2$ C_{2v}
$T_0 = 12262.7$ gas LF[6] $\tilde{a}$-$\tilde{X}$ 661–815 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_2 scissors	996	gas	LF	6
	3	C=Se stretch	667	gas	LF	6
b_1	4	OPLA	208[b]	gas	LF	6
b_2	6	DCSe bend	563H	gas	LF	6

$\tilde{X}\ ^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	C=Se stretch	789T	gas	LF	6

$A_0 = 4.87(2)$; $B_0 = 0.344$; $C_0 = 0.321$ MW^4LF^7

[a] $\upsilon_4 = 1$.
[b] From fit to double minimum potential. Barrier to inversion 13.1 for H_2CSe, 16.2 for D_2CSe.[6]

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H_2SiO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Si=O stretch	1202	Ar	IR	1,2
		SiH_2 deform.	697	Ar	IR	2

D_2SiO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Si=O stretch	1189	Ar	IR	1,2
		SiD_2 deform.	533	Ar	IR	2

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HSiOH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3661	Ar	IR	1,2
	2	SiH stretch	1882[a]	Ar	IR	1,2
			1847			
	3	HSiO bend	937	Ar	IR	1,2
	4	SiO stretch	851	Ar	IR	1,2
	5	SiOH bend	723	Ar	IR	1,2
a"	6	Torsion	595	Ar	IR	1,2

DSiOD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2667	Ar	IR	2
	2	SiD stretch	1354	Ar	IR	1,2
	3	DSiO bend	715	Ar	IR	1,2
			701[b]	Ar	IR	1
	4	SiO stretch	847[b]	Ar	IR	1,2
			841	Ar	IR	1,2
	5	SiOD bend	521	Ar	IR	1,2
a"	6	Torsion	447	Ar	IR	1,2

[a] Fermi resonance splitting.
[b] Less stable rotamer, presumed to have the *cis-* structure.

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H_2GeO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		GeH_2 stretch	2079.6	Ar	IR	1
		GeH_2 stretch	2076.6	Ar	IR	1
		Ge=O stretch	961.9	Ar	IR	1
		GeH_2 scissors	803.8	Ar	IR	1

D_2GeO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		GeD_2 a-stretch	1495.7	Ar	IR	1
		GeD_2 s-stretch	1490.1	Ar	IR	1
		Ge=O stretch	963.2	Ar	IR	1
		D_2GeO wag	615.4	Ar	IR	1
		GeH_2 scissors	577	Ar	IR	1

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HGeOH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3652.0	Ar	IR	2
	2	GeH stretch	1741.3	Ar	IR	1,2
	3	GeOH bend	885.2	Ar	IR	2
	4	HGeO bend	708.7	Ar	IR	2
	5	GeO stretch	657.6	Ar	IR	1,2
a"	6	Torsion	566.2	Ar	IR	1,2

DGeOD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2695.1	Ar	IR	2
	2	GeD stretch	1257.6	Ar	IR	2
	3	GeOD bend	685.4	Ar	IR	2
	4	GeO stretch	642.0	Ar	IR	2
	5	DGeO bend	503.0	Ar	IR	2
a"	6	Torsion	420.3	Ar	IR	2

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HSnOH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	SnH stretch	1608.0	Ar	IR	1
			1597.7			
	4	HSnO bend	782.6	Ar	IR	1
	5	SnO stretch	569.3	Ar	IR	1
a"	6	Torsion	475.5	Ar	IR	1

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H_2CF^+

$\tilde{X}\ ^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF stretch	1450(30)	gas	PE	1

D_2CF^+

$\tilde{X}\ ^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF stretch	1530(30)	gas	PE	1

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[1]L. Andrews, J. M. Dyke, N. Jonathan, N. Keddar, A. Morris, and A. Ridha, J. Phys. Chem. **88**, 2364 (1984).

H_2CCl^+

$\tilde{X}\ ^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCl stretch	1040(30)	gas	PE	1,2

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H_2CBr^+

$\tilde{X}\ ^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CBr stretch	860(30)	gas	PE	1,2

D_2CBr^+

$\tilde{X}\ ^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_2 scissors	1130(30)	gas	PE	2
	3	CBr stretch	780(30)	gas	PE	2

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t–N_2H_2

$\tilde{C}\ ^1B_u$ [a] C_{2h}
T_0 = 67894 gas AB[9] $\tilde{C}$–$\tilde{X}$ 135–147 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2	Bend	1180	gas	AB	9
	3	NN stretch	1849	gas	AB	9

$\tilde{B}\ ^1B_u$ C_{2h} Structure: AB[9]
T_0 = 57926.5 gas AB[2,9] $\tilde{B}$–$\tilde{X}$ 150–175 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	NH stretch	3092	gas	AB	9
	2	Bend	1180	gas	AB	2,9
	3	NN stretch	1875	gas	AB	2,9

A_0 = 15.63; B_0 = 1.32; C_0 = 1.22 AB[9]

$\tilde{A}\ ^1B_g$ C_{2h}
T^c = 23896 gas AB[4,5,8] $\tilde{A}$–$\tilde{X}$ 300–440 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2	Bend	1215(15)	gas	AB	5
	3	NN stretch	1550(20)	gas	AB	5

$\tilde{X}\ ^1A_g$ C_{2h} Structure: IR[2,6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	NH stretch	3128	N_2	Ra	3
	2	NH bend	1583	N_2	Ra	3
	3	N=N stretch	1529	N_2	Ra	3
a_u	4	Torsion	1288.64	gas	IR	10
			1283	Ar	IR	7
			1286	N_2	IR,Ra	1,3,7
b_u	5	NH stretch	3120.28	gas	IR	2,6,10
			3118	Ar	IR	7
			3137	N_2	IR	7
	6	NH bend	1316.4i	gas	IR	10
			1313	Ar	IR	7
			1321	N_2	IR	3,7

A_0 = 10.000; B_0 = 1.304; C_0 = 1.150 IR[6,10]

t-N_2D_2

$\tilde{B}\ ^1B_u$ C_{2h}
$T_0 \cong 58086$[d] gas AB[2] $\tilde{B}$-$\tilde{X}$ 159–172 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2	Bend	950	gas	AB	2

$\tilde{A}\ ^1B_g$ C_{2h}
gas AB[5] $\tilde{A}$-$\tilde{X}$ 320–430 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2	Bend	910(10)	gas	AB	5
	3	NN stretch	1440(20)	gas	AB	5

$\tilde{X}\ ^1A_g$ C_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2	ND bend	1215	N_2	Ra	3
	3	N=N stretch	1539	N_2	Ra	3
a_u	4	Torsion	946	N_2	IR	1,3,7
b_u	5	ND stretch	2315	gas	IR	6
			2308	N_2	IR	7
	6	ND bend	972	N_2	IR	7

A_0 = 6.025; B_0 = 1.089; C_0 = 0.920 IR[6]

[a] $4p\pi$ Rydberg transition.
[b] $3p\pi$ Rydberg transition.
[c] 5_0^1 vibronic band origin.[8]
[d] 1–0 subband origin.

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H_2NN

Photolyzes on irradiation of the sample by visible light; solid solution in 2-methyltetrahydrofuran at 80 K shows structured absorption between 500 and 730 nm, with maximum near 636 nm.[1]

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NH stretch	2862.0s	Ar	IR	1,2
	2	NH_2 scissors	1644.7w	Ar	IR	2
	3	N=N stretch	1574.2m	Ar	IR	1,2
b_1	4	OPLA	1002.7vs	Ar	IR	1,2
b_2	5	NH stretch	2804.6m	Ar	IR	1,2
	6	NH_2 rock	1287.5vw	Ar	IR	2

D_2NN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ND stretch	2140.2vs	Ar	IR	2
	2	N=N stretch	1599.0wm	Ar	IR	1,2
b_1	4	OPLA	793.5ms	Ar	IR	1,2
b_2	5	ND stretch	2107.0s	Ar	IR	1,2

References

[1]A. P. Sylwester and P. B. Dervan, J. Am. Chem. Soc. **106**, 4648 (1984).
[2]J. H. Teles, G. Maier, B. A. Hess, Jr., and L. J. Schaad, Chem. Ber. **122**, 749 (1989).

H_2NO^+

$\tilde{A}\ ^1A_2$ C_{2v}
T_0 = 19280(160) gas PE[1]

$\tilde{a}\ ^3A_2$ C_{2v}
T_0 = 13720(160) gas PE[1]

$X\ ^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	NO stretch	1640(40)	gas	PE	1

D_2NO^+

$\tilde{A}\ ^1A_2$ C_{2v}
T_0 = 19440(160) gas PE[1]

$\tilde{a}\ ^3A_2$ C_{2v}
T_0 = 13880(160) gas PE[1]

$X\ ^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	NO stretch	1710(60)	gas	PE	1

References

[1]J. Baker, V. Butcher, J. M. Dyke, and A. Morris, J. Chem. Soc., Faraday Trans. **86**, 3843 (1990).

H_2CS^-

Threshold for electron detachment from ground-state H_2CS^- = 3750(185) gas PE[1,2]

$\tilde{X}$ C_{2v} Structure: PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CS stretch	860(220)	gas	PE	1,2
b_1	4	OPLA	450(120)	gas	PE	1,2

References

[1]S. Moran and G. B. Ellison, Int. J. Mass Spectrom. Ion Proc. **80**, 83 (1987).
[2]S. Moran and G. B. Ellison, J. Phys. Chem. **92**, 1794 (1988).

H_2CF

5p Rydberg state C_{2v}
T_0 = 67265(10) gas MPI[8]

4p Rydberg state C_{2v}
T_0 = 63275(10) gas MPI[8] $4p$–$\tilde{X}$ 147–158 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF stretch	1580(20)	gas	MPI	8
	3	CH_2 scissors	1443(20)	gas	MPI	8
b_1	4	OPLA	1259(20)	gas	MPI	8

3p Rydberg state C_{2v}
T_0 = 52863(10) gas MPI[8] $3p$–$\tilde{X}$ 167–193 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF stretch	1575(20)	gas	MPI	8
	3	CH_2 scissors	1420(20)	gas	MPI	8
b_1	4	OPLA	1223(20)	gas	MPI	8

Threshold for photodecomposition, producing CF, observed[5] near 280 nm in an argon matrix.

$\tilde{X}$ $^2B_1$ C_{2v} Structure: ESR[1]MW[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CF stretch	1170.42	gas	DL	7
			1163m	Ar	IR	2,3,5
b_1	4	OPLA	300(30)	gas	MW	6
			260(30)	gas	MPI	8

A_0 = 8.846; B_0 = 1.032; C_0 = 0.925 LMR[4]MW[6]

D_2CF

5p Rydberg state C_{2v}
T_0 = 67186(10) gas MPI[8]

4p Rydberg state C_{2v}
T_0 = 63195(10) gas MPI[8] $4p$–$\tilde{X}$ 154–159 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_2 s-stretch	2190(20)	gas	MPI	8
	2	CF stretch	1513(20)	gas	MPI	8
	3	CD_2 scissors	1076(20)	gas	MPI	8
b_1	4	OPLA	1004(20)	gas	MPI	8

3p Rydberg state C_{2v}
T_0 = 52786(10) gas MPI[8] $3p$–$\tilde{X}$ 167–193 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_2 s-stretch	2176(20)	gas	MPI	8
	2	CF stretch	1504(20)	gas	MPI	8
	3	CD_2 scissors	1080(20)	gas	MPI	8
b_1	4	OPLA	976(10)	gas	MPI	8

$\tilde{X}$ $^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF stretch	1191m	Ar	IR	2,3,5
	3	CD_2 scissors	1013w	Ar	IR	5
b_1	4	OPLA	170(30)	gas	MPI	8

References

[1]R. W. Fessenden and R. H. Schuler, J. Chem. Phys. **43**, 2704 (1965).
[2]M. E. Jacox and D. E. Milligan, J. Chem. Phys. **50**, 3252 (1969).
[3]J. I. Raymond and L. Andrews, J. Phys. Chem. **75**, 3235 (1971).
[4]J. A. Mucha, D. A. Jennings, K. M. Evenson, and J. T. Hougen, J. Mol. Spectrosc. **68**, 122 (1977).
[5]M. E. Jacox, Chem. Phys. **59**, 199 (1981).
[6]Y. Endo, C. Yamada, S. Saito, and E. Hirota, J. Chem. Phys. **79**, 1605 (1983).
[7]C. Yamada and E. Hirota, J. Mol. Spectrosc. **116**, 101 (1986).
[8]J. W. Hudgens, C. S. Dulcey, G. R. Long, and D. J. Bogan, J. Chem. Phys. **87**, 4546 (1987).

H_2CCl

$\tilde{X}$ C_{2v} Structure: ESR[3]MW[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_2 scissors	1391wm	Ar	IR	2
	3	CCl stretch	827s	Ar	IR	1,2
b_1	4	OPLA	402s	Ar	IR	1,2

A_0 = 9.152(3); B_0 = 0.532; C_0 = 0.502 MW[4]

D_2CCl

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_2 scissors	1045m	Ar	IR	1,2
	3	CCl stretch	788m	Ar	IR	1,2
b_1	4	OPLA	291m	Ar	IR	1,2

References

[1]M. E. Jacox and D. E. Milligan, J. Chem. Phys. **53**, 2688 (1970).
[2]L. Andrews and D. W. Smith, J. Chem. Phys. **53**, 2956 (1970).
[3]J. P. Michaut and J. Roncin, Chem. Phys. Lett. **12**, 95 (1971).
[4]Y. Endo, S. Saito, and E. Hirota, Can. J. Phys. **62**, 1347 (1984).

H_2CBr

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_2 scissors	1355.7s	Ar	IR	1,2
		CH_2 rock	953w	Ar	IR	1
		CBr stretch	693.4s	Ar	IR	1,2
		Umbrella	368vs	Ar	IR	1,2

D_2CBr

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD_2 scissors	1016.4s	Ar	IR	1,2
		CD_2 rock	708w	Ar	IR	1
		CBr stretch	656.6m	Ar	IR	1,2
		Umbrella	263vs	Ar	IR	1,2

References

[1]D. W. Smith and L. Andrews, J. Chem. Phys. **55**, 5295 (1971).
[2]L. Andrews, J. H. Miller, and E. S. Prochaska, J. Am. Chem. Soc. **101**, 7158 (1979).

H_2Cl

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3050T	gas	IR	2
		CH_2 scissors	1330T	gas	IR	2
			1331.5s	Ar	IR	1
		Cl stretch	611wm	Ar	IR	1
		Umbrella	375s	Ar	IR	1

D_2Cl

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD_2 scissors	994m	Ar	IR	1
		Cl stretch	578w	Ar	IR	1
		Umbrella	271s	Ar	IR	1

References

[1]D. W. Smith and L. Andrews, J. Chem. Phys. **58**, 5222 (1973).
[2]S. L. Baughcum and S. R. Leone, J. Chem. Phys. **72**, 6531 (1980).

H_2GeCl

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		GeH stretch	1856wm	Ar	IR	1
		GeH stretch	1810vs	Ar	IR	1
		GeH_2 scissors	734w	Ar	IR	1
		GeH_2 wag	715m	Ar	IR	1
		GeH_2 twist	685w	Ar	IR	1
		GeCl stretch	385s	Ar	IR	1

D_2GeCl

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		GeD stretch	1336w	Ar	IR	1
		GeD stretch	1304ms	Ar	IR	1
		GeD_2 scissors	533vw	Ar	IR	1
		GeD_2 wag	516w	Ar	IR	1
		GeD_2 twist	495vw	Ar	IR	1

References

[1]R. J. Isabel and W. A. Guillory, J. Chem. Phys. **55**, 1197 (1971).

H_2GeBr

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		GeH stretch	1859T	Ar	IR	1
		GeH stretch	1816s	Ar	IR	1
		GeH_2 wag	691m	Ar	IR	1
		GeH_2 twist	661wm	Ar	IR	1
		GeBr stretch	280s	Ar	IR	1

D_2GeBr

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		GeD stretch	1352s	Ar	IR	1
		GeD stretch	1339s	Ar	IR	1
		GeD_2 wag	498w	Ar	IR	1
		GeD_2 twist	472wm	Ar	IR	1
		GeBr stretch	279ms	Ar	IR	1

References

[1]R. J. Isabel and W. A. Guillory, J. Chem. Phys. **57**, 1116 (1972).

H_2NO

$\tilde{X}$ C_{2v} Structure: LMR^1MW^2
$A_0 = 10.642$; $B_0 = 1.139$; $C_0 = 1.029$ MW^2

References

[1]P. B. Davies, P. Dransfeld, F. Temps, and H. Gg. Wagner, J. Chem. Phys. **81**, 3763 (1984).
[2]H. Mikami, S. Saito, and S. Yamamoto, J. Chem. Phys. **94**, 3415 (1991).

H_2PO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		PH stretch	2275.7	Ar	IR	1
			2273.8			
		P=O stretch	1153.1	Ar	IR	1
			1151.7			
			1147.7			
		PH_2 rock	833.2	Ar	IR	1
		PH_2 wag	791.6	Ar	IR	1

D_2PO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		PD stretch	1648.2	Ar	IR	1
		P=O stretch	1147.3	Ar	IR	1
			1141.7			
			1137.7			
		PD_2 rock	628.4	Ar	IR	1
		PD_2 wag	602.9	Ar	IR	1

References

[1]R. Withnall and L. Andrews, J. Phys. Chem. **92**, 4610 (1988).

HPOH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		POH deform.	1094.4	Ar	IR	1
		HPO deform.	955.7	Ar	IR	1
		P–O stretch	817.7	Ar	IR	1
		Torsion	406.3	Ar	IR	1

DPOD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OD stretch	2689.0	Ar	IR	1
		POD deform.	821.8	Ar	IR	1
			820.2			
		P–O stretch	816.6	Ar	IR	1
		DPO deform.	710.5	Ar	IR	1
		Torsion	303	Ar	IR	1

References

[1]R. Withnall and L. Andrews, J. Phys. Chem. **92**, 4610 (1988).

NH_2F^+

$\tilde{C},\tilde{D}\ ^2A'',^2A'$ C_s
$T^a = 52300(1000)$ gas PE[1]

$\tilde{B}\ ^2A'$ C_s
$T^a = 34500(1000)$ gas PE[1]

$\tilde{A}\ ^2A''$ C_s
$T^a = 21220(160)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			550T	gas	PE	1

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			300T[b]	gas	PE	1

[a] From vertical ionization potentials.
[b] Separation characteristic of higher vibrational spacings.

References

[1]H. Baumgärtel, H.-W. Jochims, E. Rühl, H. Bock, R. Dammel, J. Minkwitz, and R. Nass, Inorg. Chem. **28**, 943 (1989).

H_2NCl^+

$\tilde{D}\ ^2A''$ C_s
T^a = 61720(560) gas PE[1,2]

$\tilde{C}\ ^2A'$ C_s
T^a = 47360(560) gas PE[1,2]

$\tilde{B}\ ^2A'$ C_s
T_0 = 26630(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	4	NCl stretch	450(40)	gas	PE	1,2

$\tilde{A}\ ^2A''$ C_s
T_0 = 16700(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH stretch	3040(40)	gas	PE	2
			970(40)	gas	PE	2
			580(40)	gas	PE	1,2

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			760(40)	gas	PE	2

[a] From vertical ionization potential.

References

[1]M. K. Livett, E. Nagy–Felsobuki, J. B. Peel, and G. D. Willett, Inorg. Chem. **17**, 1608 (1978).
[2]D. Colbourne, D. C. Frost, C. A. McDowell, and N. P. C. Westwood, J. Chem. Phys. **68**, 3574 (1978).

H_2NBr^+

$\tilde{C}\ ^2A'$ C_s
T^a = 42600(900) gas PE[1,2]

$\tilde{B}\ ^2A'$ C_s
T^a = 23960(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		NBr stretch	370(60)	gas	PE	1

$\tilde{A}\ ^2A''$ C_s
T^a = 11860(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			840(50)	gas	PE	2

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			650(50)	gas	PE	1,2

[a] From vertical ionization potential.

References

[1]E. Nagy–Felsobuki, J. B. Peel, and G. D. Willett, J. Electron Spectrosc. Relat. Phenom. **13**, 17 (1978).
[2]D. Colbourne, D. C. Frost, C. A. McDowell, and N. P. C. Westwood, Can. J. Chem. **57**, 1279 (1979).

AsH_2F

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	AsH stretch	2108	Ar	IR	1
	2	AsH_2 scissors	984	Ar	IR	1
	3	AsH_2 deform.	842w	Ar	IR	1
	4	AsF stretch	649s	Ar	IR	1
a''	5	AsH stretch	2117	Ar	IR	1

AsD_2F

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	AsD stretch	1518	Ar	IR	1
	3	AsF stretch	662s	Ar	IR	1
	4	AsD_2 deform.	606m	Ar	IR	1
a''	5	AsD stretch	1526	Ar	IR	1

References

[1]L. Andrews and T. C. McInnis, Inorg. Chem. **30**, 2990 (1991).

$HOOH^+$

$\tilde{C},\tilde{D}\ ^2A,^2B$ C_2
T^a = 55190(320) gas PE[1,2]

$\tilde{B}\ ^2A$ C_2
T^a = 38400(400) gas PE[1,2]

$\tilde{A}\ ^2A$ C_2
T^a = 16800(500) gas PE[1,2]

$\tilde{X}\ ^2B$ C_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a		Deformation	1080(50)	gas	PE	2

[a] From vertical ionization potential. The first ionization potential of HOOH is taken to equal 10.54 eV, as in Ref. 2.

References

[1]K. Osafune and K. Kimura, Chem. Phys. Lett. **25**, 47 (1974).
[2]R. S. Brown, Can. J. Chem. **53**, 3439 (1975).

$HSSH^+$

$\tilde{D}\ ^2A$ C_2
T^a = 46700(1200) gas PE[3]

$\tilde{C}\ ^2B$ C_2
T^a = 37200(400) gas PE[3]

$\tilde{B}\ ^2A$ C_2
T^a = 25900(400) gas PE[3]

$\tilde{A}\ ^2B$ C_2
T^a = 7020(400) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	3	S–S stretch	500(30)	gas	PE	2

$\tilde{X}\ ^2A$ C_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	3	S–S stretch	480(30)	gas	PE	2

[a] From vertical ionization potential.

References

[1]G. Wagner and H. Bock, Chem. Ber. **107**, 68 (1974).
[2]D. C. Frost, S. T. Lee, C. A. McDowell, and N. P. C. Westwood, J. Electron Spectrosc. Relat. Phenom. **12**, 95 (1977).
[3]B. Solouki and H. Bock, Inorg. Chem. **16**, 665 (1977).

NH_2F

$\tilde{X}$ C_s Structure: MW^2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH_2 s–stretch	3269 HF	Ar	IR	1
			3234	N_2	IR	3
	2	NH_2 scissors	1568 HF	Ar	IR	1
			1564	N_2	IR	3
	3	NH_2 wag	1244 HF	Ar	IR	1
			1241	N_2	IR	3
			1233			
	4	NF stretch	934 HF	Ar	IR	1
			891	N_2	IR	3
a"	5	NH_2 a–stretch	3346	N_2	IR	3

Barrier to inversion = 5250 MW^2
A_0 = 8.782; B_0 = 0.879; C_0 = 0.845 MW^2

ND_2F

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ND_2 s–stretch	2399 DF	Ar	IR	1
	2	ND_2 scissors	1151 DF	Ar	IR	1
	3	ND_2 wag	968 DF	Ar	IR	1
	4	NF stretch	924 DF	Ar	IR	1

A_0 = 4.612; B_0 = 0.784; C_0 = 0.726 MW^2

References

[1]L. Andrews and R. Lascola, J. Am. Chem. Soc. **109**, 6243 (1987).
[2]D. Christen, R. Minkwitz, and R. Nass, J. Am. Chem. Soc. **109**, 7020 (1987).
[3]H. Baumgärtel, H.-W. Jochims, E. Rühl, H. Bock, R. Dammel, J. Minkwitz, and R. Nass, Inorg. Chem. **28**, 943 (1989).

PH_2F

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	PH_2 s–stretch	2304	Ar	IR	1
	2	PH_2 scissors	1090	Ar	IR	1
	3	PH_2 s–deform.	934	Ar	IR	1
	4	PF stretch	795vs	Ar	IR	1
a"	5	PH_2 a–stretch	2310	Ar	IR	1

PD_2F

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	PD_2 s–stretch	1673	Ar	IR	1
	3	PF stretch	798	Ar	IR	1
	4	PD_2 s–deform.	701	Ar	IR	1
a"	5	PD_2 a–stretch	1680	Ar	IR	1

References

[1]L. Andrews and R. Withnall, Inorg. Chem. **28**, 494 (1989).

HOOH

Continuous absorption, 120–300 nm.[1,2,7,12]

$\tilde{X}$ C_2 Structure: $IR^{4,19,21}MW^{8,21}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	OH s–stretch	3617.95[a]	gas	IR,Ra	3,4,10,
			3609.8			17
			3593	Ar	Ra	11

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	OH s-bend	1393.5	gas	Ra	10
			1385	Ar	Ra	11
	3	OO stretch	877.93[a]	gas	IR	20
			865.94	gas	Ra,IR	10,20
			869	Ar	Ra	11
	4	Torsion	370.89[a]	gas	IR	6,17,18,
			254.55			19
			372br	Ar	IR	9
			264			
			378vs,br	N_2	IR	5,9
b	5	OH a-stretch	3618.84[a]	gas	IR	3,4,17
			3610.66			
			3597	Ar	IR	9
			3589			
			3587s	N_2	IR	5,9
			3582s			
	6	OH a-bend	1273.68[a]	gas	IR,DL	3,16
			1264.58			
			1277ms	Ar	IR	9
			1271vs			
			1294vs	N_2	IR	5,9

A_0 = 10.069; B_0 = 0.874; C_0 = 0.838 IR[4,17,20] MW[8,13-15]

DOOD

$\tilde{X}$ C_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	OD s-stretch	2668	gas	Ra	10
			2653.5	Ar	Ra	11
	2	OD s-bend	1029	gas	Ra	10
			1021.5	Ar	Ra	11
	3	OO stretch	867	gas	Ra	10
			871	Ar	Ra	11
	4	Torsion	251	Ar	IR	9
			286br	N_2	IR	9
b	5	OD a-stretch	2661m	gas	IR	3
			2646	Ar	IR	9
			2646	N_2	IR	9
	6	OD a-bend	947s	gas	IR	3
			951vs	Ar	IR	9
			966vs	N_2	IR	9

[a] Transitions to two lowest torsional levels associated with this fundamental are given.

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HSOH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3425w	Ar	IR	1
		HOS bend	1177m	Ar	IR	1
		SO stretch	763s	Ar	IR	1
		Torsion	445m	Ar	IR	1

DSOD

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OD stretch	2661wm	Ar	IR	1
		DOS bend	866m	Ar	IR	1
		SO stretch	775ms	Ar	IR	1
		DSO bend	737wm	Ar	IR	1
		Torsion	332wm	Ar	IR	1

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HSSH

$\tilde{X}$ C_2 Structure: MW,IR[13,14]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	SH s-stretch	2555.78	gas	IR	3,5
	3	SS stretch	514.5T	gas	IR	3
	4	Torsion	417.48	gas	IR	2,3,11
b	5	SH a-stretch	2558.64	gas	IR	1,3,5
	6	Deformation	882.0	gas	IR	1,3

A_0 = 4.899; B_0 = 0.233; C_0 = 0.232 MW[4,8,9,12]IR[10,12]

DSSD

$\tilde{X}$ C_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	4	Torsion	306	gas	IR	3
b	5	SD a-stretch	1863	gas	IR	3
	6	Deformation	646.4	gas	IR	3

A_0 = 2.550; B_0 = 0.218; C_0 = 0.218 MW[4,6,7,13]IR[13]

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6.6. Four-Atomic Monohydrides

CaCCH

$\tilde{A}\ ^2\Pi$ $C_{\infty v}$
T_0 = 15521.55 gas LF[1-3] $\tilde{A}$–$\tilde{X}$ 640–665 nm
A = 70.466 gas LF[1-3]
B_0 = 0.118 LF[2,3]

$\tilde{X}\ ^2\Sigma^+$ $C_{\infty v}$ Structure: LF[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	CaC stretch	399(10)	gas	LF	1
Π	5	CaCC bend	91(5)H	gas	LF	1

B_0 = 0.116 LF[2,3]

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SrCCH

$\tilde{A}\ ^2\Pi$ $C_{\infty v}$
T_0 = 14176(10) gas LF[1] $\tilde{A}$–$\tilde{X}$ 685–725 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	SrC stretch	354(10)	gas	LF	1

A = 275(10) gas LF[1]

$\tilde{X}\ ^2\Sigma^+$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	SrC stretch	343(10)	gas	LF	1
Π	5	SrCC bend	70(5)H	gas	LF	1

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HFe_2F

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		HFe stretch	1713.9	Ar	IR	1
		FeF stretch	651.6	Ar	IR	1

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cyc–HC_3

$\tilde{X}\ ^2B_2$ C_{2v} Structure: MW[2]
A_0 = 1.486; B_0 = 1.135; C_0 = 0.640 MW[1,3]

cyc–DC_3

$\tilde{X}\ ^2B_2$ C_{2v}
A_0 = 1.485; B_0 = 0.931; C_0 = 0.570 MW[2,3]

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HC_3

$\tilde{X}\ ^2\Pi_{1/2}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3238.0w	Ar	IR	5,6
	2	C_3 a–stretch	1832.6m 1824.7s	Ar	IR	1,5,6
	3	C_3 s–stretch	1167br 1159.8w	Ar	IR	5,6
Π	4	HCC bend	28[a]	gas	MW	4

A = 14.44 gas MW[2–4]
B_0 = 0.373 MW[2–4]

DC_3

$\tilde{X}\ ^2\Pi_{1/2}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2424.0wmT	Ar	IR	5,6
	2	C_3 a–stretch	1778.8sh 1771.5m	Ar	IR	1,5,6
	3	C_3 s–stretch	1148br 1140.4w	Ar	IR	5,6

A = 12.53 gas MW[4]
B_0 = 0.337 MW[4]

[a] $^2\Sigma^u$ component.

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HCCN

$^3\Sigma^-$?

In the gas phase, a prominent absorption band system beginning at 340 nm has been attributed[2,3] to HCCN, but has not been analyzed. An absorption band system assigned to HCCN was observed in an argon matrix between 240 and 340 nm, with band separations of approximately 1050.[4]

$\tilde{X}\ ^3\Sigma^-$ $C_{\infty v}$[a] Structure: ESR[1]MW[5–7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3246.66	gas	CC	8
			3229s	Ar	IR	4
	2	CCN a–stretch	1735s	Ar	IR	4
	3	CCN s–stretch	1178m	Ar	IR	4
Π	4	H deform.	458mT[b]	Ar	IR	4
	5	Skel. deform.	187(20)	gas	CC	8

B_0 = 0.366 MW[5,7]

DCCN

$\tilde{X}\ ^3\Sigma^-$ $C_{\infty v}$[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2424ms	Ar	IR	4
	2	CCN a–stretch	1730s	Ar	IR	4
	3	CCN s–stretch	1127w	Ar	IR	4
Π	4	CCN bend	405wmT	Ar	IR	4
	5	D deform.	318msT	Ar	IR	4

B_0 = 0.330 MW[6]

[a] Quasi–linear.[6,7]
[b] Ref. 8 attributes a gas–phase band at 383(20) to ν_4 and suggests that an argon–matrix absorption reported by Ref. 4 at 369 may, alternatively, be assigned to that fundamental. The argon–matrix absorption at 458 might then be assigned to $2\nu_5$. However, the 383(20) band lies closer to twice the 198(20) frequency determined[8] for ν_5.

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HCCO

On flash photolysis of oxazole or isoxazole (C_3H_3NO), absorption band systems appear between 367 and 340 nm and between 340 and 308 nm which have tentatively been assigned to HCCO.[1] Band separations of 1057 and 1074 were identified in the first of these transitions and of 423 and 969 in the second, with some evidence for a "hot band" at 505 in the second transition.

Analysis of the submillimeter-wave spectrum[2] indicates that HCCO possesses a low-lying excited electronic state which, together with the ground state, is derived from a Π state by Renner–Teller interaction.

$\tilde{X}\ ^2A''$ C_s Structure: MW[2,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CCO a-stretch	2022.64	gas	DL	4
			2019.5	Ar	IR	3

A_0 = 41.5(1.5); B_0 = 0.363; C_0 = 0.359 MW[2,5]

DCCO

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CCO a-stretch	1989.9	Ar	IR	3

A_0 = 21.75(12); B_0 = 0.331; C_0 = 0.325 MW[2]

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HCCS

$\tilde{A}\ ^2\Pi$ $C_{\infty v}$

T_0 = 24299.690(6) gas $AB^{1,2}EM^3LF^4$ $\tilde{A}$–$\tilde{X}$ 377–452 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	CC stretch	1843T	gas	AB	2
	3	CS stretch	740	gas	AB	1,2
Π	5	CCS bend	328H	gas	AB,EM	2,3

B_0 = 0.174 AB^2

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$ Structure: MW[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	CC stretch	2189T	gas	EM	3
	3	CS stretch	782	gas	EM	3
Π	5	CCS bend	411H	gas	EM	3

$A \cong -185$ gas MW[5]
B_0 = 0.196 AB^2MW^5

DCCS

$\tilde{A}\ ^2\Pi$ $C_{\infty v}$

T_0 = 24359 gas AB^2LF^4 $\tilde{A}$–$\tilde{X}$ 376–420 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	CC stretch	1718T	gas	AB	2
	3	CS stretch	725	gas	AB	2

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HSCC

T_0 = 27475.5 gas AB^1 330–380 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		HSC bend	1062	gas	AB	1
		C–S stretch	746	gas	AB	1
			290	gas	AB	1

$\tilde{X}$?

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			373	gas	AB	1

DSCC

T_0 = 27501.1 gas AB^1 330–380 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		DSC bend	854	gas	AB	1
		C–S stretch	650	gas	AB	1

A_0 = 2.258; B_0 = 0.225; C_0 = 0.192 AB^1

$\tilde{X}$?

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			207	gas	AB	1

A_0 = 2.936; B_0 = 0.232; C_0 = 0.215 AB^1

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$HCCF^+$

$\tilde{C}\ ^2\Sigma$ $C_{\infty v}$

T^a = 80200(1000) gas PE[2]

$\tilde{B}\ ^2\Sigma$ $C_{\infty v}$

$T^a \cong$ 54400 gas PE[1,2]

$\tilde{A}\ ^2\Pi$ $C_{\infty v}$

T^a = 52800(1000) gas PE[1,2]

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	C≡C stretch	2180(80)	gas	PE	1
	3	CF stretch	1210(80)	gas	PE	1

[a] From vertical ionization potential.

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$HC\equiv CCl^+$

$\tilde{A}\ ^2\Pi_{3/2}$ $C_{\infty v}$

T_0 = 27021.3 gas $PE^1EF^{3,4}LF^5$ $\tilde{A}$–$\tilde{X}$ 331–470 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3249.4(2)	gas	LF	5
	2	C≡C stretch	2063.8(2)	gas	LF	5
	3	CCl stretch	595.7(3)	gas	EF,LF	3–5
Π	5	CCCl bend	224	gas	EF	3

τ_1 = 17(3) ns gas EF^1; ≤ 25 ns gas $PIFCO^2$
τ_2 = 430(90) ns gas EF^1; 450(45) ns gas $PIFCO^2$
A = −400(160) gas PE^1
B_0 = 0.171 LF^5

$\tilde{X}\ ^2\Pi_{3/2}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3146T	gas	EF	3
	2	C≡C stretch	1984.5(3)	gas	EF	3,4
	3	CCl stretch	836.8(3)	gas	EF	3,4
Π	4	HCC bend	595T	gas	EF	3
	5	CCCl bend	235T	gas	EF	3

$A \cong -150$ gas PE^1
B_0 = 0.195 LF^5

$DC\equiv CCl^+$

$\tilde{A}\ ^2\Pi_{3/2}$ $C_{\infty v}$

T_0 = 26997.5 gas $EF^{3,4}LF^5$ $\tilde{A}$–$\tilde{X}$ 328–488 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2561.5(2)	gas	LF	5
	2	C≡C stretch	1919.7(2)	gas	LF	5
	3	CCl stretch	587.2(3)	gas	EF,LF	3–5
Π	5	CCCl bend	216	gas	EF	3

τ_1 = 17(3) ns gas EF^2; ≤ 30 ns gas $PIFCO^2$
τ_2 = 430(90) ns gas EF^2; 500(50) ns gas $PIFCO^2$
B_0 = 0.156 LF^5

$\tilde{X}\ ^2\Pi_{3/2}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2475T	gas	EF	3
	2	C≡C stretch	1882.0(3)	gas	EF	3,4
	3	CCl stretch	817.0(3)	gas	EF	3,4
Π	4	DCC bend	476	gas	EF	3

B_0 = 0.177 LF^5

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$HC\equiv CBr^+$

$\tilde{A}\ ^2\Pi_{3/2}$ $C_{\infty v}$ Structure: LF^3

T_0 = 20550.82(4) gas $PE^1LF^{2,3}EF^4$ $\tilde{A}$–$\tilde{X}$ 416–613 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	C≡C stretch	2051(3)	gas	LF	2
	3	CBr stretch	492(2)	gas	LF,EF	2,4
Π	4	CCH bend	629(3)	gas	LF	2
	5	CCBr bend	207(3)	gas	LF	2

τ_1 = 12(2) ns gas EF^1
τ_2 = 270(54) ns gas EF^1
A = −1610(160) gas PE^1
B_0 = 0.121 LF^3

$\tilde{X}\ ^2\Pi_{3/2}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3280(2)	gas	EF	4
	2	C≡C stretch	1931(2)	gas	EF	4
	3	CBr stretch	673(2)	gas	LF,EF	2,4
Π	4	CCH bend	618(10)	gas	EF	4
	5	CCBr bend	273(10)H	gas	EF	4

$A = -1000(160)$ gas PE[1]
$B_0 = 0.138$ LF[3]

$DC \equiv CBr^+$

$\tilde{A}\ ^2\Pi_{3/2}$ $C_{\infty v}$
$T_0 = 20546.43(4)$ gas LF[2,3]EF[4] $\tilde{A}-\tilde{X}$ 416–604 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2548(3)	gas	LF	2
	2	C≡C stretch	1939(3)	gas	LF	2
	3	CBr stretch	484(2)	gas	LF,EF	2,4
Π	4	CCD bend	488(3)	gas	LF	2
	5	CCBr bend	200(3)	gas	LF	2

$B_0 = 0.111$ LF[3]

$\tilde{X}\ ^2\Pi_{3/2}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2482(2)	gas	EF	4
	2	C≡C stretch	1866(2)	gas	EF	4
	3	CBr stretch	658(2)	gas	EF	4
Π	4	CCD bend	544(10)	gas	EF	4
	5	CCBr bend	258(10)H	gas	EF	4

$B_0 = 0.126$ LF[3]

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[3]M. A. King, J. P. Maier, L. Misev, and M. Ochsner, Can. J. Phys. **62**, 1437 (1984).
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$HC \equiv Cl^+$

$\tilde{A}\ ^2\Pi_{3/2}$ $C_{\infty v}$ Structure: LF[2]
$T_0 = 17373.94(3)$ gas PE[1]LF[2]EF[3] $\tilde{A}-\tilde{X}$ 521–750 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	C≡C stretch	1822(2)T	gas	LF	2
	3	CI stretch	407(2)	gas	LF,EF	2,3

$\tilde{A}\ ^2\Pi_{3/2}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	4	HCC bend	612(2)HT	gas	LF	2
	5	CCI bend	212	gas	EF	3

$\tau_1 = 18(4)$ ns gas EF[1]
$\tau_2 = 500(100)$ ns gas EF[1]
$A = -2020(160)$ gas PE[1]
$B_0 = 0.097$ LF[2]

$\tilde{X}\ ^2\Pi_{3/2}$ $C_{\infty v}$ Structure: LF[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3258(2)	gas	EF	3
	2	C≡C stretch	1805(10)	gas	EF	3
	3	CI stretch	578(2)	gas	EF	3
Π	4	HCC bend	542(10)H	gas	EF	3
	5	CCI bend	237(2)	gas	EF	3

$A = -3230(160)$ gas PE[1]
$B_0 = 0.110$ LF[2]

$DC \equiv Cl^+$

$\tilde{A}\ ^2\Pi_{3/2}$ $C_{\infty v}$
$T_0 = 17388.07(3)$ gas LF[2] $\tilde{A}-\tilde{X}$ 517–575 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	C≡C stretch	1792(2)T	gas	LF	2
	3	CI stretch	398(2)	gas	LF,EF	2,3
Π	4	DCC bend	480(2)H	gas	LF	2
	5	CCI bend	224(2)H	gas	LF,EF	2,3

$B_0 = 0.089$ LF[2]

$\tilde{X}\ ^2\Pi_{3/2}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2618(2)	gas	EF	3
	2	C≡C stretch	1742(10)	gas	EF	3
	3	CI stretch	563(2)	gas	EF	3
Π	5	CCI bend	223(2)	gas	EF	3

$B_0 = 0.100$ LF[2]

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[2]J. P. Maier and M. Ochsner, J. Chem. Soc., Faraday Trans. 2 **81**, 1587 (1985).
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HNCN

$\tilde{B}\ ^2A'$ C_s Structure: AB^1
T_0 = 28994.1 gas AB^1LF^2 $\tilde{B}-\tilde{X}$ 344–365 nm
τ_0 = 20(5) ns gas LF^2
A_0 = 22.30; B_0 = 0.376; C_0 = 0.369 AB^1LF^2

$\tilde{X}\ ^2A''$ C_s Structure: AB^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a''	6	NCN deform.	440T	gas	LF	2

A_0 = 21.30(2); B_0 = 0.370; C_0 = 0.362 AB^1LF^2

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HPCN

By analogy with HNCN, weak, diffuse absorption bands between 314 and 338 nm produced in the flash photolysis of PH_3–C_2N_2–N_2 mixtures have been tentatively assigned to HPCN.[1]

References

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$HNCO^+$

$\tilde{D}\ ^2\Sigma$ $C_{\infty v}$?
T^a = 61480(320) gas PE^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1000(50)	gas	PE	1

$\tilde{C}\ ^2\Sigma$ $C_{\infty v}$?
T^a = 47440(320) gas PE^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			460(50)	gas	PE	1

$\tilde{B}\ ^2\Pi$ $C_{\infty v}$?
T^a = 33730(1000) gas PE^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NCO s–stretch	1120(50)	gas	PE	1

$\tilde{A}\ ^2A'$ C_s
T^a = 5490(320) gas PE^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		NH deform.	610(50)	gas	PE	1

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	NCO a–stretch	1980(50)	gas	PE	1
	3	NCO s–stretch	1080(50)	gas	PE	1

$DNCO^+$

$\tilde{D}\ ^2\Sigma$ $C_{\infty v}$?
T^a = 61480(320) gas PE^1

$\tilde{C}\ ^2\Sigma$ $C_{\infty v}$?
T^a = 47440(320) gas PE^1

$\tilde{B}\ ^2\Pi$ $C_{\infty v}$?
T^a = 33730(1000) gas PE^1

$\tilde{A}\ ^2A'$ C_s
T^a = 5490(320) gas PE^1

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	NCO a–stretch	2070(50)	gas	PE	1

[a] From vertical ionization potentials.

References

[1]S. Cradock, E. A. V. Ebsworth, and J. D. Murdoch, J. Chem. Soc. Faraday Trans. 2 **68**, 86 (1972).

$HNCS^+$

$\tilde{C}\ ^2\Sigma$ $C_{\infty v}$?
T^a = 41790(320) gas PE^1

$\tilde{B}\ ^2\Pi$ $C_{\infty v}$?
T^a = 27190(320) gas PE^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		NCS s–stretch	850(50)	gas	PE	1

$\tilde{A}\ ^2A'$ C_s
T^a = 2900(1000) gas PE^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		NH deform.	600(50)	gas	PE	1

$\tilde{X}\ ^2A''$ C_s

[a] From vertical ionization potentials.

References

[1]S. Cradock, E. A. V. Ebsworth, and J. D. Murdoch, J. Chem. Soc., Faraday Trans. 2 **68**, 86 (1972).

HCNN

$\tilde{A}$

T_0 = 30500 gas AB[1,2,4,5] $\tilde{A}$–$\tilde{X}$ 289–328 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1048	gas	AB	4

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3233wm	Ar	IR	3
			3229m	N_2	IR	3
		CNN a–stretch	1787s	Ar	IR	3
			1784s	Kr	IR	3
			1800s	N_2	IR	3
		H deform.	861vs	Ar	IR	3
			860vs	Kr	IR	3
			871m	N_2	IR	3
			863m			

DCNN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CNN a–stretch	1771vs	Ar	IR	3
		D deform.	725vs	Ar	IR	3

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$HCNO^+$

$\tilde{C}\ ^2\Sigma^+$ $C_{\infty v}$

T_0 = 66720(1000) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3000(80)	gas	PE	1

$\tilde{B}\ ^2\Sigma^+$ $C_{\infty v}$

T_0 = 56160(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	CNO a–stretch	2420(80)	gas	PE	1
	3	CNO s–stretch	1070(80)	gas	PE	1

$\tilde{A}\ ^2\Pi$ $C_{\infty v}$

T_0 = 36070(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	CNO s–stretch	1100T	gas	PE	1

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	CNO a–stretch	1700(80)	gas	PE	1
	3	CNO s–stretch	1290(80)	gas	PE	1

References

[1]J. Bastide and J. P. Maier, Chem. Phys. **12**, 177 (1976).

HN_3^+

$\tilde{E}\ ^2A'$ C_s

T^a = 87620(1000) gas PE[3]

$\tilde{D}\ ^2A''$ C_s

T^a = 77130(1000) gas PE[2,3]

$\tilde{C}\ ^2A'$ C_s

T^a = 48890(320) gas PE[1–3]

$\tilde{B}\ ^2A'$ C_s

T_0 = 38000(320) gas PE[1–3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	N_3 a–stretch	2380(80)	gas	PE	1–3
	4	N_3 s–stretch	930(80)	gas	PE	1–3
	5	N_3 deform.	570(80)	gas	PE	1–3

$\tilde{A}\ ^2A'$ C_s
T_0 = 7750(320) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	5	N_3 deform.	480T	gas	PE	1–3

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	N_3 a–stretch	1850(80)	gas	PE	1,3
	4	N_3 s–stretch	850(80)	gas	PE	1,3

DN_3^+

$\tilde{E}\ ^2A'$ C_s
T^a = 87620(1000) gas PE[3]

$\tilde{D}\ ^2A''$ C_s
T^a = 77130(1000) gas PE[1,3]

$\tilde{C}\ ^2A'$ C_s
T^a = 48890(320) gas PE[1,3]

$\tilde{B}\ ^2A'$ C_s
T_0 = 38000(320) gas PE[1,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	N_3 a–stretch	2300(80)	gas	PE	1,3
	4	N_3 s–stretch	900(80)	gas	PE	1,3
	5	N_3 deform.	490(80)	gas	PE	1,3

$\tilde{A}\ ^2A'$ C_s
T_0 = 7750(320) gas PE[1,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	5	N_3 deform.	400T	gas	PE	3

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	N_3 a–stretch	1850(80)	gas	PE	1,3
	4	N_3 s–stretch	850(80)	gas	PE	1,3

[a] From vertical ionization potential.

References

[1]S. Cradock, E. A. V. Ebsworth, and J. D. Murdoch, J. Chem. Soc., Faraday Trans. 2 **68**, 86 (1972).
[2]T. H. Lee, R. J. Colton, M. G. White, and J. W. Rabalais, J. Am. Chem. Soc. **97**, 4845 (1975).
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HOBO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3681	Ar	IR	1
		OBO a–stretch	2023	Ar	IR	1
		HOB deform.	904	Ar	IR	1
		OBO deform.	516	Ar	IR	1
		HOB deform.	447T	Ar	IR	1

DOBO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OD stretch	2713	Ar	IR	1
		OBO a–stretch	2013	Ar	IR	1

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[1]L. Andrews and T. R. Burkholder, J. Chem. Phys. **97**, 7203 (1992).

HFC=C:

$\tilde{b}\ ^3A'$ C_s
T_0 = 10965(70) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1100(100)	gas	PE	1
			600(50)	gas	PE	1

$\tilde{a}\ ^3A''$ C_s
T_0 = 10650(70) gas PE[1]

$\tilde{X}\ ^1A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	C=C stretch	1680(30)	gas	PE	1
	4	CF stretch	960(30)	gas	PE	1
	5	CCF bend	205(30)	gas	PE	1

References

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HNCO

Between 132.5 and 120 nm, continuous absorption, with some diffuse bands.[5]

Relatively sharp absorption bands at 72940, 73910, and 74680 (137.1, 135.3, and 133.9 nm), which may be contributed by a Rydberg transition.[5]

Between 147 and 163 nm, diffuse bands are superposed on a continuum, with maximum near 157 nm.[5]

Continuous absorption between 163 and 185 nm, with a maximum near 166 nm.[5]

Continuous absorption has its onset near 41000 (244 nm), and extends beyond 200 nm.[4]

$\tilde{A}\ ^1A''$ C_s gas AB^4 $\tilde{A}-\tilde{X}$ 228–282 nm

Complicated group of progressions, possibly resulting from the occurrence of *cis*– and *trans*– rotamers in the excited state.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		NCO bend	555T	gas	AB	4

$A \cong 4.37$; $B \cong 0.388$; $C \cong 0.357$ AB^4

$\tilde{X}\ ^1A'$ C_s Structure: MW^7

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH stretch	3538.25s	gas	IR	1,2,12
						14
			3516.8wm	Ar	IR	12
			3505.7wm			
	2	NCO a–stretch	2268.89vs	gas	IR	1,2,9,10
			2259.0vs	Ar	IR	12,13
	3	NCO s–stretch	1327vw	gas	IR	1,2
	4	HNC, NCO bend	776.62wm	gas	IR	6
			769.8wm	Ar	IR	12,13
	5	HNC, NCO bend	577.35w	gas	IR	1,2,6
			573.7wm	Ar	IR	12,13
a''	6	Torsion	656.29	gas	IR	6,11

$A_0 = 30.638$; $B_0 = 0.369$; $C_0 = 0.364$ MW^7IR^{14}

DNCO

$\tilde{X}\ ^1A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ND stretch	2637.20	gas	IR	8
			2606.9m	Ar	IR	12
	2	NCO a–stretch	2235vs	gas	IR	3
			2231.0vs	Ar	IR	12
	3	NCO s–stretch	1310	gas	IR	3
	4	DNC, NCO bend	578.6w	Ar	IR	12
	5	DNC, NCO bend	475.4w	Ar	IR	12
a''	6	Torsion	602.9	gas	IR	3

$A_0 = 17.09$; $B_0 = 0.344$; $C_0 = 0.336$ MW^7

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HOCN

$\tilde{X}$ C_s Structure: MO^{2-4}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3610	Ne	IR	5
			3569.6s	Ar	IR	1,6
			3506s	N_2	IR	1
	2	C≡N stretch	2294	Ne	IR	5
			2286.3vs	Ar	IR	1,6,7
			2294s	N_2	IR	1
	3	OH deform.	1227	Ne	IR	5
			1227.9s	Ar	IR	1,6,7
			1241m	N_2	IR	1
	4	C–O stretch	1082	Ne	IR	5
			1081.3m	Ar	IR	1,6,7
			1098s	N_2	IR	1
	5	OCN deform.	460wm	N_2	IR	1

DOCN

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2635.0vs	Ar	IR	1,6
			2590sh	N_2	IR	1
	2	C≡N stretch	2284.6vs	Ar	IR	1,6
			2292s	N_2	IR	1
	3	OD deform.	1077.8ms	Ar	IR	1,6
			1093m	N_2	IR	1
	4	C–O stretch	949.4m	Ar	IR	1,6
			957m	N_2	IR	1
	5	OCN deform.	437wm	N_2	IR	1

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HCNO

$\tilde{A}$ C_s

$T_0 \leq 35053$ gas AB[8] $\tilde{A}-\tilde{X}$ 244–285 nm

Underlying absorption continuum, with increasing intensity at shorter wavelengths.[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Bend	345(5)	gas	AB	8

$\tilde{X}$ $C_{\infty v}$[a] Structure: MW,IR[13]MO[15]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3336.1	gas	IR	1,10
			3338	Ne	IR	14
			3317.2s	Ar	IR	17
			3311	N_2	IR	17
	2	CNO a–stretch	2195.8	gas	IR	1,2,10
			2200	Ne	IR	14
			2192.7vs	Ar	IR	17
			2200	N_2	IR	17
	3	CNO s–stretch	1253.4	gas	IR	1,2,10
			1250	Ne	IR	14
			1244.1m	Ar	IR	17
			1232	N_2	IR	17
Π	4	CNO bend	537.25	gas	IR	1,2,9,16
			539	Ne	IR	14
			538.2w	Ar	IR	17
			536.9w			
			528	N_2	IR	17
	5	HCN bend	224.11	gas	IR	9,11
			560	Ne	IR	17
			566.6m	Ar	IR	17
			582	N_2	IR	17

$B_0 = 0.383$ $MW^{3,4}$

DCNO

$\tilde{X}$ $C_{\infty v}$[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2620.73	gas	IR	7
			2612.7vs	Ar	IR	17
	2	CNO a–stretch	2070.92	gas	IR	12
			2063.2s	Ar	IR	17

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	3	CNO s–stretch	1254	gas	IR	2,6
			1218.5m	Ar	IR	17
Π	5	DCN bend	162.7	gas	IR	9
			418.5wm	Ar	IR	17

$B_0 = 0.343$ $MW^{3,5}IR^7$

[a] Quasilinear. See discussion in Refs. 13, 15, and 17.

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[17]J. H. Teles, G. Maier, B. A. Hess, Jr., L. J. Schaad, M. Winnewisser, and B. P. Winnewisser, Chem. Ber. **122**, 753, 1219 (1989).

HONC

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3443.7vs	Ar	IR	1,2
	2	NC stretch	2190.1wm	Ar	IR	1,2
	3	HON bend	1232.4m	Ar	IR	1,2
	4	NO stretch	628.4w	Ar	IR	1,2
	5	ONC bend	361.2w	Ar	IR	1,2
a''	6	Torsion	379.3w	Ar	IR	1,2

DONC

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2545.2vs	Ar	IR	1,2
	2	NC stretch	2190.3wm	Ar	IR	1,2
	3	DON bend	902.6m	Ar	IR	1,2
	4	NO stretch	623.1w	Ar	IR	1,2
	5	ONC bend	357.3w	Ar	IR	2
a''	6	ONC bend	362.1w	Ar	IR	1,2

References

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[2]J. H. Teles, G. Maier, B. A. Hess, Jr., L. J. Schaad, M. Winnewisser, and B. P. Winnewisser, Chem. Ber. **122**, 753 (1989).

$HOCO^+$

$\tilde{X}$ C_s Structure: MW^5

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3375.37	gas	LD	2,3
	2	OCO a-stretch	2300T	gas	PI	6
	3	OCO s-stretch	1500T	gas	PI	6

$A_0 = 26.350$; $B_0 = 0.359$; $C_0 = 0.354$ $MW^{1,4,5}LD^{2,3}$

$DOCO^+$

$\tilde{X}$ C_s

$A_0 = 14.44$; $B_0 = 0.339$; $C_0 = 0.331$ $MW^{4,5}$

References

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$HOCS^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OH stretch	3435.16	gas	LD	1

$A_0 = 26.11$; $B_0 = 0.192$; $C_0 = 0.190$ LD^1

References

[1]T. Nakanaga and T. Amano, Mol. Phys. **61**, 313 (1987).

$HONN^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OH stretch	3330.91	gas	LD	1

$A_0 = 20.88$; $B_0 = 0.377$; $C_0 = 0.370$ $LD^1MW^{2,3}$

$DONN^+$

$\tilde{X}$

$A_0 = 11.64$; $B_0 = 0.358$; $C_0 = 0.347$ MW^3

References

[1]T. Amano, Chem. Phys. Lett. **127**, 101 (1986).
[2]M. Bogey, C. Demuynck, J. L. Destombes, and A. R. W. McKellar, Astron. Astrophys. **167**, L13 (1986).
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HPCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	CO stretch	1997.8s	Ar	IR	1
	3	HPC bend	907.3w	Ar	IR	1

DPCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	CO stretch	1998.9	Ar	IR	1

References

[1]Z. Mielke and L. Andrews, Chem. Phys. Lett. **181**, 355 (1991).

HBF_2^+

$\tilde{F}$ $^2A_1$ C_{2v}

$T_0 = 57000(500)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	BF stretch	1010(40)	gas	PE	1

$\tilde{E}\ ^2A_1$ C_{2v}
T^a = 43000(800) gas PE[1]

$\tilde{D}\ ^2B_2$ C_{2v}
T_0 = 36800(560) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	BF stretch	1025(40)	gas	PE	1

$\tilde{C}\ ^2B_1$ C_{2v}
T_0 = 32280(500) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	BF stretch	950(40)	gas	PE	1

$\tilde{A},\tilde{B}\ ^2B_2,^2A_2$ C_{2v}
T_0 = 16140(1200) gas PE[1]

$\tilde{X}\ ^2A_1$ [b] C_{2v}

[a] From vertical ionization potential.
[b] Possibly dissociative.

References

[1]D. P. Chong, C. Kirby, W. M. Lau, T. Minato, and N. P. C. Westwood, Chem. Phys. **59**, 75 (1981).

$HBCl_2^+$

$\tilde{F}\ ^2A_1$ C_{2v}
T_0 = 46800(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	BH stretch	2510(40)	gas	PE	1
	2	BCl stretch	670(60)	gas	PE	1

$\tilde{E}\ ^2A_1$ C_{2v}
T_0 = 27270(560) gas PE[1]

$\tilde{D}\ ^2B_2$ C_{2v}
T_0 = 22110(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	BCl stretch	610(40)	gas	PE	1

$\tilde{C}\ ^2B_1$ C_{2v}
T_0 = 13640(320) gas PE[1]

$\tilde{A},\tilde{B}\ ^2A_1,^2A_2$ C_{2v}
T_0 = 3550(320) gas PE[1]

$\tilde{X}\ ^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	BCl stretch	860(40)	gas	PE	1

References

[1]D. C. Frost, C. Kirby, C. A. McDowell, and N. P. C. Westwood, J. Am. Chem. Soc. **103**, 4428 (1981).

$HBBr_2^+$

$\tilde{F}\ ^2A_1$ C_{2v}
$T_0 \cong$ 50700 gas PE[1]

$\tilde{E}\ ^2A_1$ C_{2v}
T_0 = 27760(320) gas PE[1]

$\tilde{D}\ ^2B_2$ C_{2v}
T_0 = 23160(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	BBr stretch	500(60)	gas	PE	1

$\tilde{C}\ ^2B_1$ C_{2v}
T_0 = 13470(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	BBr stretch	430(60)	gas	PE	1

$\tilde{B}\ ^2A_2$ C_{2v}
T_0 = 4030(320) gas PE[1]

$\tilde{A}\ ^2A_1$ C_{2v}
T_0 = 3230(320) gas PE[1]

$\tilde{X}\ ^2B_2$

References

[1]D. C. Frost, C. Kirby, C. A. McDowell, and N. P. C. Westwood, J. Am. Chem. Soc. **103**, 4428 (1981).

t-HOCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3635.70	gas	LD	7
			3631.7wm	Ne	IR	8
			3628.1wm			
			3602.9	Ar	IR	2
			3456	CO	IR	1
	2	C=O stretch	1852.57	gas	DL	4
			1848.0s	Ne	IR	8
			1843.6	Ar	IR	2
			1833	CO	IR	1
	3	HOC bend	1210.4m	Ne	IR	8
			1211.2	Ar	IR	2
			1261	CO	IR	1
	4	C–O stretch	1050.4wm	Ne	IR	8
			1064.6	Ar	IR	2
			1077	CO	IR	1
	5	OCO bend	615	CO	IR	1
a"	6	Torsion	508.1wm	Ne	IR	8
			515	Ar	IR	2

A_0 = 5.596; B_0 = 0.381; C_0 = 0.356 MW^3LMR^5

t-DOCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2684.10	gas	LD	6
			2680.7wm	Ne	IR	8
			2678.1wm			
			2558	CO	IR	1
	2	C=O stretch	1851.65	gas	DL	4
			1848.0m	Ne	IR	8
			1846.2s			
			1841.7	Ar	IR	2
			1825	CO	IR	1
	3	Mixed	1082.5m	Ne	IR	8
			1092.6	Ar	IR	2
			1117	CO	IR	1
	5	OCO bend	610m	CO	IR	1
a"	6	Torsion	472wm	CO	IR	1

A_0 = 5.160; B_0 = 0.356; C_0 = 0.333 MW^3LD^6

References

[1]D. E. Milligan and M. E. Jacox, J. Chem. Phys. **54**, 927 (1971).
[2]M. E. Jacox, J. Chem. Phys. **88**, 4598 (1988).
[3]H. E. Radford, W. Wei, and T. J. Sears, J. Chem. Phys. **97**, 3989 (1992).
[4]T. J. Sears, W. M. Fawzy, and P. M. Johnson, J. Chem. Phys. **97**, 3996 (1992).
[5]T. J. Sears, H. E. Radford, and M. A. Moore, J. Chem. Phys. **98**, 6624 (1993).
[6]J.T. Petty and C. B. Moore, J. Chem. Phys. **99**, 47 (1993).
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[8]D. Forney, W. E. Thompson, and M. E. Jacox, unpublished data.

c-HOCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3316wm	CO	IR	1
	2	C=O stretch	1797s	CO	IR	1
	3	HOC bend	1261s	CO	IR	1
	4	C–O stretch	1088s	CO	IR	1
	5	OCO bend	620m	CO	IR	1

c-DOCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2456m	CO	IR	1
	2	C=O stretch	1798s	CO	IR	1
	3	C–O stretch + DOC bend	1148s	CO	IR	1
	5	OCO bend	563w	CO	IR	1
a"	6	Torsion	497wm	CO	IR	1

References

[1]D. E. Milligan and M. E. Jacox, J. Chem. Phys. **54**, 927 (1971).

t-HSCS

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SH stretch	2527.5w	Ar	IR	1
	2	C=S stretch[a]	1275.2vs	Ar	IR	1
			1227.8s	Ar	IR	1
	3	HSC deform.	941.4s	Ar	IR	1
	4	C–S stretch	627.9wm	Ar	IR	1
a"	6	Torsion	412.9m	Ar	IR	1

t-DSCS

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SD stretch	1805.3	Ar	IR	1
	2	C=S stretch[a]	1249.7	Ar	IR	1
			1213.1	Ar	IR	1
	3	DSC deform.	713.8	Ar	IR	1
	4	C–S stretch	614.8	Ar	IR	1

[a] In Fermi resonance with $2\nu_4$.

References

[1]R. B. Bohn, G. D. Brabson, and L. Andrews, J. Phys. Chem. **96**, 1582 (1992).

HCS_2

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1252.9T	Ar	IR	1
			1004.5T	Ar	IR	1

DCS_2

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1065.5T	Ar	IR	1
			853.0T	Ar	IR	1

References

[1]R. B. Bohn, G. D. Brabson, and L. Andrews, J. Phys. Chem. **96**, 1582 (1992).

$HFC{=}C{:}^-$

Threshold for electron detachment from ground-state $HFC{=}C{:}^-$ = 13860(50) gas PE[1]

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CF stretch	710(35)	gas	PE	1
			485(30)	gas	PE	1

References

[1]M. K. Gilles, W. C. Lineberger, and K. M. Ervin, J. Am. Chem. Soc. **115**, 1031 (1993).

HFCN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CH stretch	3016	Ar	IR	1
	2	C≡N stretch	1672s	Ar	IR	1
		CF stretch	1057vs	Ar	IR	1
		FCN bend	536m	Ar	IR	1

DFCN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CD stretch	2252	Ar	IR	1
	2	C≡N stretch	1651m	Ar	IR	1
		CF stretch	1047vs	Ar	IR	1
		FCN bend	530wm	Ar	IR	1

References

[1]R. D. Hunt and L. Andrews, Inorg. Chem. **26**, 3051 (1987).

$HFCO^+$

$\tilde{D}\ ^2A'$ C_s

T^a = 55100(1000) gas PE[1]

$\tilde{C}\ ^2A''$ C_s

T_0 = 42760(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			800(50)	gas	PE	1
			580(50)	gas	PE	1

$\tilde{B}\ ^2A'$ C_s

T^a = 24850(1000) gas PE[1]

$\tilde{A}\ ^2A''$ C_s

T_0 = 12830(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1290(50)	gas	PE	1

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1450(50)	gas	PE	1
			1130(50)	gas	PE	1

[a] From vertical ionization potential.

References

[1]K. Wittel, J. Electron Spectrosc. Relat. Phenom. **8**, 245 (1976).

$HCOCl^+$

$\tilde{E}\ ^2A'$ C_s

T^a = 45900(1300) gas PE[1]

$\tilde{D}\ ^2A'$ C_s

T_0 = 38490(240) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1250(60)	gas	PE	1

$\tilde{C}\ ^2A''$ C_s

T_0 = 28720(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CO stretch	1690(30)	gas	PE	1
	4	CCl stretch	770(40)	gas	PE	1
	5	ClCO deform.	340(40)	gas	PE	1

$\tilde{B}\ ^2A'$ C_s

T^a = 7660(320) gas PE[1]

$\tilde{A}\ ^2A''$ C_s

T^a = 7020(320) gas PE[1]

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CH deform.	1390(50)	gas	PE	1
	4	CCl stretch	830(40)	gas	PE	1
	5	ClCO deform.	610(70)	gas	PE	1

[a] From vertical ionization potential.

References

[1]D. C. Frost, C. A. McDowell, and N. P. C. Westwood, Chem. Phys. Lett. **51**, 607 (1977).

$HNSO^+$

$\tilde{E}\ ^2A'$ C_s

T^a = 41310(160) gas PE[1]

$\tilde{D}\ ^2A'$ C_s

T^a = 32110(160) gas PE[1]

$\tilde{C}\ ^2A''$ C_s

T^a = 28240(160) gas PE[1]

$\tilde{B}\ ^2A'$ C_s

T^a = 7420(160) gas PE[1]

$\tilde{X},\tilde{A}\ ^2A'',^2A'$ C_s

[a] From vertical ionization potentials.

References

[1]B. Solouki, P. Rosmus, and H. Bock, Angew. Chem. **88**, 381 (1976).

$HAlCl_2$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	AlH stretch	1968s	Ar	IR	1
	2	AlCl s–stretch	481s	Ar	IR	1
b_1	4	OPLA	472s	Ar	IR	1
b_2	5	AlCl a–stretch	579m	Ar	IR	1
	6	H deformation	654vs	Ar	IR	1

$DAlCl_2$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	AlD stretch	1430	Ar	IR	1
	2	AlCl s–stretch	478	Ar	IR	1
b_1	4	OPLA	355	Ar	IR	1
b_2	6	AlCl a–stretch	598	Ar	IR	1

References

[1]H. Schnöckel, J. Mol. Struct. **50**, 275 (1978).

$HGaCl_2$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	GaH stretch	2015.3s	Ar	IR	1
	2	$GaCl_2$ s–stretch	414.3wm	Ar	IR	1
b_1	4	OPLA	464.3ms	Ar	IR	1
b_2	5	H deform.	607.5vs	Ar	IR	1
	6	$GaCl_2$ a–stretch	437.3s	Ar	IR	1

$DGaCl_2$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	GaD stretch	1450.2	Ar	IR	1
	2	$GaCl_2$ s–stretch	414.5	Ar	IR	1
b_2	5	Mixed	469.6	Ar	IR	1
	6	Mixed	420.4	Ar	IR	1

References

[1]R. Köppe, M.Tacke, and H. Schnöckel, Z. Anorg. Allg. Chem. **605**, 35 (1991).

HCOCl

$\tilde{A}\ ^1A''$ C_s

T_0 = 32754.7 gas AB[5,6] $\tilde{A}$–$\tilde{X}$ 230–314 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CO stretch	1153.8	gas	AB	5
	4	CCl stretch	633.6	gas	AB	5
	5	ClCO deform.	306.3	gas	AB	5
a''	6	Umbrella (OPLA)	779.5	gas	AB	5

Barrier to planarity = 1608.8 gas AB[5]

$\tilde{X}\ ^1A'$ C_s Structure: MW[2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	2929.18w	gas	IR	1,3,6
	2	CO stretch	1784.13vs	gas	IR	1,3,6
	3	CH bend	1307.21m	gas	IR	1,3,6,7
	4	CCl stretch	738.80vs	gas	IR	1,3,6
	5	CCl bend	458vw	gas	IR	1,6
a''	6	OPLA	932.14vw	gas	IR	1,3,6

A_0 = 2.601; B_0 = 0.205; C_0 = 0.190 MW[2,4]IR[7]

DCOCl

$\tilde{A}\ ^1A''$ C_s

T_0 = 32775.3 gas AB[5] $\tilde{A}$–$\tilde{X}$ 283–313 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CO stretch	1092.0	gas	AB	5
	4	CCl stretch	633.4	gas	AB	5
	5	ClCO deform.	303.1	gas	AB	5
a''	6	Umbrella (OPLA)	566.5	gas	AB	5

$\tilde{X}\ ^1A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CD stretch	2215.0	gas	IR	4
	2	CO stretch	1748.5	gas	IR	4
	3	CD bend	986.2	gas	IR	4
	4	CCl stretch	700.4	gas	IR	4

A_0 = 1.904; B_0 = 0.203; C_0 = 0.184 MW[2,4]

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HCOBr

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	2911.9	gas	IR	1
	2	CO stretch	1797.9[a]	gas	IR	1
	3	H deform.	1270.9[b]	gas	IR	1
	4	CBr stretch	646.3	gas	IR	1
a''	6	OPLA	893.4	gas	IR	1

DCOBr

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CD stretch	2205.4	gas	IR	1
	2	CO stretch	1748.3	gas	IR	1
	3	D deform.	975.5[c]	gas	IR	1
	4	CBr stretch	605.2	gas	IR	1
	5	CBr deform.	358T	gas	IR	1
a''	6	OPLA	746.8	gas	IR	1

[a] Uncorrected for Fermi resonance with $2\nu_6$.
[b] Uncorrected for Fermi resonance with $2\nu_4$.
[c] Uncorrected for Fermi resonance with $(\nu_4 + \nu_5)$.

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[1]G. Yarwood, H. Niki, and P. D. Maker, J. Phys. Chem. **95**, 4773 (1991).

HCF_2^+

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	5	CF_2 stretch	1608s 1605s	Ar	IR	1

DCF_2^+

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	5	CF_2 stretch	1599s 1596s	Ar Ar	IR IR	1 1

References

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$HCFCl^+$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CF stretch	1436m 1430m	Ar	IR	1
		CH deform.	1296wm	Ar	IR	1
		CCl stretch	920(40)	gas	PE	2

$DCFCl^+$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CF stretch	1414m 1406m	Ar	IR	1

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[2]L. Andrews, J. M. Dyke, N. Jonathan, N. Keddar, and A. Morris, J. Am. Chem. Soc. **106**, 299 (1984).

$HCFBr^+$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CF stretch	1401s	Ar	IR	1
		CH deform.	1149m	Ar	IR	1

References

[1]F. T. Prochaska and L. Andrews, J. Chem. Phys. **73**, 2651 (1980).

$HCFI^+$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CF stretch	1359m	Ar	IR	1

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$HCCl_2^+$

A broad, unstructured absorption observed near 250 nm in argon–matrix experiments[2] in which infrared absorptions of $HCCl_2^+$ are prominent has been attributed to an excited state of $HCCl_2^+$ which can undergo proton transfer to the matrix.

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	3032.8w	Ar	IR	3
	2	CCl stretch	860(30)	gas	PE	4,5
			845w	Ar	IR	3
b_2	5	H deformation	1291m	Ar	IR	1–3
	6	CCl stretch	1044s	Ar	IR	1–3

$DCCl_2^+$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCl stretch	790(30)	gas	PE	4,5
b_2	5	CCl stretch	1122s	Ar	IR	1,2
	6	D deformation	864wm	Ar	IR	1,2

References

[1]M. E. Jacox and D. E. Milligan, J. Chem. Phys. **54**, 3935 (1971).
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$HCClBr^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CCl stretch	994m	Ar	IR	1

$DCClBr^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1077s	Ar	IR	1

References

[1]L. Andrews, C. A. Wight, F. T. Prochaska, S. A. McDonald, and B. S. Ault, J. Mol. Spectrosc. **73**, 120 (1978).

$HCBr_2^+$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	5	H deformation	1229m	Ar	IR	1,2
	6	CBr stretch	897vs	Ar	IR	1–3

$DCBr_2^+$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	5	D deformation	1015vs	Ar	IR	1,2
	6	CBr stretch	781s	Ar	IR	1,2

References

[1]L. Andrews, C. A. Wight, F. T. Prochaska, S. A. McDonald, and B. S. Ault, J. Mol. Spectrosc. **73**, 120 (1978).
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HClSi=S

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SiH stretch	2199.9wm	Ar	IR	1
	2	HSiCl deform.	836.0s	Ar	IR	1
	3	SiS stretch	755.0wm	Ar	IR	1
	4	SiCl stretch	525.5wm	Ar	IR	1

DClSi=S

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SiD stretch	1603.1	Ar	IR	1
	2	SiS stretch	775.7	Ar	IR	1
	3	DSiCl deform.	581.0	Ar	IR	1
	4	SiCl stretch	516.4	Ar	IR	1

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[1]R. Köppe and H. Schnöckel, Z. Anorg. Allg. Chem. **607**, 41 (1992).

t–HONO

$\tilde{B}$

An intense, unstructured absorption between 200 and 275 nm, with a maximum near 46500 (215 nm), has been attributed[13] to HONO.

$\tilde{A}$ $^1A''$ C_s

T_0 = 26034 gas AB[1–3,6] $\tilde{A}$–$\tilde{X}$ 315–385 nm

Diffuse bands; predissociated into OH + NO.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		NO stretch	1117	gas	AB	6

$\tilde{X}$ $^1A'$ C_s Structure: MW[9,11,12]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3590.71m	gas	IR	4,5,8,16 17,21
			3558	N_2	IR	7
	2	N=O stretch	1699.76s	gas	IR,LS DL	4,5,8,14 16–18,23
			1688.0	Ar	IR	10,20
			1684	N_2	IR	7
	3	HON bend	1263.21s	gas	IR,DL	4,5,8,16 17,19,23
			1298	N_2	IR	7
	4	O–N stretch	790.12s	gas	IR	4,5,8,16 17,22
			795.1	Ar	IR	10,20
			815	N_2	IR	7
	5	ONO bend	595.6s	gas	IR	4,5,8,17
			625	N_2	IR	7
a''	6	Torsion	543.0m	gas	IR	4,5,8,17
			550	Ar	IR	10
			583	N_2	IR	7

A_0 = 3.099; B_0 = 0.418; C_0 = 0.367 MW[9,11,15]IR[21]

t–DONO

$\tilde{A}$ $^1A''$ C_s

T_0 = 26050(10) gas AB[2,3,6] $\tilde{A}$–$\tilde{X}$ 315–385 nm

Diffuse bands; predissociated into OD + NO.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		NO stretch	1147(20)	gas	AB	6

$\tilde{X}$ $^1A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2651.13	gas	IR	4,5,8,17
			2620	N_2	IR	7
	2	N=O stretch	1693.98	gas	IR	4,5,8,17
			1682	N_2	IR	7
	3	DON bend	1012.68	gas	IR	4,5,8,17
			1030	N_2	IR	7
	4	O–N stretch	736.27	gas	IR	4,5,8,17
			769	N_2	IR	7
	5	ONO bend	590.4	gas	IR	4,5,8,17
			618	N_2	IR	7
a''	6	Torsion	416.1	gas	IR	4,8,17
			444	N_2	IR	7

A_0 = 2.981; B_0 = 0.389; C_0 = 0.344 MW[9,11]

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[9]A. P. Cox and R. L. Kuczkowski, J. Am. Chem. Soc. **88**, 5071 (1966).
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[19]A. G. Maki, J. Mol. Spectrosc. **127**, 104 (1988).
[20]J. N. Crowley and J. R. Sodeau, J. Phys. Chem. **93**, 4785 (1989).
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c–HONO

$\tilde{B}$

An intense, unstructured absorption between 200 and 275 nm, with a maximum near 46500 (215 nm), has been attributed[13] to HONO.

$\tilde{A}\ ^1A''$ C_s

T_0 = 26320 gas AB[1–3,6] $\tilde{A}$–$\tilde{X}$ 315–385 nm

Diffuse bands; predissociated into OH + NO.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		NO stretch	1107	gas	AB	6

$\tilde{X}\ ^1A'$ C_s Structure: MW[10,11]

141(35) higher in energy than t–HONO ($\tilde{X}$). MW[12]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3426.20w	gas	IR	4,5,8,16 17,21
			3412	Ar	IR	9
			3410	N_2	IR	7
	2	N=O stretch	1640.52m	gas	IR,LS	4,5,8,14 16,21
			1632.6	Ar	IR	9,19
			1633	N_2	IR	7
	3	HON bend	1261w	gas	IR	8
			1263.3	Ar	IR	9,19

$\tilde{X}\ ^1A'$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	4	O–N stretch	851.94s	gas	IR,DL	4,5,8 16–18,20
			849.6	Ar	IR	9,19
			865	N_2	IR	7
	5	ONO bend	609.0w	gas	IR	8,17
			608	Ar	IR	9,19
a''	6	Torsion	638.5m	gas	IR	4,5,8,17
			637	Ar	IR	9,19
			658	N_2	IR	7

A_0 = 2.805; B_0 = 0.439; C_0 = 0.379 MW[10,15]DL[18]IR[21]

c–DONO

$\tilde{A}\ ^1A''$ C_s

gas AB[2,3] $\tilde{A}$–$\tilde{X}$ 315–385 nm

Diffuse bands; predissociated into OD + NO.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	4	O–N stretch	660T	gas	AB	6

$\tilde{X}\ ^1A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2525	gas	IR	4,5,8
			2518	N_2	IR	7
	2	N=O stretch	1625	gas	IR	5,8
			1612	N_2	IR	7
	3	DON bend	1008	gas	IR	8
	4	O–N stretch	813.50	gas	IR	4,5,8,17
			828	N_2	IR	7
	5	ONO bend	601	gas	IR	8
a''	6	Torsion	508.2	gas	IR	4,8,17
			522	N_2	IR	7

A_0 = 2.362; B_0 = 0.430; C_0 = 0.363 MW[10]

References

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[3]G. Porter, J. Chem. Phys. **19**, 1278 (1951).
[4]L. H. Jones, R. M. Badger, and G. E. Moore, J. Chem. Phys. **19**, 1599 (1951).
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[6]G. W. King and D. Moule, Can. J. Chem. **40**, 2057 (1962).
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[16]R. H. Kagann and A. G. Maki, J. Quant. Spectrosc. Radiat. Transfer **30**, 37 (1983).
[17]C. M. Deeley and I. M. Mills, J. Mol. Struct. **100**, 199 (1983).
[18]A. G. Maki and R. L. Sams, J. Mol. Struct. **100**, 215 (1983).
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[20]I. Kleiner, J. M. Guilmot, M. Carleer, and M. Herman, J. Mol. Spectrosc. **149**, 341 (1991).
[21]J.-M. Guilmot, F. Mélen, and M. Herman, J. Mol. Spectrosc. **160**, 401 (1993).

c–HOPO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3550.7	Ar	IR	1
	2	P=O stretch	1252.6	Ar	IR	1
	4	P–O stretch	841.5	Ar	IR	1
a"	6	Torsion	523.9	Ar	IR	1

c–DOPO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2620.4	Ar	IR	1
	2	P=O stretch	1253.0	Ar	IR	1

References

[1]R. Withnall and L. Andrews, J. Phys. Chem. **92**, 4610 (1988).

t–HONS

Threshold for photoisomerization into t–HSNO < 16400.[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3528.0	Ar	IR	1
	2	HON bend	1363.3	Ar	IR	1
	3	NS stretch	969.5	Ar	IR	1
	4	NO stretch	842.1	Ar	IR	1
	5	ONS bend	476.5	Ar	IR	1
a"	6	Torsion	531.3	Ar	IR	1

t–DONS

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2608.0	Ar	IR	1
	2	DON bend	1103.0	Ar	IR	1
	3	NS stretch	951.8	Ar	IR	1
	4	NO stretch	783.0	Ar	IR	1
	5	ONS bend	465.5	Ar	IR	1

References

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c–HSNO

In an argon matrix, conversion[2] to t–HSNO and photolysis[1,2] to SNO occur on exposure of the sample to 250 nm radiation.

In an argon matrix, slow conversion to t–HSNO occurs on prolonged exposure of the sample to infrared radiation with $\lambda \geq 2$ μ.[2]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SH stretch	2566vw	Ar	IR	2
	2	NO stretch	1570vs	Ar	IR	1,2
	3	HSN bend	858.5m	Ar	IR	2
	4	SN stretch	503m[a]	Ar	IR	1,2
	5	SNO bend	307wm	Ar	IR	2
a"	6	Torsion	406.5w	Ar	IR	2

c–DSNO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	NO stretch	1568vs	Ar	IR	2
	3	DNS bend	715	Ar	IR	2
	4	SN stretch	435	Ar	IR	2
	5	SNO bend	305.5	Ar	IR	2

[a] Assigned in Ref. 1 to the *trans*– rotamer.

References

[1]P. O. Tchir and R. D. Spratley, Can. J. Chem. **53**, 2318 (1975).
[2]R. P. Müller, M. Nonella, P. Russegger, and J. R. Huber, Chem. Phys. **87**, 351 (1984).

t–HSNO

In an argon matrix, converted to c–HSNO by irradiation at 585 nm.[2]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SH stretch	2613vw 2607vw	Ar	IR	2
	2	NO stretch	1596vs	Ar	IR	1,2
	3	HSN bend	877.5m	Ar	IR	1,2
	4	SN stretch	543.5m	Ar	IR	1,2
	5	SNO bend	297m	Ar	IR	1,2
a"	6	Torsion	386.5w	Ar	IR	2

t–DSNO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	NO stretch	1595vs	Ar	IR	1,2
	3	DSN bend	724m	Ar	IR	1,2
	4	SN stretch	485.5m	Ar	IR	1,2
	5	SNO bend	297m	Ar	IR	1,2

References

[1]P. O. Tchir and R. D. Spratley, Can. J. Chem. **53**, 2318 (1975).
[2]R. P. Müller, M. Nonella, P. Russegger, and J. R. Huber, Chem. Phys. **87**, 351 (1984).

c–HNSO [a]

gas AB^3 238–269 nm

Diffuse absorption merges into continuum with maximum near 217 nm.[3]

Photolysis in an argon matrix by 254 nm radiation leads to rapid formation of *c*–HOSN.[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	5	NSO bend	285T	gas	AB	3

$\tilde{a}$ $^3A'$ [b] C_s

Weak, unstructured absorption 325–350 nm.[3]

In an argon matrix, converted to *t*–HNSO by irradiation at wavelengths longer than 300 nm.[6]

$\tilde{X}$ $^1A'$ C_s Structure: MW[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH stretch	3345w	gas	IR	1
			3308wm	Ar	IR	3,4
			3303	N_2	IR	4
	2	SO stretch	1261s	gas	IR	1
			1249vs	Ar	IR	3,4
			1252	N_2	IR	4
	3	NS stretch	1090w	gas	IR	1
			1083s	Ar	IR	3,4
			1094	N_2	IR	4
	4	HNS bend	911m	gas	IR	1
			900s	Ar	IR	3,4
			923	N_2	IR	4
	5	NSO bend	453m	gas	IR	1
			447s	Ar	IR	3,4
			455	N_2	IR	4
a"	6	Torsion	759s	gas	IR	1
			755vs	Ar	IR	3,4
			774	N_2	IR	4

c–DNSO

gas AB^3 242–264 nm

Diffuse, merges into continuum.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	5	NSO bend	285T	gas	AB	3

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ND stretch	2480w	gas	IR	1
			2453	Ar	IR	3,4
	2	SO stretch	1257s	gas	IR	1
			1245	Ar	IR	3,4
	3	NS stretch	1055w	gas	IR	1
			1048	Ar	IR	3,4
	4	DNS bend	757m	gas	IR	1
			752	Ar	IR	3,4
	5	NSO bend	410mT	gas	IR	1
			400	Ar	IR	3,4
a"	6	Torsion	594s	gas	IR	1
			594	Ar	IR	3,4

[a] Stable rotamer.
[b] Tentative assignment.

References

[1]H. Richert, Z. Anorg. Allg. Chem. **309**, 171 (1961).
[2]W. H. Kirchhoff, J. Am. Chem. Soc. **91**, 2437 (1969).
[3]J. M. Allegretti and A. J. Merer, Can. J. Phys. **50**, 404 (1972).
[4]P. O. Tchir and R. D. Spratley, Can. J. Chem. **53**, 2311 (1975).
[5]P. O. Tchir and R. D. Spratley, Can. J. Chem. **53**, 2318 (1975).
[6]P. O. Tchir and R. D. Spratley, Can. J. Chem. **53**, 2331 (1975).

t–HNSO

In an argon matrix, prolonged photolysis of *c*–HNSO samples with 340 nm radiation, the condition under which *t*–HNSO is formed,[1] leads to the formation of *c*– and *t*–HSNO.[2]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	SO stretch	1382	Ar	IR	1
	3	NS stretch	986	Ar	IR	1
	4	HNS bend	881	Ar	IR	1
a"	6	Torsion	651	Ar	IR	1

t–DNSO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	2	SO stretch	1380	Ar	IR	1
	3	NS stretch	951	Ar	IR	1

References

[1]P. O. Tchir and R. D. Spratley, Can. J. Chem. **53**, 2331 (1975).
[2]R. P. Müller, M. Nonella, P. Russegger, and J. R. Huber, Chem. Phys. **87**, 351 (1984).

c–HOSN

Photolyzes in an argon matrix on prolonged exposure of the sample to 254–nm radiation, producing *c*– and *t*–HSNO.[1,2]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	OH stretch	3520m	Ar	IR	1
	2	SN stretch	1321w	Ar	IR	1
	3	HOS bend	992w	Ar	IR	1
	4	SO stretch	674vs	Ar	IR	1
	5	OSN bend	374	Ar	IR	1
a″	6	Torsion	418m	Ar	IR	1

c–DOSN

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	OD stretch	2597m	Ar	IR	1
	2	SN stretch	1319w	Ar	IR	1
	4	SO stretch	671vs	Ar	IR	1
a″	6	Torsion	325m	Ar	IR	1

References

[1]P. O. Tchir and R. D. Spratley, Can. J. Chem. **53**, 2318 (1975).
[2]R. P. Müller, M. Nonella, P. Russegger, and J. R. Huber, Chem. Phys. **87**, 351 (1984).

HCF_2

$\tilde{F}$ ***3p Rydberg state*** C_{2v}
T_0 = 49312(10) gas MPI[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF stretch	1365(8)	gas	MPI	4
	3	CF_2 scissors	660(20)	gas	MPI	4
b_1	4	OPLA	1022(1)	gas	MPI	4

$\tilde{X}$ C_s Structure: ESR[1]MPI[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	2	CF s–stretch	1164s	Ar	IR	2,3
	3	Umbrella	949(10)	gas	MPI	4
a″	5	HCF deform.	1317m	Ar	IR	2,3
	6	CF a–stretch	1173vs	Ar	IR	2,3

Barrier to inversion = 2800(500) gas MPI[4]

DCF_2

$\tilde{F}$ ***3p Rydberg state*** C_{2v}
T_0 = 49323(10) gas MPI[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF stretch	1300(21)	gas	MPI	4
	3	CF_2 scissors	650(15)	gas	MPI	4
b_1	4	OPLA	864(2)	gas	MPI	4

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	2	CF s–stretch	1143m	Ar	IR	2,3
	3	Umbrella	794(4)	gas	MPI	4
a″	5	CF a–stretch	1214s	Ar	IR	2,3
	6	DCF deform.	933wm	Ar	IR	2,3

References

[1]R. W. Fessenden and R. H. Schuler, J. Chem. Phys. **43**, 2704 (1965).
[2]T. G. Carver and L. Andrews, J. Chem. Phys. **50**, 5100 (1969).
[3]M. E. Jacox, J. Mol. Spectrosc. **81**, 349 (1980).
[4]D. V. Dearden, J. W. Hudgens, R. D. Johnson III, B. P. Tsai, and S. A. Kafafi, J. Phys. Chem. **96**, 585 (1992).

HCFCl

$\tilde{J}$ ***3d Rydberg state*** C_s
T_0 = 55250(20) gas MPI[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	3	CH deform.	1280(30)	gas	MPI	3
	4	CCl stretch	910(30)	gas	MPI	3
	5	FCCl scissors	440(30)	gas	MPI	3
a″	6	OPLA	980(30)	gas	MPI	3

F* 3p *Rydberg state C_s

T_0 = 49160(20) gas MPI[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CH deform.	1280(30)	gas	MPI	3
	4	CCl stretch	910(30)	gas	MPI	3
	5	FCCl scissors	440(30)	gas	MPI	3
a''	6	OPLA	980(30)	gas	MPI	3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	H deform.	1283s	Ar	IR	1
	3	CF stretch	1151s	Ar	IR	1
	4	CCl stretch	757m	Ar	IR	1
	6	Umbrella	540(30)	gas	MPI	3

Barrier to inversion = 1190 gas MPI[3]

DCFCl

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1154s	Ar	IR	1
		CD deform.	960m	Ar	IR	1,2

References

[1]F. T. Prochaska, B. W. Keelan, and L. Andrews, J. Mol. Spectrosc. **76**, 142 (1979).
[2]F. T. Prochaska and L. Andrews, J. Chem. Phys. **73**, 2651 (1980).
[3]J. W. Hudgens, R. D. Johnson III, and B. P. Tsai, J. Chem. Phys. **98**, 1925 (1993).

HCFBr

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		H deform.	1266m	Ar	IR	1,2
		CF stretch	1149s	Ar	IR	1,2
		CBr stretch	650wmT	Ar	IR	1

DCFBr

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1162s	Ar	IR	1
		D deform.	913m	Ar	IR	1

References

[1]F. T. Prochaska, B. W. Keelan, and L. Andrews, J. Mol. Spectrosc. **76**, 142 (1979).
[2]F. T. Prochaska and L. Andrews, J. Chem. Phys. **73**, 2651 (1980).

HCFI

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		H deform.	1256s	Ar	IR	1,2
		CF stretch	1138s	Ar	IR	1,2
		CI stretch	560m	Ar	IR	1,2

References

[1]F. T. Prochaska, B. W. Keelan, and L. Andrews, J. Mol. Spectrosc. **76**, 142 (1979).
[2]F. T. Prochaska and L. Andrews, J. Chem. Phys. **73**, 2651 (1980).

$HCCl_2$

3d Rydberg state C_{2v}

T_0 = 54024(10) gas MPI[3] $3d$–$\tilde{X}$ 179–185 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCl_2 s–stretch	845(10)	gas	MPI	3

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	5	HCCl deform.	1226m	Ar	IR	1
	6	CCl_2 a–stretch	902vs	Ar	IR	1

$DCCl_2$

3d Rydberg state C_{2v}

T_0 = 53980(10) gas MPI[3] $3d$–$\tilde{X}$ 180–185 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCl_2 s–stretch	814(10)	gas	MPI	3

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	5	DCCl deform.	974vs	Ar	IR	1,2
	6	CCl_2 a–stretch	814s	Ar	IR	1,2

References

[1]T. G. Carver and L. Andrews, J. Chem. Phys. **50**, 4235 (1969).
[2]E. E. Rogers, S. Abramowitz, M. E. Jacox, and D. E. Milligan, J. Chem. Phys. **52**, 2198 (1970).
[3]G. R. Long and J. W. Hudgens, J. Phys. Chem. **91**, 5870 (1987).

HCClBr

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	H deformation	1196m	Ar	IR	1
	3	CCl stretch	866s	Ar	IR	1

References

[1]T. G. Carver and L. Andrews, J. Chem. Phys. **50**, 4235 (1969).

$HCBr_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CBr s–stretch	633wm	Ar	IR	1
a''	5	HCBr deform.	1165s	Ar	IR	1–4
	6	CBr a–stretch	778vs	Ar	IR	1–5

$DCBr_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CBr s–stretch	616w	Ar	IR	1
a''	5	DCBr deform.	898vs	Ar	IR	1,3,4
	6	CBr a–stretch	725s	Ar	IR	1,3,4

References

[1]T. G. Carver and L. Andrews, J. Chem. Phys. **50**, 4223 (1969).
[2]E. E. Rogers, S. Abramowitz, M. E. Jacox, and D. E. Milligan, J. Chem. Phys. **52**, 2198 (1970).
[3]L. Andrews, C. A. Wight, F. T. Prochaska, S. A. McDonald, and B. S. Ault, J. Mol. Spectrosc. **73**, 120 (1978).
[4]L. Andrews, F. T. Prochaska, and B. S. Ault, J. Am. Chem. Soc. **101**, 9 (1979).
[5]B. J. Kelsall and L. Andrews, J. Mol. Spectrosc. **97**, 362 (1983).

HCl_2

$\tilde{X}$ C_s (C_{2v} ?)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	5	HCl deform.	1106	Ar	IR	1
	6	Cl stretch	716	Ar	IR	1

DCl_2

$\tilde{X}$ C_s (C_{2v} ?)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	5	DCl deform.	850	Ar	IR	1
	6	Cl stretch	653	Ar	IR	1

References

[1]D. W. Smith and L. Andrews, J. Phys. Chem. **76**, 2718 (1972).

HNF_2^+

$\tilde{F}\ ^2A'$ C_s
T_e^a = 66480(1100) gas PE[1]

$\tilde{E}\ ^2A''$ C_s
T_e^a = 60270(1450) gas PE[1]

$\tilde{D}\ ^2A'$ C_s
T_e^a = 52280(1100) gas PE[1]

$\tilde{C}\ ^2A''$ C_s
T_e^a = 35900(900) gas PE[1]

$\tilde{B}\ ^2A'$ C_s
T_e^a = 32350(900) gas PE[1]

$\tilde{A}\ ^2A''$ C_s
T_e^a = 31220(1450) gas PE[1]

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	4	NF_2 scissors	580(30)	gas	PE	1

DNF_2^+

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	4	NF_2 scissors	530(30)	gas	PE	1

[a] From vertical ionization potential.

References

[1]D. Colbourne, D. C. Frost, C. A. McDowell, and N. P. C. Westwood, Chem. Phys. Lett. **72**, 247 (1980).

$HNCl_2^+$

$\tilde{F}\ ^2A'$ C_s
T^a = 59800(560) gas PE[1,2]

$\tilde{E}\ ^2A''$ C_s
T^a = 49460(560) gas PE[1,2]

$\tilde{D}\ ^2A'$ C_s
T^a = 37030(560) gas PE[1,2]

$\tilde{C}\ ^2A''$ C_s
T^a = 20330(800) gas PE[1,2]

$\tilde{B}\ ^2A'$ C_s
T^a = 19450(560) gas PE[1,2]

$\tilde{A}\ ^2A''$ C_s
T^a = 15330(560) gas PE[1,2]

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			560(50)	gas	PE	1

[a] From vertical ionization potential.

References

[1]M. K. Livett, E. Nagy-Felsobuki, J. B. Peel, and G. D. Willett, Inorg. Chem. **17**, 1608 (1978).
[2]D. Colbourne, D. C. Frost, C. A. McDowell, and N. P. C. Westwood, J. Chem. Phys. **69**, 1078 (1978).

$HNBr_2^+$

$\tilde{F}\ ^2A'$ C_s
T^a = 53250(2000) gas PE[1]

$\tilde{E}\ ^2A''$ C_s
T^a = 41150(2000) gas PE[1]

$\tilde{D}\ ^2A'$ C_s
T^a = 21800(2000) gas PE[1]

$\tilde{C}\ ^2A'$ C_s
T^a = 11860(1000) gas PE[1,2]

$\tilde{B}\ ^2A''$ C_s
T^a = 10730(1000) gas PE[1,2]

$\tilde{A}\ ^2A''$ C_s
T^a = 7260(2000) gas PE[1]

$\tilde{X}\ ^2A'$ C_s

[a] From vertical ionization potentials.

References

[1]E. Nagy-Felsobuki and J. B. Peel, J. Electron Spectrosc. Relat. Phenom. **15**, 61 (1979).
[2]D. Colbourne, D. C. Frost, C. A. McDowell, and N. P. C. Westwood, Can. J. Chem. **57**, 1279 (1979).

HPF_2^+

$\tilde{G}\ ^2A'$ C_s
T^a = 58900(1600) gas PE[1,2]

$\tilde{F}\ ^2A'$ C_s
T^a = 53250(1600) gas PE[1,2]

$\tilde{B},\tilde{C},\tilde{D},\tilde{E}\ ^2A'',^2A'',^2A',^2A''$ C_s
T^a = 38700(1600) gas PE[1,2]

$\tilde{A}\ ^2A'$ C_s
T^a = 33100(1600) gas PE[1,2]

$\tilde{X}\ ^2A'$ C_s

[a] From vertical ionization potentials.

References

[1]S. Cradock and D. W. H. Rankin, J. Chem. Soc., Faraday Trans. 2 **68**, 940 (1972).
[2]A. H. Cowley, R. A. Kemp, M. Lattman, and M. L. McKee, Inorg. Chem. **21**, 85 (1982).

$HAsF_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		AsH stretch	2099	Ar	IR	1
		AsF stretch	668T	Ar	IR	1

$DAsF_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		AsD stretch	1513	Ar	IR	1
		AsF stretch	668T	Ar	IR	1

References

[1]L. Andrews and T. C. McInnis, Inorg. Chem. **30**, 2990 (1991).

6.7. Four–Atomic Nonhydrides

Li_4

$2\,^1B_{1u}$ D_{2h}
T^a = 23618 gas DPI[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			145T	gas	DPI	1

$2\,^1B_{2u}$ D_{2h}
T^a = 21386 gas DPI[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			210	gas	DPI	1

$2\,^1B_{3u}$ D_{2h}
T^a = 16807 gas DPI[1]

$1\,^1B_{2u}$ D_{2h}
T^a = 14750 gas DPI[1]

$1\,^1B_{3u}$ D_{2h}
T^a = 14526 gas DPI[1]

[a] Band maximum.

References

[1]M. Broyer, J. Chevaleyre, Ph. Dugourd, J. P. Wolf, and L. Wöste, Phys. Rev. A **42**, 6954 (1990).

Li_2Na_2

$2^1B_{1u}, 3^1B_{1u}$ D_{2h}
T^a = 23300 gas DPI[1] $2^1B_{1u}, 3^1B_{1u}$–$\tilde{X}$ 429 nm

$2^1B_{2u}, 3^1B_{2u}$ D_{2h}
T^a = 21400 gas DPI[1] $2^1B_{2u}, 3^1B_{2u}$–$\tilde{X}$ 468 nm

1^1B_{1u} D_{2h}
T^a = 19100 gas DPI[1] 1^1B_{1u}–$\tilde{X}$ 524 nm

2^1B_{3u} D_{2h}
T^a = 16300 gas DPI[1] 2^1B_{3u}–$\tilde{X}$ 614 nm

1^1B_{3u} D_{2h}
T^a = 14300 gas DPI[1] 1^1B_{3u}–$\tilde{X}$ 701 nm

$\tilde{X}\,^1A_g$ D_{2h}

[a] Band maximum.

References

[1]S. Pollack, C. R. C. Wang, T. A. Dahlseid, and M. M. Kappes, J. Chem. Phys. **96**, 4918 (1992).

$LiNa_3$

$\tilde{E}$ C_{2v}
T^a = 22900 gas DPI[1] $\tilde{E}$–$\tilde{X}$ 437 nm

$\tilde{D}$ C_{2v}
T^a = 20700 gas DPI[1] $\tilde{D}$–$\tilde{X}$ 484 nm

$\tilde{C}$ C_{2v}
T^a = 18600 gas DPI[1] $\tilde{C}$–$\tilde{X}$ 537 nm

$\tilde{B}$ C_{2v}
T^a = 16000 gas DPI[1] $\tilde{B}$–$\tilde{X}$ 626 nm

$\tilde{A}$ C_{2v}
T^a = 14450 gas DPI[1] $\tilde{A}$–$\tilde{X}$ 692 nm

$\tilde{X}\,^1A_1$ C_{2v}

[a] Band maximum.

References

[1]S. Pollack, C. R. C. Wang, T. A. Dahlseid, and M. M. Kappes, J. Chem. Phys. **96**, 4918 (1992).

Na_4

$\tilde{H}\,^1B_{2u}$ D_{2h}
T^a = 26900 gas DPI[2]

$\tilde{G}\,^1B_{1u}, ^1B_{3u}$ D_{2h}
T^a = 25400 gas DPI[2]

$\tilde{F}\,^1B_{1u}$ D_{2h}
T^a = 22400 gas DPI[1,2]
Maximum also observed[2] at 23000.

$\tilde{E}\,^1B_{2u}$ D_{2h}
T^a = 20200 gas DPI[1,2]
Maximum also observed[2] at 21200.

$\tilde{D}\,^1B_{1u}$ D_{2h}
T^a = 17600 gas DPI[1,2]

$\tilde{C}\,^1B_{3u}$ D_{2h}
T^a = 16000 gas DPI[1,2]

$\tilde{B}\,^1B_{3u}$ D_{2h}
T^a = 14500 gas DPI[1,2]

$\tilde{A}\,^1B_{2u}$ D_{2h}
T^a = 13200 gas DPI[1,2]

[a] Band maximum.

References

[1]C. R. C. Wang, S. Pollack, and M. M. Kappes, Chem. Phys. Lett. **166**, 26 (1990).
[2]C. R. C. Wang, S. Pollack, D. Cameron, and M. M. Kappes, J. Chem. Phys. **93**, 3787 (1990).

BBNN

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NN stretch	1912.6	Ar	IR	2
			1934.2	N_2	IR	1
		BB stretch	1484.8	Ar	IR	2
			1480.0	N_2	IR	1

References

[1]P. Hassanzadeh and L. Andrews, J. Phys. Chem. **96**, 9177 (1992).
[2]L. Andrews, P. Hassanzadeh, T. R. Burkholder, and J. M. L. Martin, J. Chem. Phys. **98**, 922 (1993).

BNBN

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BNB a–stretch	1958.8	Ar	IR	2
			1965.4	N_2	IR	1

References

[1]P. Hassanzadeh and L. Andrews, J. Phys. Chem. **96**, 9177 (1992).
[2]L. Andrews, P. Hassanzadeh, T. R. Burkholder, and J. M. L. Martin, J. Chem. Phys. **98**, 922 (1993).

cyc–$(BN)_2$

$\tilde{X}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}			1029.2	N_2	IR	1

References

[1]P. Hassanzadeh and L. Andrews, J. Phys. Chem. **96**, 9177 (1992).

C_4

$^1\Delta_g$ $D_{\infty h}$
T_0 = 2640(50) gas PE[7]

$\tilde{X}$ $^3\Sigma_g^-$ $D_{\infty h}$ [a] Structure: ESR[2,6]DL[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	2032(50)	gas	PE	7
Σ_u^+	3	Asym. stretch	1548.94	gas	DL	4
			1543.4	Ar	IR	1

$\tilde{X}$ $^3\Sigma_g^-$ —Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_g	4	Bend	339(55)	gas	PE	7
Π_u	5	Bend	172.4	Ar	IR	5
			170.4			

B_0 = 0.165 DL[4]

[a] ESR measurements[2,6] and the infrared detection[3] of the $\nu_3 + \nu_5$ combination band suggest that C_4 may deviate by a few degrees from the linear structure.

References

[1]L. N. Shen and W. R. M. Graham, J. Chem. Phys. **91**, 5115 (1989).
[2]H. M. Cheung and W. R. M. Graham, J. Chem. Phys. **91**, 6664 (1989).
[3]L. N. Shen, P. A. Withey, and W. R. M. Graham, J. Chem. Phys. **94**, 2395 (1991).
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Si_2C_2

$\tilde{X}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{1u}	3		982.9vs	Ar	IR	1
b_{2u}	4		382.2wm	Ar	IR	1

References

[1]J. D. Presilla-Márquez, C. M. L. Rittby, and W. R. M. Graham, Paper TG11, 48th International Symposium on Molecular Spectroscopy, Columbus, Ohio, 1993.

Si_3C

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Ring breathing	658.2	Ar	IR	1
	2	Si_3 s–deform.	511.8	Ar	IR	1
	3	SiCSi s–deform.	309.5	Ar	IR	1
b_2	5	SiCSi a–stretch	1101.4	Ar	IR	1
	6	Si_3 a–stretch	357.6	Ar	IR	1

References

[1]J. D. Presilla-Márquez and W. R. M. Graham, J. Chem. Phys. **96**, 6509 (1992).

Si_4

$\tilde{C}$

T_0 = 16220(80) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			450(65)	gas	PE	1

$\tilde{B}$

T_0 = 11700(80) gas PE[1]

$\tilde{A}$

T_0 = 6540(80) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			300(25)	gas	PE	1

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			360(25)	gas	PE	1

References

[1]T. N. Kitsopoulos, C. J. Chick, A. Weaver, and D. M. Neumark, J. Chem. Phys. **93**, 6108 (1990).

CaNCO[a]

$\tilde{B}\ ^2\Sigma^+$ $C_{\infty v}$

T_0 = 17180(30) gas LF[1] $\tilde{B}$–$\tilde{X}$ 582 nm

$\tilde{A}\ ^2\Pi$ $C_{\infty v}$

T_0 = 16230(5) gas LF[1] $\tilde{A}$–$\tilde{X}$ 610–635 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	CaN stretch	395(5)	gas	LF	1
Π	4	NCO bend	650T[b]	gas	LF	1

A = 68(7) gas LF[1]

$\tilde{X}\ ^2\Sigma^+$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NCO a-stretch	2200(5)	gas	LF	1
	3	CaN stretch	390(5)	gas	LF	1
Π	4	NCO bend	640T	gas	LF	1
	5	CaNC bend	50T[b]	gas	LF	1

[a] Originally assigned to CaOCN. For reassignment, see Ref. 2.
[b] This value may correspond to $2\nu_5$.

References

[1]L. C. Ellingboe, A. M. R. P. Bopegedera, C. R. Brazier, and P. F. Bernath, Chem. Phys. Lett. **126**, 285 (1986).
[2]L. C. O'Brien and P. F. Bernath, J. Chem. Phys. **88**, 2117 (1988).

SrNCO

$\tilde{B}\ ^2\Sigma^+$ $C_{\infty v}$

T_0 = 16016(30) gas LF[1] $\tilde{B}$–$\tilde{X}$ 624 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	SrN stretch	314(30)	gas	LF	1

$\tilde{A}\ ^2\Pi$ $C_{\infty v}$

T_0 = 15069.62 gas LF[1,2] $\tilde{A}$–$\tilde{X}$ 650–685 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	SrN stretch	320(30)[a]	gas	LF	1

A = 292.57 gas LF[1,2]
B_0 = 0.043 LF[2]

$\tilde{X}\ ^2\Sigma^+$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	SrN stretch	297(30)	gas	LF	1

B_0 = 0.043 LF[2]

[a] For $^2\Pi_{3/2}$ state.

References

[1]L. C. Ellingboe, A. M. R. P. Bopegedera, C. R. Brazier, and P. F. Bernath, Chem. Phys. Lett. **126**, 285 (1986).
[2]L. C. O'Brien and P. F. Bernath, J. Chem. Phys. **88**, 2117 (1988).

CaN_3

$\tilde{B}\ ^2\Sigma^+$ $C_{\infty v}$

T_0 = 17079 gas LF[1] $\tilde{B}$–$\tilde{X}$ 570–590 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	CaN stretch	384	gas	LF	1
Π	5	CaNN bend	42.5H	gas	LF	1

$\tilde{A}\ ^2\Pi$ $C_{\infty v}$

T_0 = 16255 gas LF[1] $\tilde{A}$–$\tilde{X}$ 600–710 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	CaN stretch	389	gas	LF	1

A = 76 gas LF[1]

$\tilde{X}\ ^2\Sigma^+$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	N_3 a–stretch	2114	gas	LF	1
	2	N_3 s–stretch	1364	gas	LF	1
	3	CaN stretch	396	gas	LF	1
Π	5	CaNN bend	43H	gas	LF	1

References

[1]C. R. Brazier and P. F. Bernath, J. Chem. Phys. **88**, 2112 (1988).

SrN_3

$\tilde{B}\ ^2\Sigma^+$ $C_{\infty v}$

T_0 = 15872 gas LF[1] $\tilde{B}$–$\tilde{X}$ 630 nm

$\tilde{A}\ ^2\Pi$ $C_{\infty v}$

T_0 = 15057.69 gas LF[1] $\tilde{A}$–$\tilde{X}$ 640–690 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	SrN stretch	321	gas	LF	1

A = 296.43 gas LF[1]
B_0 = 0.045 LF[1]

$\tilde{X}\ ^2\Sigma^+$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	SrN stretch	316	gas	LF	1
Π	5	SrNN bend	41H	gas	LF	1

B_0 = 0.045 LF[1]

References

[1]C. R. Brazier and P. F. Bernath, J. Chem. Phys. **88**, 2112 (1988).

$B_2O_2^+$

$\tilde{C}\ ^2\Sigma_u$ $D_{\infty h}$

T_0 = 18560(320) gas PE[1]

$\tilde{B}\ ^2\Sigma_g$ $D_{\infty h}$

T_0 = 13720(320) gas PE[1]

$\tilde{A}\ ^2\Pi_u$ $D_{\infty h}$

T_0 = 5080(320) gas PE[1]

$\tilde{X}\ ^2\Pi_g$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	BO stretch	1922[a]	gas	PE	1
	2	BB stretch	499[a]	gas	PE	1

[a] Obtained from Franck–Condon fit to partially resolved structure in the first photoelectron band.

References

[1]B. M. Ruscic, L. A. Curtiss, and J. Berkowitz, J. Chem. Phys. **80**, 3962 (1984).

C_4^-

Threshold for electron detachment from ground-state C_4^- = 31320(80) gas PE[1,2]

References

[1]S. Yang, K. J. Taylor, M. J. Craycraft, J. Conceicao, C. L. Pettiette, O. Cheshnovsky, and R. E. Smalley, Chem. Phys. Lett. **144**, 431 (1988).
[2]D. W. Arnold, S. E. Bradforth, T. N. Kitsopoulos, and D. M. Neumark, J. Chem. Phys. **95**, 8753 (1991).

Si_4^-

Threshold for electron detachment from ground-state Si_4^- = 17350(80) gas PE[1]

References

[1]T. N. Kitsopoulos, C. J. Chick, A. Weaver, and D. M. Neumark, J. Chem. Phys. **93**, 6108 (1990).

CCCN

$\tilde{X}\ ^2\Sigma^+$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	5	Bend	179T	gas	MW	3

B_0 = 0.165 MW[1,2]

References

[1]M. Guélin, F. Friberg, and A. Mezaoui, Astron. Astrophys. **109**, 23 (1981).
[2]C. A. Gottlieb, E. W. Gottlieb, P. Thaddeus, and H. Kawamura, Astrophys. J. **275**, 916 (1983).
[3]H. Mikami, S. Yamamoto, S. Saito, and M. Guélin, Astron. Astrophys. **217**, L5 (1989).

$N{\equiv}C{-}C{\equiv}N^+$

$\tilde{C}\ ^2\Pi_u$ $D_{\infty h}$

T_0 =			
17020(160)	gas	PE[1]
17056(6)	Ne	AB[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡N stretch	2020(10)	Ne	AB	2
	2	C–C stretch	710(40)	gas	PE	1
			740(10)	Ne	AB	2
Π_g	4	Bend	422	Ne	AB	2

$\tilde{B}\ ^2\Sigma_u^+$ $D_{\infty h}$

T_0 = 12100(160) gas PE[1]
12285(40) Ne AB[2]

$\tilde{A}\ ^2\Sigma_g^+$ $D_{\infty h}$

T_0 = 9120(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡N stretch	1860(40)	gas	PE	1

$\tilde{X}\ ^2\Pi_g$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡N stretch	2120(40)	gas	PE	1

References

[1]C. Baker and D. W. Turner, Proc. Roy. Soc. (London) **A308**, 19 (1968).
[2]J. Fulara, S. Leutwyler, J. P. Maier, and U. Spittel, J. Phys. Chem. **89**, 3190 (1985).

$CNCN^+$ [a]

$\tilde{C}$ $C_{\infty v}$

T_0 = 26080(80) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			710(40)	gas	PE	1

$\tilde{B}$ $C_{\infty v}$

T_0 = 12240(80) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2075(40)	gas	PE	1
			1160(40)	gas	PE	1

$\tilde{A}$ $C_{\infty v}$

T_0 = 310(80) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2270(40)	gas	PE	1
			1300(40)	gas	PE	1

[a] The molecule studied in Ref. 1 was at that time believed to be CNNC. Subsequent infrared studies[2] demonstrated that it is CNCN.

References

[1]O. Grabandt, C. A. De Lange, R. Mooyman, T. van der Does, and F. Bickelhaupt, Chem. Phys. Lett. **155**, 221 (1989).
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NNBN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NN stretch	2091.7	Ar	IR	2
			2124.8	N_2	IR	1
	2	BN stretch	1802.0	Ar	IR	2
			1806.1	N_2	IR	1
	3	N_2–BN stretch	760.3w	Ar	IR	2
			750.4	N_2	IR	1

References

[1]P. Hassanzadeh and L. Andrews, J. Phys. Chem. **96**, 9177 (1992).
[2]L. Andrews, P. Hassanzadeh, T. R. Burkholder, and J. M. L. Martin, J. Chem. Phys. **98**, 922 (1993).

B_2O_2

$\tilde{X}$ $D_{\infty h}$ Structure: MO,PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	BO stretch	1898.9	Ar	IR	1,2,4
			1894.6	Kr	IR	4
Π_u	5	Bend	213	Ar	IR	1,2

References

[1]Yu. N. Sekachev, L. V. Serebrennikov, and A. A. Mal'tsev, Vestnik Mosk. Univ. Khim. **20**, 589 (1979).
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[4]T. R. Burkholder and L. Andrews, J. Chem. Phys. **95**, 8697 (1991).

AlOAlO

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1176.3	Ar	IR	2
			945.4	Ar	IR	1,2

References

[1]I. L. Rozhanskii, G. V. Chertikhin, L. V. Serebrennikov, and V. F. Shevel'kov, Zh. Fiz. Khim. **62**, 2351 (1988); Russ. J. Phys. Chem. **62**, 1215 (1988).
[2]L. Andrews, T. R. Burkholder, and J. T. Yustein, J. Phys. Chem. **96**, 10182 (1992).

GaOGaO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			967.0	Ar	IR	1

References

[1]T. R. Burkholder, J. T. Yustein, and L. Andrews, J. Phys. Chem. **96**, 10189 (1992).

cyc–GaO_2Ga

$\tilde{X}$ D_{2h} ?

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		GaO stretch	463.0	Ar	IR	1
			458.6	N_2	IR	1

References

[1]M. J. Zehe, D. A. Lynch, Jr., B. J. Kelsall, and K. D. Carlson, J. Phys. Chem. **83**, 656 (1979).

InOInO

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			816.6s	Ar	IR	1
			552.7	Ar	IR	1

References

[1]T. R. Burkholder, J. T. Yustein, and L. Andrews, J. Phys. Chem. **96**, 10189 (1992).

cyc–InO_2In

$\tilde{X}$ D_{2h} ?

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		InO stretch	454.9	Ar	IR	1,2
			443.2	N_2	IR	1

References

[1]M. J. Zehe, D. A. Lynch, Jr., B. J. Kelsall, and K. D. Carlson, J. Phys. Chem. **83**, 656 (1979).
[2]T. R. Burkholder, J. T. Yustein, and L. Andrews, J. Phys. Chem. **96**, 10189 (1992).

CNCN

$\tilde{X}$ $C_{\infty v}$ Structure: MW[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡N s–stretch	2302.00	gas	IR	1
			2294.4	Ar	IR	2
	2	C≡N a–stretch	2059.73	gas	IR	1
			2053.7	Ar	IR	2
	3	N–C stretch	975T	gas	IR	1
			979.2	Ar	IR	2
Π	4	Bend	463.69	gas	IR	2,5
			468.5	Ar	IR	2
			467.2			
	5	Bend	194.75	gas	IR	1
			200T[b]	Ar	IR	1

B_0 = 0.173 IR[1,3]MW[1,3–5]

[a] From combination bands.

References

[1]F. Stroh and M. Winnewisser, Chem. Phys. Lett. **155**, 21 (1989).
[2]F. Stroh, B. P. Winnewisser, M. Winnewisser, H. P. Reisenauer, G. Maier, S. J. Goede, and F. Bickelhaupt, Chem. Phys. Lett. **160**, 105 (1989); Chem. Phys. Lett. **162**, 253 (1989).
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[4]M. C. L. Gerry, F. Stroh, and M. Winnewisser, J. Mol. Spectrosc. **140**, 147 (1990).
[5]M. Winnewisser, J. W. G. Seibert, and K. M. T. Yamada, J. Mol. Spectrosc. **153**, 635 (1992).

CNNC

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3		1997.0	Ar	IR	1,2
			2001.3	N_2	IR	2

References

[1]F. Stroh, B. P. Winnewisser, M. Winnewisser, H. P. Reisenauer, G. Maier, S. J. Goede, and F. Bickelhaupt, Chem. Phys. Lett. **160**, 105 (1989); Chem. Phys. Lett. **162**, 253 (1989).
[2]G. Maier, H. P. Reisenauer, J. Eckwert, C. Sierakowski, and T. Stumpf, Angew. Chem. **104**, 1287 (1992); Angew. Chem. Int. Ed. Engl. **31**, 1218 (1992).

CCCO

$\tilde{X}$ $C_{\infty v}$ Structure: MW[4,7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1		2257.22	gas	IR	8
			2243vs	Ar	IR	1,5–7
	2		1907.0m	Ar	IR	5,7
	3		939.1vw	Ar	IR	7
Π	4		580m	Ar	IR	5,7

B_0 = 0.160 MW[2–4]IR[8]

References

[1]R. L. DeKock and W. Weltner, Jr., J. Am. Chem. Soc. **93**, 7106 (1971).
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CCCS

In an argon matrix, a weak absorption maximum at 26460 (378 nm) has been assigned[2] to CCCS.

$\tilde{X}\ ^1\Sigma$ $C_{\infty v}$ Structure: MW[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1		2046.2vs	Ar	IR	2
	2		1533.2wm	Ar	IR	2
	3		725.6w	Ar	IR	2

B_0 = 0.096 MW[1,4]

References

[1]S. Yamamoto, S. Saito, K. Kawaguchi, N. Kaifu, H. Suzuki, and M. Ohishi, Astrophys. J. **317**, L119 (1987).
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OBCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CO stretch	1863.4	Ar	IR	1

References

[1]T. R. Burkholder, L. Andrews, and R. J. Bartlett, J. Phys. Chem. **97**, 3500 (1993).

$ONCN^+$

$\tilde{F}\ ^2A'$ C_s
T_0 = 65100(1200) gas PE[1]

$\tilde{E}\ ^2A''$ C_s
T_0 = 61100(1200) gas PE[1]

$\tilde{D}\ ^2A'$ C_s
T_0 = 47120(800) gas PE[1]

$\tilde{C}\ ^2A''$ C_s
T^a = 28400(560) gas PE[1]

$\tilde{B}\ ^2A'$ C_s
T^a = 23080(560) gas PE[1]

$\tilde{A}\ ^2A'$ C_s
T^a = 21220(560) gas PE[1]

$\tilde{X}\ ^2A'$ C_s

[a] From vertical ionization potential.

References

[1]G. Jonkers, R. Mooyman, and C. A. de Lange, Chem. Phys. **57**, 97 (1981).

t–$OCCO^+$

$\tilde{B}$
gas PD[2] $\tilde{B}$–$\tilde{X}$ 270–330 nm
Superposed on continuum.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g			475(20)	gas	PD	2

$\tilde{X}\ ^2B_u$ C_{2h} Structure: ESR,MO[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	CO s–stretch	2076T[a]	Ne	IR	4
			526(30)T	gas	PD	2
b_u	5	CO a–stretch	2056.6	Ne	IR	3,4

[a] Calculated using observed values for asymmetrically substituted species.

References

[1]L. B. Knight, Jr., J. Steadman, P. K. Miller, D. E. Bowman, E. R. Davidson, and D. Feller, J. Chem. Phys. **80**, 4593 (1984).
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N_4^+

$\tilde{A}, \tilde{B}$

A broad, unstructured absorption[1-3] between 270 and 650 nm, with a maximum near 330 nm, leads to the formation of $N_2^+ + N_2$. Detection of the fluorescence of N_2^+ (B) at the higher energies in this range suggests that the potential energy surface for a bound excited state of N_4^+ which correlates with N_2^+ (B) has an avoided crossing with the surface for the dissociative $\tilde{A}$ state.[3]

$\tilde{X}\ ^2\Sigma_u$ $D_{\infty h}$ Structure: ESR,MO[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	N≡N s-stretch	2283T[a]	Ne	IR	6
Σ_u^+	3	N≡N a-stretch	2237.6	Ne	IR	5,6

[a] Calculated using observed values for asymmetrically ^{15}N-substituted species.

References

[1]G. P. Smith and L. C. Lee, J. Chem. Phys. **69**, 5393 (1978).
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P_4^+

$\tilde{C}\ ^2T_2$ T_d

$T_0^a \cong 42400$ gas PE[1,2]
Jahn-Teller splitting ≅ 9300 gas PE[1,2]

$\tilde{B}\ ^2A_1$ T_d

T_0^a = 22800(100) gas PE[1,2,5]
22936(5) Ar AB[3] $\tilde{B}-\tilde{X}$ 398–436 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	577(5)	gas	PE	1,2,5
			550(10)	Ar	AB	3

$\tilde{A}\ ^2T_2$ T_d

T_0^a = 9280(800) gas PE[1,2,5]
A weak, broad absorption maximum observed[3] in an argon matrix at 9570 has been tentatively assigned to the $\tilde{A}-\tilde{X}$ transition of P_4^+.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
t_2	3		400(10)	gas	PE	5

Jahn-Teller splitting ≅ 1130 gas PE[1,2]

$\tilde{X}\ ^2E$ T_d

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	2		315(10)[b]	gas	PE	4
			275(10)[c]	gas	PE	4

Separation of band maxima associated with Jahn-Teller splitting = 3710(160) gas PE[1,2,4,5]

[a] The adiabatic first ionization potential of P_4 is taken as 8.95 eV, the value obtained in the linear Jahn-Teller fit of Ref. 4.
[b] Lower frequency component of Jahn-Teller doublet.
[c] Higher frequency component of Jahn-Teller doublet.

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As_4^+

$\tilde{B}\ ^2A_1$ T_d

T_0^a = 25710(100) gas PE[1,2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1		350(6)	gas	PE	4

$\tilde{A}\ ^2T_2$ T_d

T_0^a = 13500(900) gas PE[1,2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
t_2	3		240T	gas	PE	4

$\tilde{X}\ ^2E$ T_d

Separation of band maxima associated with Jahn-Teller splitting = 3310(160) gas PE[3,4]

[a] The adiabatic first ionization potential of As_4 is taken as 7.83 eV, the value obtained in the linear Jahn-Teller fit of Ref. 3.

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SCCS

A very prominent, unstructured absorption with threshold near 43500 (230 nm) has been attributed[1] to SCCS.

$\tilde{A}\ ^3\Sigma_u^-$ $D_{\infty h}$

T_0 = 25523(6) Ar AB[1-3] $\tilde{A}$–$\tilde{X}$ 361–392 nm

Exposure of the sample to 392-nm radiation leads to a decrease in the intensity of the absorptions attributed to SCCS and to a growth in the absorption of CS.[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	2	CS s-stretch	532(6)	Ar	AB	3
Π_u	5	Bend	219HT[a]	Ar	AB	3

$\tilde{X}\ ^3\Sigma_g^-$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	CC stretch	1904T	Ar	IR	1
	2	CS s-stretch	546T	Ar	IR	1
Σ_u^+	3	CS a-stretch	1179.7	Ar	IR	1-3

[a]Ref. 3 assigns a progression beginning at 25960 to vibronically allowed transitions to ν_4 (Π_g) + $n\nu_2$ upper state energy levels. It seems more likely that this progression involves $2\nu_5 + n\nu_2$ excitation.

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Si_2O_2

$\tilde{X}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{1u}	4	Deformation	79	Ar	IR	2
b_{2u}	5	SiO stretch	809.5	Ne	IR	2
			803.2	Ar	IR	1-4
			804.7	N_2	IR	1
b_{3u}	6	SiO stretch	766.7	Ne	IR	2
			768.2	Ar	IR	1-4
			766.3	N_2	IR	1

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Ge_2O_2

$\tilde{X}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}	5	GeO stretch	667.7	Ar	IR	1,2
			667	N_2	IR	1
b_{3u}	6	GeO stretch	600.0	Ar	IR	1,2
			599	N_2	IR	1

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NCNO

An absorption maximum has been reported[3,9] at 216 nm, with absorption extending beyond 200 nm.

A weaker absorption maximum occurs near 270 nm, with a long wavelength threshold near 400 nm.[9]

$\tilde{A}\ ^1A''$ C_s Structure: PF[11]

T_0 = 11339 gas AB[1,3,7]PF[11] $\tilde{A}$–$\tilde{X}$ 540–971 nm

Threshold for photodissociation into CN and NO at 17085.[9,10] Extensively perturbed by interaction with high vibrational levels of the ground state.[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	C≡N stretch	1956	gas	PF	11
	2	N=O stretch	1485	gas	PF	11
	3	C–N stretch	918	gas	PF	11
	4	NCN bend	543	gas	AB,PF	7,11
	5	CNO bend	212.5	gas	AB,PF	7,11
a''	6	Torsion	411	gas	PF	11

$\tau_{rad} \cong 14$ μs gas LF[8,12]. $\tau_{fluor} > 40$ μs for all levels below D_0 (17085) LF[12].

A = 4.76(2); B = 0.167(3) PF[11]

$\tilde{X}$ C_s Structure: MW[2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	C≡N stretch	2170.0	gas	IR	6
	2	N=O stretch	1501.0	gas	IR	6
	3	C–N stretch	820.0	gas	IR	3,6
	4	NCN bend	588.5	gas	IR	6
	5	CNO bend	212.0(2)	gas	IR	5
a''	6	Torsion	264.2	gas	IR	5

A_0 = 2.709; B_0 = 0.180; C_0 = 0.168 MW[2,4]IR[5]

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ClCCN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2118s	Ar	IR	1
			2113s	Ar	IR	1
			1945s	Ar	IR	1
			1025m	Ar	IR	1
			996ms	Ar	IR	1

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BrCCN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2102m	Ar	IR	1
			1923ms	Ar	IR	1
			1035vw	Ar	IR	1
			984vs	Ar	IR	1

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Sb_4

$\tilde{a}\ ^3T_2$ T_d

T_0 = 9700T gas PE[3]

Jahn–Teller distortion occurs.

$\tilde{X}\ ^1A_1$ T_d

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1		242.1(5)	Ne	Ra	1,2
			241.5(3)	Ar	Ra	2
			239.6(3)	Kr	Ra	2
e	2		137.1(3)	Ar	Ra	2
			135.8(3)	Kr	Ra	2
t_2	3		179.1(5)	Ne	Ra	1,2
			178.5(3)	Ar	Ra	2
			177.1(3)	Kr	Ra	2

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Bi_4

$\tilde{B}$ T_d

T_0 = 15312 Ne LF[1] $\tilde{B}$–$\tilde{X}$ 600–710 nm
15250 Ar LF[1] $\tilde{B}$–$\tilde{X}$ 600–670 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1		129.1	Ne	LF	1
			131	Ar	LF	1
e	2		82.4	Ne	LF	1
t_2	3		104.9	Ne	LF	1

$\tau < 20$ ns Ne LF[1]

A weak emission band system with origin at 13424 which terminates in Bi_4 ($\tilde{X}$) was observed by Ref. 4 in neon matrix studies of the laser excitation of Bi_4 ($\tilde{B}$).

$\tilde{A}$ T_d

T_0 = 12535 Ne AB^2LF^2 $\tilde{A}$–$\tilde{X}$ 725–765 nm
12396 Ar LF[1] $\tilde{A}$–$\tilde{X}$ 740–765 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1		123	Ar	LF	1

$\tau \cong 1.5$ μs Ne LF[1]

$\tilde{X}$ T_d

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1		149.7	Ne	LF	1
			151	Ar	LF,Ra	1,4
			152	Kr	Ra	3
e	2		89.8	Ne	LF	1
t_2	3		120.4	Ne	LF	1

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OBSO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BO stretch	2006.3	Ar	IR	1
			1049.6T	Ar	IR	1

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OAlOO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1092.5	Ar	IR	1

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OGaOO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			865.9	Ar	IR	1

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t–OCCO$^-$

In solid neon, threshold for electron detachment < 18000.[1,2]

$\tilde{X}$ C_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	3	Bend	524[a]	Ne	IR	2
b_u	5	CO a–stretch	1517.7	Ne	IR	1,2

[a] $(\nu_3 + \nu_5) - \nu_5$. Tentative assignment of combination band.

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$C_2F_2^+$

$\tilde{D}\ ^2\Sigma_u$ $D_{\infty h}$
T^a = 84880(1000) gas PE[2]

$\tilde{C}\ ^2\Sigma_g$ $D_{\infty h}$
T^a = 76000(1000) gas PE[1,2]

$\tilde{B}\ ^2\Pi_u$ $D_{\infty h}$
T^a = 59060(1000) gas PE[1,2]

$\tilde{A}\ ^2\Pi_g$ $D_{\infty h}$
T^a = 52600(1000) gas PE[1,2]

$\tilde{X}\ ^2\Pi_u$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2420(80)	gas	PE	2
	2	CF s–stretch	825(80)	gas	PE	2

[a] From vertical ionization potential.

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$C_2Cl_2^+$

$\tilde{D}\ ^2\Sigma_u^+$ $D_{\infty h}$
T_0 = 62287(160) gas PE[1]

$\tilde{C}\ ^2\Sigma_g^+$ $D_{\infty h}$
T_0 = 53816(160) gas PE[1]

$\tilde{B}\ ^2\Pi_u$ $D_{\infty h}$
T_0 = 35178(160) gas PE[1]
$\tau \cong 2850$ ns gas PEFCO[4]

$\tilde{A}\ ^2\Pi_{g,3/2}$ $D_{\infty h}$
T_0 = 26962.8(3) gas EF[5,8]LF[7] $\tilde{A}$–$\tilde{X}$ 360–496 nm
26637(10) Ne AB[6] $\tilde{A}$–$\tilde{X}$ 341–375 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2223(5)	Ne	AB	6
	2	CCl stretch	484.2(3)[a]	gas	EF,LF	5,7,8
			486(5)	Ne	AB	6
Π_u	5	Bend	205(3)H	gas	LF	7
			207(5)H	Ne	AB	6

τ = 13(2) ns gas EF[2]PEFCO[4]; ≤ 30 ns gas PIFCO[3]
A = −565(80) gas EF[5]

$\tilde{X}\ ^2\Pi_{u,3/2}$ $D_{\infty h}$ Structure: UV[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2107.2(3)[b]	gas	EF,LF	5,7,8
	2	CCl stretch	503.8(3)[c]	gas	EF,LF	5,7,8
Π_g	4	Bend	317.8(3)H	gas	EF,LF	5,7,8
Π_u	5	Bend	233H	gas	LF	7

$A = -240(120)$ gas EF[5]

[a] 495 for $\tilde{A}\ ^2\Pi_{g,1/2}$.
[b] 2101.0(3) for $\tilde{X}\ ^2\Pi_{u,1/2}$.[8]
[c] 514.0(3) for $\tilde{X}\ ^2\Pi_{u,1/2}$.[8]

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$ClC{\equiv}CBr^+$

$\tilde{D}\ ^2\Sigma^+$ $C_{\infty v}$
$T_0 = 60432(160)$ gas PE[1]

$\tilde{C}\ ^2\Sigma^+$ $C_{\infty v}$
$T_0 = 49136(160)$ gas PE[1]

$\tilde{B}\ ^2\Pi$ $C_{\infty v}$
$T_0 = 33080(160)$ gas PE[1]
$\tau \geq 1100$ ns gas PEFCO[2]

$\tilde{A}\ ^2\Pi_{3/2}$ $C_{\infty v}$
$T_0 = 21441$ gas EF[3] $\tilde{A}$–$\tilde{X}$ 426–550 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡C stretch	2172(2)	gas	EF	3
	2	CCl stretch	878(2)	gas	EF	3
	3	CBr stretch	334(2)	gas	EF	3
Π	4	CCCl bend	304(2)T	gas	EF	3
	5	CCBr bend	182(2)HT	gas	EF	3

$\tau = 21(2)$ ns gas PEFCO[3]
$A = \cong -1900$ gas EF[3]

$\tilde{X}\ ^2\Pi_{3/2}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡C stretch	2011(2)	gas	EF	3
	2	CCl stretch	1017(2)	gas	EF	3
	3	CBr stretch	405(2)	gas	EF	3
Π	5	CCBr bend	246(2)T	gas	LF	3

$A = \cong -1000$ gas EF[3]

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$C_2Br_2^+$

$\tilde{D}\ ^2\Sigma_u^+$ $D_{\infty h}$
$T_0 = 58334(160)$ gas PE[1]

$\tilde{C}\ ^2\Sigma_g^+$ $D_{\infty h}$
$T_0 = 48168(160)$ gas PE[1]

$\tilde{B}\ ^2\Pi_u$ $D_{\infty h}$
$T_0 = 29369(160)$ gas PE[1]
$\tau \geq 1500$ ns gas PEFCO[3]
$A = -323(160)$ gas PE[1]

$\tilde{A}\ ^2\Pi_{g,1/2}$ $D_{\infty h}$
$T_0 = 22188(80)$ gas PE[1]EF[4] $\tilde{A}$–$\tilde{X}$ 467–648 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	2	CBr stretch	278	gas	EF	4
Π_g	4	Bend	257HT	gas	EF	4
Π_u	5	Bend	112H	gas	EF	4

$\tau = 27(3)$ ns gas EF[2]; 25(3) ns gas PEFCO[3]

$\tilde{A}\ ^2\Pi_{g,3/2}$ $D_{\infty h}$
$T_0 = 19855.9(3)$ gas EF[4,7],LF[6] $\tilde{A}$–$\tilde{X}$ 438–648 nm
19548(4) Ne AB[5] $\tilde{A}$–$\tilde{X}$ 448–511 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2190	gas	EF,LF	4,6
			2194(5)	Ne	AB	5
	2	CBr stretch	282.7(3)	gas	EF,LF	4,6,7
			293(5)	Ne	AB	5
Π_g	4	Bend	263H	gas	EF	4
			259(5)H	Ne	AB	5
			240(5)H			
Π_u	5	Bend	119H	gas	EF,LF	4,6
			135(5)H	Ne	AB	5
			126(5)H			

$\tau = 29(3)$ ns gas EF[2]; 31(3) ns gas PEFCO[3]

$\tilde{X}\ ^2\Pi_{u,1/2}$ $D_{\infty h}$

T_0 = 1372(80) gas PE[1]EF[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2065.1(3)	gas	EF	4,7
	2	CBr stretch	318.4(3)	gas	EF	4,7
Π_g	4	Bend	294.5(3)H	gas	EF	4,7
Π_u	5	Bend	132.6(3)H	gas	EF	4,7

$\tilde{X}\ ^2\Pi_{u,3/2}$ $D_{\infty h}$ Structure: UV[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2067.0(3)	gas	EF,LF	4,6,7
	2	CBr stretch	320.7(3)	gas	EF,LF	4,6,7
Π_g	4	Deformation	299.0(3)H	gas	EF,LF	4,6,7
Π_u	5	Deformation	134.9(3)H	gas	EF,LF	4,6,7

References

[1]E. Heilbronner, V. Hornung, and E. Kloster-Jensen, Helv. Chim. Acta **53**, 331 (1970).
[2]M. Allan, E. Kloster-Jensen, and J. P. Maier, J. Chem. Soc., Faraday Trans. 2 **73**, 1417 (1977).
[3]J. P. Maier and F. Thommen, Chem. Phys. **70**, 325 (1982).
[4]D. Klapstein, J. P. Maier, and W. Zambach, Chem. Phys. **77**, 463 (1983).
[5]S. Leutwyler, J. P. Maier, and U. Spittel, Mol. Phys. **51**, 437 (1984).
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[7] D. Klapstein, R. Kuhn, and J. P. Maier, J. Electron Spectrosc. Relat. Phenom. **35**, 171 (1985).

$C_2I_2^+$

$\tilde{D}\ ^2\Sigma_u^+$ $D_{\infty h}$

T_0 = 52040(160) gas PE[1]

$\tilde{C}\ ^2\Sigma_g^+$ $D_{\infty h}$

T_0 = 41874(160) gas PE[1]

$\tilde{B}\ ^2\Pi_u$ $D_{\infty h}$

T_0 = 25334(160) gas PE[1]
$\tau \geq 3000$ ns gas PEFCO[3]
$A = -1694(160)$ gas PE[1]

$\tilde{A}\ ^2\Pi_{g,1/2}$ $D_{\infty h}$

T_0 = 17912(80) gas PE[1]EF[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	2	CI stretch	195	gas	EF	4
Π_g	4	Bend	224	gas	EF	4

τ = 52(3) ns gas EF[2]PEFCO[3]

$\tilde{A}\ ^2\Pi_{g,3/2}$ $D_{\infty h}$

T_0 = 12971 gas EF[4] $\tilde{A}$–$\tilde{X}$ 670–846 nm
12987(3) Ne AB[5] $\tilde{A}$–$\tilde{X}$ 613–770 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2146(5)	Ne	AB	5
	2	CI stretch	204	gas	EF	4
			195(5)	Ne	AB	5
Π_g	4	Bend	225HT	gas	EF	4
			227(5)H	Ne	AB	5

τ = 25(3) ns gas PEFCO[3]

$\tilde{X}\ ^2\Pi_{u,1/2}$ $D_{\infty h}$

T_0 = 3630(80) gas PE[1]EF[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	1990	gas	EF	4
	2	CI stretch	234	gas	EF	4
Π_g	4	Bend	214H	gas	EF	4
Π_u	5	Bend	94H	gas	EF	4

$\tilde{X}\ ^2\Pi_{u,3/2}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	2	CI stretch	242	gas	EF	4
Π_g	4	Bend	221H	gas	EF	4
Π_u	5	Bend	101H	gas	EF	4

References

[1]E. Heilbronner, V. Hornung, and E. Kloster-Jensen, Helv. Chim. Acta **53**, 331 (1970).
[2]M. Allan, E. Kloster-Jensen, and J. P. Maier, J. Chem. Soc., Faraday Trans. 2 **73**, 1417 (1977).
[3]J. P. Maier and F. Thommen, Chem. Phys. **70**, 325 (1982).
[4]D. Klapstein, J. P. Maier, and W. Zambach, Chem. Phys. **77**, 463 (1983).
[5]S. Leutwyler, J. P. Maier, and U. Spittel, Mol. Phys. **51**, 437 (1984).

FNCN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C≡N stretch	2068s	Ar	IR	1
		NF stretch	874s	Ar	IR	1

References

[1]D. E. Milligan and M. E. Jacox, J. Chem. Phys. **48**, 4811 (1968).

$CINCO^+$

$\tilde{F}\ ^2A'$ C_s

T^a = 63660(240) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1100(80)	gas	PE	1

$\tilde{E}\ ^2A'$ C_s

T^a = 55430(240) gas PE[1]

Structure with band spacings of either 950 or 1900(50).

$\tilde{D}\ ^2A''$ C_s

T^a = 45180(240) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			910(80)	gas	PE	1

$\tilde{B},\tilde{C}\ ^2A'',^2A'$ C_s

T^a = 25420(240) gas PE[1]

$\tilde{A}\ ^2A'$ C_s

T^a = 7420(240) gas PE[1]

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1110(40)	gas	PE	1
			600(40)	gas	PE	1

[a] From vertical ionization potential.

References

[1]D. C. Frost, C. B. MacDonald, C. A. McDowell, and N. P. C. Westwood, Chem. Phys. **47**, 111 (1980).

$BrNCO^+$

$\tilde{F}\ ^2A'$ C_s

T^a = 62040(240) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			750(80)	gas	PE	1

$\tilde{E}\ ^2A'$ C_s

T^a = 53740(240) gas PE[1]

Structured, with band separations varying from 700 to 850.

$\tilde{D}\ ^2A''$ C_s

T^a = 44540(240) gas PE[1]

$\tilde{C}\ ^2A'$ C_s

T^a = 22190(240) gas PE[1]

$\tilde{B}\ ^2A''$ C_s

T^a = 20820(240) gas PE[1]

$\tilde{A}\ ^2A'$ C_s

T^a = 5970(240) gas PE[1]

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1100(40)	gas	PE	1
			520(40)	gas	PE	1

[a] From vertical ionization potential.

References

[1]D. C. Frost, C. B. MacDonald, C. A. McDowell, and N. P. C. Westwood, Chem. Phys. **47**, 111 (1980).

$INCO^+$

$\tilde{F}\ ^2A'$ C_s

T^a = 61800(240) gas PE[1]

$\tilde{E}\ ^2A'$ C_s

T^a = 52440(240) gas PE[1]

$\tilde{D}\ ^2A''$ C_s

T^a = 46070(240) gas PE[1]

$\tilde{C}\ ^2A'$ C_s

T^a = 21300(240) gas PE[1]

$\tilde{B}\ ^2A''$ C_s

T^a = 18320(240) gas PE[1]

$\tilde{A}\ ^2A'$ C_s

T^a = 5570(240) gas PE[1]

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			2070(40)	gas	PE	1
			420(40)	gas	PE	1

[a] From vertical ionization potential.

References

[1]D. C. Frost, C. B. MacDonald, C. A. McDowell, and N. P. C. Westwood, Chem. Phys. **47**, 111 (1980).

$FSCN^+$

$\tilde{G}\ ^2A'$ C_s

T^a = 68300(1000) gas PE[1]

$\tilde{F}\ ^2A'$ C_s
T^a = 53800(1000) gas PE[1]

$\tilde{E}\ ^2A''$ C_s
T^a = 52200(1000) gas PE[1]

$\tilde{D}\ ^2A'$ C_s
T^a = 34450(320) gas PE[1]

$\tilde{C}\ ^2A''$ C_s
T^a = 23960(1000) gas PE[1]

$\tilde{B}\ ^2A'$ C_s
T^a = 21460(320) gas PE[1]

$\tilde{A}\ ^2A'$ C_s
T^a = 19900(1000) gas PE[1]

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		SF stretch	840(50)	gas	PE	1

[a] From vertical ionization potential.

References

[1]G. Jonkers, O. Grabandt, R. Mooyman, and C. A. de Lange, J. Electron Spectrosc. Relat. Phenom. **26**, 147 (1982).

ClSCN$^+$

$\tilde{G}\ ^2A'$ C_s
T^a = 57280(560) gas PE[1]

$\tilde{F}\ ^2A'$ C_s
T^a = 40260(320) gas PE[1]

$\tilde{E}\ ^2A''$ C_s
T^a = 32440(320) gas PE[1]

$\tilde{D}\ ^2A'$ C_s
T^a = 25900(320) gas PE[1]

$\tilde{C}\ ^2A''$ [b] C_s
T^a = 22830(320) gas PE[1]

$\tilde{B}\ ^2A'$ C_s
T^a = 20980(320) gas PE[1]

$\tilde{A}\ ^2A'$ C_s
T^a = 17910(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			680(40)	gas	PE	2

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		SCl stretch	570(50)	gas	PE	1

[a] From vertical ionization potential.
[b] May be a vibrational component of the $\tilde{B}$ state.

References

[1]D. C. Frost, C. B. MacDonald, C. A. McDowell, and N. P. C. Westwood, J. Am. Chem. Soc. **103**, 4423 (1981).
[2]H. Leung, R. J. Suffolk, and J. D. Watts, Chem. Phys. **109**, 289 (1986).

BrSCN$^+$

$\tilde{G}\ ^2A'$ C_s
T^a = 55830(560) gas PE[1]

$\tilde{F}\ ^2A'$ C_s
T^a = 37680(320) gas PE[1]

$\tilde{E}\ ^2A''$ C_s
T^a = 30180(320) gas PE[1]

$\tilde{D}\ ^2A'$ C_s
T^a = 25580(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			400(60)	gas	PE	1

$\tilde{C}\ ^2A''$ C_s
T^a = 19280(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CN stretch	2050(60)	gas	PE	1

$\tilde{B}\ ^2A'$ C_s
T^a = 17180(320) gas PE[1]

$\tilde{A}\ ^2A'$ C_s
T^a = 13150(320) gas PE[1]

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		SBr stretch	450(50)	gas	PE	1

References

[1]D. C. Frost, C. B. MacDonald, C. A. McDowell, and N. P. C. Westwood, J. Am. Chem. Soc. **103**, 4423 (1981).

$ISCN^+$

$\tilde{D}\ ^2A'$ C_s
T^a = 24500(800) gas PE[1]

$\tilde{C}\ ^2A''$ C_s
T^a = 18000(800) gas PE[1]

$\tilde{B}\ ^2A'$ C_s
T^a = 17020(800) gas PE[1]

$\tilde{A}\ ^2A'$ C_s
T^a = 13960(800) gas PE[1]

$\tilde{X}\ ^2A''$ C_s

[a] From vertical ionization potentials.

References

[1]H. Leung, R. J. Suffolk, and J. D. Watts, Chem. Phys. **109**, 289 (1986).

$ClSeCN^+$

$\tilde{G}\ ^2A'$ C_s
T^a = 54540(320) gas PE[1]

$\tilde{F}\ ^2A'$ C_s
T^a = 38000(320) gas PE[1]

$\tilde{E}\ ^2A''$ C_s
T^a = 29530(320) gas PE[1]

$\tilde{D}\ ^2A'$ C_s
T^a = 26620(320) gas PE[1]

$\tilde{B},\tilde{C}\ ^2A'',^2A'$ C_s
$T^a \cong$ 21800 gas PE[1]

$\tilde{A}\ ^2A'$ C_s
T^a = 18070(320) gas PE[1]

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		SeCl stretch	440(50)	gas	PE	1

[a] From vertical ionization potentials.

References

[1]G. Jonkers, R. Mooyman, and C. A. de Lange, Mol. Phys. **43**, 655 (1981).

$BrSeCN^+$

$\tilde{G}\ ^2A'$ C_s
T^a = 54620(320) gas PE[1]

$\tilde{F}\ ^2A'$ C_s
T^a = 35660(320) gas PE[1]

$\tilde{E}\ ^2A''$ C_s
T^a = 28640(320) gas PE[1]

$\tilde{D}\ ^2A'$ C_s
T^a = 26300(320) gas PE[1]

$\tilde{C}\ ^2A'$ C_s
T^a = 20740(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CN stretch	1850(50)	gas	PE	1

$\tilde{B}\ ^2A''$ C_s
T^a = 18150(320) gas PE[1]

$\tilde{A}\ ^2A'$ C_s
T^a = 13720(320) gas PE[1]

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		SeBr stretch	360(50)	gas	PE	1

[a] From vertical ionization potentials.

References

[1]G. Jonkers, R. Mooyman, and C. A. de Lange, Mol. Phys. **43**, 655 (1981).

$(NO)_2^+$

$\tilde{A}$

Dissociates into NO + NO^+, with onset at 10700(1000) and maximum at 16400(1000). AB[1-4,6]PE[7]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO s-stretch	2090	gas	PI,PE TPE	5,7,9
	2	NNO s-bend	323	gas	TPE	9
	4	Torsion	118	gas	TPE	9
	5	NO a-stretch	1787.3T	Ne	IR	8

References

[1]J. A. Vanderhoff, J. Chem. Phys. **67**, 2332 (1977).
[2]R. R. Burke and R. P. Wayne, Int. J. Mass Spectrom. Ion Phys. **25**, 199 (1977).
[3]G. P. Smith, P. C. Cosby, and J. T. Moseley, J. Chem. Phys. **67**, 3818 (1977).
[4]G. P. Smith and L. C. Lee, J. Chem. Phys. **69**, 5393 (1978).
[5]S. H. Linn, Y. Ono, and C. Y. Ng, J. Chem. Phys. **74**, 3342 (1981).
[6]M. F. Jarrold, A. J. Illies, and M. T. Bowers, J. Chem. Phys. **79**, 6086 (1983).
[7]F. Carnovale, J. B. Peel, and R. G. Rothwell, J. Chem. Phys. **84**, 6526 (1986).
[8]M. E. Jacox and W. E. Thompson, J. Chem. Phys. **93**, 7609 (1990).
[9]I. Fischer, A. Strobel, J. Staecker, G. Niedner-Schatteburg, K. Müller-Dethlefs, and V. E. Bondybey, J. Chem. Phys. **96**, 7171 (1992).

$N_2S_2^+$

T^{ab}= 51310(320) gas PE[1,2]

T^{ab} = 32190(320) gas PE[1,2]

$\tilde{C}\ ^2B_{2u}$ D_{2h}

T^a = 15090(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			790(80)	gas	PE	1
			450(80)	gas	PE	1

$\tilde{B}\ ^2B_{3u}$ D_{2h}

T^a = 5160(320) gas PE[1,2]

$\tilde{A}\ ^2B_{3g}$ D_{2h}

T^a = 3630(320) gas PE[1,2]

$\tilde{X}\ ^2B_{2g}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			810(80)	gas	PE	1
			470(80)	gas	PE	1

[a] From vertical ionization potential.
[b] A large number of transitions have been calculated[3] to occur in this energy region.

References

[1]D. C. Frost, M. R. LeGeyt, N. L. Paddock, and N. P. C. Westwood, J. Chem. Soc., Chem. Commun. 217 (1977).
[2]R. H. Findlay, M. H. Palmer, A. J. Downs, R. G. Egdell, and R. Evans, Inorg. Chem. **19**, 1307 (1980).
[3]W. von Niessen, J. Schirmer, and L. S. Cederbaum, J. Chem. Soc., Faraday Trans. 2 **82**, 1489 (1986).

FN_3^+

$\tilde{E}\ ^2A'$ C_s

T^a = 58000(1050) gas PE[1]

$\tilde{D}\ ^2A'$ C_s

T^a = 45670(480) gas PE[1]

$\tilde{C}\ ^2A''$ C_s

T^a = 39450(1050) gas PE[1]

$\tilde{B}\ ^2A'$ C_s

T^a = 37030(1050) gas PE[1]

$\tilde{A}\ ^2A'$ C_s

T^a = 21860(480) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	N_3 a–stretch	1800T	gas	PE	1

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	N_3 s–stretch	800T	gas	PE	1

[a] From vertical ionization potentials.

References

[1]P. Rademacher, A. J. Bittner, G. Schatte, and H. Willner, Chem. Ber. **121**, 555 (1988).

ClN_3^+

$\tilde{F}\ ^2A'$ C_s

T^a = 67210(500) gas PE[1]

$\tilde{E}\ ^2A''$ C_s

T^a = 58010(500) gas PE[1]

$\tilde{D}\ ^2A'$ C_s

T^a = 46470(240) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			2100(60)	gas	PE	1
			1280(60)	gas	PE	1

$\tilde{B},\tilde{C}\ ^2A'',^2A'$ C_s

T^a = 25740(240) gas PE[1]

$\tilde{A}\ ^2A'$ C_s

T^a = 14520(240) gas PE[1]

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			730(60)	gas	PE	1

[a] From vertical ionization potential. The adiabatic ground–state ionization potential may lie 730(60) lower, increasing each T value by that amount.

References

[1]D. C. Frost, C. B. MacDonald, C. A. McDowell, and N. P. C. Westwood, Chem. Phys. **47**, 111 (1980).

BrN_3^+

$\tilde{F}\ ^2A'$ C_s
T^a = 64630(500) gas PE[1]

$\tilde{E}\ ^2A''$ C_s
T^a = 56800(500) gas PE[1]

$\tilde{D}\ ^2A'$ C_s
T^a = 45340(240) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1940(80)	gas	PE	1

$\tilde{C}\ ^2A'$ C_s
T^a = 22190(240) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1970(80)	gas	PE	1

$\tilde{B}\ ^2A''$ C_s
T^a = 19690(240) gas PE[1]

$\tilde{A}\ ^2A'$ C_s
T^a = 11130(240) gas PE[1]

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			710(60)	gas	PE	1

[a] From vertical ionization potential. The adiabatic ground–state ionization potential may lie 710(60) lower, increasing each T value by that amount.

References

[1]D. C. Frost, C. B. MacDonald, C. A. McDowell, and N. P. C. Westwood, Chem. Phys. **47**, 111 (1980).

Sb_4^-

Threshold for electron detachment from ground–state Sb_4^- < 8070(800) gas PE[1]

References

[1]M. L. Polak, G. Gerber, J. Ho, and W. C. Lineberger, J. Chem. Phys. **97**, 8990 (1992).

Bi_4^-

Threshold for electron detachment from ground–state Bi_4^- < 8470(800) gas PE[1,2]

References

[1]M. L. Polak, J. Ho, G. Gerber, and W. C. Lineberger, J. Chem. Phys. **95**, 3053 (1991).
[2]M. L. Polak, G. Gerber, J. Ho, and W. C. Lineberger, J. Chem. Phys. **97**, 8990 (1992).

FCCF

$\tilde{X}$ $D_{\infty h}$ Structure: IR[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	CC stretch	2436[a]	gas	IR	2,4
	2	CF s–stretch	787[a]	gas	IR	2,4
Σ_u^+	3	CF a–stretch	1349.524[b]	gas	IR	2–4
			1346.9vvs	Ne	IR	2
			1340.7vvs	Ar	IR	1,2
Π_g	4	Bend	270[a]	gas	IR	2,4
Π_u	5	Bend	268[a]	gas	IR	4
			286.7vw	Ar	IR	2
			279.3vw			

B_0 = 0.119 gas IR[2,4]

[a] From combination bands.
[b] Effective value. Correction for anharmonic perturbation gives 1348.665.

References

[1]J. C. Brahms and W. P. Dailey, J. Am. Chem. Soc. **111**, 8940 (1989).
[2]H. Bürger, W. Schneider, S. Sommer, W. Thiel, and H. Willner, J. Chem. Phys. **95**, 5660 (1991).
[3]H. Bürger and S. Sommer, J. Mol. Spectrosc. **151**, 148 (1992).
[4]D. McNaughton and P. Elmes, Spectrochim. Acta **48A**, 605 (1992).

$F_2C{=}C{:}$

$\tilde{a}\ ^3A_2$ C_{2v}
T_0 = 7455(70) gas PE[2]

$\tilde{X}\ ^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	C=C stretch	1670(25)	gas	PE	2
	2	CF_2 s-stretch	905(25)	gas	PE	2
	3	CF_2 scissors	510(25)	gas	PE	2
b_2	5	CF_2 a-stretch	1247T	Ne	IR	1

References

[1]H. Bürger, W. Schneider, S. Sommer, W. Thiel, and H. Willner, J. Chem. Phys. **95**, 5660 (1991).
[2]M. K. Gilles, W. C. Lineberger, and K. M. Ervin, J. Am. Chem. Soc. **115**, 1031 (1993).

FNCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NCO a-stretch	2177s 2167s	Ar	IR	1
	3	NF stretch	861s	Ar	IR	1
	4	NCO deform.	695wm	Ar	IR	1
	5	FNC deform.	529m	Ar	IR	1
a''	6	NCO deform.	646wm	Ar	IR	1

References

[1]K. Gholivand, H. Willner, D. Bielefeldt, and A. Haas, Z. Naturforsch. **39B**, 1211 (1984).

ClNCO

$\tilde{X}$ C_s Structure: MW[3,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NCO a-stretch	2212.2vs	gas	IR	1,2,5
	2	NCO s-stretch	1306.6w	gas	IR	1,2,5
	3		707.7wm	gas	IR	1,2,5
	4		607.7vw	gas	IR	5
a''	6	NCO bend	559.0wm	gas	IR	1,2,5

A_0 = 1.720; B_0 = 0.104; C_0 = 0.098 MW[3,4]

References

[1]E. Nachbaur and W. Gottardi, Montash. Chem. **97**, 115 (1966).
[2]H. H. Eysel and E. Nachbaur, Z. Anorg. Allg. Chem. **381**, 71 (1971).
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BrNCO

In the gas phase, an absorption maximum has been observed at 292 nm.[1]

$\tilde{X}$ C_s Structure: MW[2,3,6]IR[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NCO a-stretch	2198.0vs	gas	IR	1,4,5
			2196	Ne	IR	5
			2191.9	Ar	IR	5
	2	NCO s-stretch	1294.5w	gas	IR	1,4,5
			1290.9	Ne	IR	5
			1296.9	Ar	IR	5
	3	NCO bend	687.7w	gas	IR	1,4,5
			691.1	Ne	IR	5
			686.6	Ar	IR	5
	4	NBr stretch	506.0vw	Ne	IR	5
	5	BrNC bend	137.4w	Ne	IR	5
a''	6	NCO bend	569.9w	gas	IR	1,4,5
			572.2	Ne	IR	5
			563.1	Ar	IR	5

A_0 = 1.374; B_0 = 0.073; C_0 = 0.069 MW[2,3,6]

References

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INCO

$\tilde{X}$ C_s Structure: MW[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2201.1vs	gas	IR	2
			1298.1w	gas	IR	2
			667.0w	gas	IR	2
			462.3vw	gas	IR	2
			583.3w	gas	IR	2

A_0 = 1.354; B_0 = 0.057; C_0 = 0.055 MW[1]

References

[1]H. M. Jemson, W. Lewis-Bevan, N. P. C. Westwood, and M. C. L. Gerry, J. Mol. Spectrosc. **119**, 22 (1986).
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ClSCN

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CN stretch	2170w	gas	IR	2
	2	CS stretch	678.9wm	gas	IR	2
	3	SCl stretch	533.6wm	gas	IR	2

A_0 = 0.404; B_0 = 0.097; C_0 = 0.078 MW[1]

References

[1]R. J. Richards, R. W. Davis, and M. C. L. Gerry, J. Chem. Soc., Chem. Commun. 915 (1980).
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BrSCN

$\tilde{X}$ C_s Structure: MW[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CN stretch	2145.1wm	gas	IR	1
	2	CS stretch	674.2ms	gas	IR	1
	3	BrS stretch	455.8m	gas	IR	1

A_0 = 0.337; B_0 = 0.065; C_0 = 0.054 MW[2]

References

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[2]H. N. Jemson, W. Lewis-Bevan, and M. C. L. Gerry, Can. J. Chem. **65**, 2478 (1987).

ISCN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CN stretch	2124.2vs	gas	IR	1
		CS stretch	668.0wm	gas	IR	1

References

[1]T. C. DeVore, J. Mol. Struct. **162**, 287 (1987).

ClCNO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CNO a-stretch	2281.4 2261.7	Ar	IR	1
		CNO s-stretch	1326.3	Ar	IR	1

References

[1]G. Maier and J. H. Teles, Angew Chem. **99**, 152 (1987); Angew. Chem. Int. Ed. Engl. **26**, 155 (1987).

BrCNO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CNO a-stretch	2271.3 2252.5	Ar	IR	1
		CNO s-stretch	1305.6	Ar	IR	1

References

[1]G. Maier and J. H. Teles, Angew Chem. **99**, 152 (1987); Angew. Chem. Int. Ed. Engl. **26**, 155 (1987).

FN_3

$\tilde{X}$ C_s Structure: MW[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	N≡N stretch	2037.0vs	gas	IR	2
			2031.0	Ar	IR	1,2
	2	N=N stretch	1090.0m	gas	IR	2
			1085.6	Ar	IR	1,2
	3	NF stretch	873.5s	gas	IR	2
			868.1	Ar	IR	1,2
	4	Deform.	658.0m	gas	IR	2
			652.1	Ar	IR	1,2
	5	Deform.	241.0m	gas	IR	2
			239.9	Ar	IR	2
a''	6	Deform.	504.0w	gas	IR	2
			502.8	Ar	IR	1,2

A_0 = 1.605; B_0 = 0.191; 0.170 MW[2]

References

[1]D. E. Milligan and M. E. Jacox, J. Chem. Phys. **40**, 2461 (1964).
[2]D. Christen, H. G. Mack, G. Schatte, and H. Willner, J. Am. Chem. Soc. **110**, 707 (1988).

CO_3

A broad, weak absorption with maximum at 406 nm has been assigned[4] to CO_3 trapped in a CO_2 matrix. The threshold for the photodissociation of CO_3 into CO_2 + O in this system lies near 500 nm.

$\tilde{X}$ C_{2v} Structure: IR[3]MO[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	C=O stretch	2045.1	Ne	IR	6
			2053[a]	Ar	IR	2
			2045vs	CO_2	IR	1,3
	2	O–O stretch	1070	Ar	IR	2
			1073m	CO_2	IR	1,3
	3	C–O stretch	593m	CO_2	IR	1,3
b_2	5	C–O stretch	975	Ar	IR	2
			972s	CO_2	IR	1,3
	6	O–C=O bend	564	Ar	IR	2
			568m	CO_2	IR	1,3

[a] Fermi resonance with overtone of fundamental at 975 leads to appearance of another very prominent absorption at 1894 (1880 in CO_2 matrix experiments).

References

[1]N. G. Moll, D. R. Clutter, and W. E. Thompson, J. Chem. Phys. **45**, 4469 (1966).
[2]E. Weissberger, W. H. Breckenridge, and H. Taube, J. Chem. Phys. **47**, 1764 (1967).

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[6]M. E. Jacox and W. E. Thompson, J. Phys. Chem. **95**, 2781 (1991).

c–$(NO)_2$

$\tilde{X}$ C_{2v} Structure: MW[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NO s–stretch	1868.25	gas	IR,DL	3,11,13
			1867.2	Ne	IR	12
			1866m	Ar	IR	1
			1870	N_2	IR	2
			1862m	CO_2	IR,Ra	1,6
			1866	NO	IR,Ra	4,5,8
	2	N··N stretch	262	CO_2	Ra	6
			266	NO	IR,Ra	4,5,8
	3	NNO s–bend	161	CO_2	Ra	6,8
			187	NO	Ra	4,5,8
a_2	4	Torsion	88.2[a]	gas	IR	9
			97	NO	IR,Ra	4,5,8
b_2	5	NO a–stretch	1789	gas	IR,DL	3,9,10
						11
			1780.6	Ne	IR	12
			1778.7			
			1776s	Ar	IR	1
			1785	N_2	IR	2
			1768s	CO_2	IR	1
			1762	NO	IR,Ra	5,8
	6	NNO a–bend	202	CO_2	Ra	6,8
			214	NO	Ra	4,5,8

A_0 = 0.862; B_0 = 0.187; C_0 = 0.154 MW[7]IR[13]

[a] From observation of $\nu_5 - \nu_4$ = 1700.8 cm^{-1}.

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[1]W. G. Fateley, H. A. Bent, and B. Crawford, Jr., J. Chem. Phys. **31**, 204 (1959).
[2]W. A. Guillory and C. E. Hunter, J. Chem. Phys. **50**, 3516 (1969).
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[13]B. J. Howard and A. R. W. McKellar, Mol. Phys. **78**, 55 (1993).

t–$(NO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_u	5	Asym. stretch	1762.5	Ne	IR	3
			1760.6			
			1764	N_2	IR	2
			1740	CO_2	IR	1

References

[1]W. G. Fateley, H. A. Bent, and B. Crawford, Jr., J. Chem. Phys. **31**, 204 (1959).
[2]W. A. Guillory and C. E. Hunter, J. Chem. Phys. **50**, 3516 (1969).
[3]M. E. Jacox and W. E. Thompson, J. Chem. Phys. **93**, 7609 (1990).

NS–SN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SN a–stretch	1167.5	Ar	IR	1

References

[1]P. Hassanzadeh and L. Andrews, J. Am. Chem. Soc. **114**, 83 (1992).

$(PO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		PO stretch	1155.0	Ar	IR	1

References

[1]Z. Mielke, M. McCluskey, and L. Andrews, Chem. Phys. Lett. **165**, 146 (1990).

F_2BO

$\tilde{C}\ ^2A_1$ [a] C_{2v}

T_0 = 22390.9(4) gas EM[3] $\tilde{C}$–$\tilde{X}$ 446–447 nm
gas EM[1,2] $\tilde{C}$–$\tilde{A}$ 554–633 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	BF stretch	875	gas	EM	1
	3	BF_2 scissors	480.6	gas	EM	1,2

C_0 = 0.176 EM[3]

$\tilde{A}\ ^2B_1$ [a] C_{2v}

T_0 = 5220[a] gas EM[1,2] $\tilde{C}$–$\tilde{A}$ 554–633 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	BO stretch	1369	gas	EM	1
	2	BF stretch	856.0	gas	EM	1,2
	3	BF_2 scissors	491.0	gas	EM	1,2

$\tilde{X}\ ^2B_2$ [a] C_{2v}

C_0 = 0.176 EM[3]

[a] See Ref. 4.

References

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BF_3^+

$\tilde{E}\ ^2A_1'$ D_{3h}

$T_0 \cong$ 47800 gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	BF stretch	800T	gas	PE	3

τ = 10 ns gas EM[5]

$\tilde{D}\ ^2E'$ D_{3h}

T_0 = 34860(160) gas PE[1,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	BF stretch	742(20)	gas	PE	1,4

Additional structure reported by Ref. 4 has been attributed to vibronic coupling.

$\tilde{C}\ ^2A_2''$ D_{3h}

T_0 = 27110(80) gas PE[1,2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	BF stretch	830(20)	gas	PE	2,4

$\tilde{B}\ ^2E'$ D_{3h}

T_0 = 10890(240) gas PE[1,2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	BF stretch	770(60)	gas	PE	1,4

$\tilde{A}\ ^2E''$ D_{3h}

T_0 = 5890(240) gas PE[1,4]

$\tilde{X}\ ^2A_2'$ D_{3h}

Structure reported by Ref. 4 has been attributed to vibronic coupling.

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[1]P. J. Bassett and D. R. Lloyd, J. Chem. Soc. A 1551 (1971).
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BCl_3^+

$\tilde{E}\ ^2A_1'$ D_{3h}

T_0 = 49200(560) gas PE[1]

Emission which is observed between 250 and 650 nm on excitation of BCl_3 by radiation of wavelength shorter than 70 nm (17.68 eV) has been attributed[4] to various transitions arising from the $\tilde{E}$ state of BCl_3^+.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	BCl stretch	440(60)	gas	PE	1

$\tilde{D}\ ^2E'$ D_{3h}

T_0 = 29700(320) gas PE[1]

A shoulder 1450(160) above the band maximum may result from spin–orbit coupling or from the Jahn–Teller effect.

Emission which is observed between about 300 and 650 nm on excitation of BCl_3 by radiation of wavelength shorter than 81 nm (15.36 eV) arises from the $\tilde{D}$ state of BCl_3^+.[3,4] The emission between 330 and 420 nm has been attributed to the $\tilde{D}$–$\tilde{X}$ transition of BCl_3^+, and that between 420 and 580 nm, with vibrational spacings of ca. 445, to the $\tilde{D}$–$\tilde{X}$,$\tilde{B}$ transitions.[3]

A broad absorption with maximum at 320 nm (31200) which appears on argon-resonance photolysis of BCl_3 isolated in an argon matrix and which can be destroyed by prolonged exposure of the sample to 340–600 nm radiation has been assigned[2] to the $\tilde{D}$–$\tilde{X}$ transition of BCl_3^+.

$\tilde{C}\ ^2A_2''$ D_{3h}

T_0 = 20800(320) gas PE[1]

Emission which is observed between 400 and 550 nm on excitation of BCl_3 by radiation of wavelength shorter than 88 nm has been attributed to the $\tilde{C}$–$\tilde{X}$ transition of BCl_3^+, and emission between 550 and 750 nm has been attributed to the $\tilde{C}$–$\tilde{A}$ transition of this species.[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	BCl stretch	440(30)	gas	PE	1

$\tilde{B}\ ^2E'$
T^a = 8230(240) gas PE[1]

$\tilde{A}\ ^2E''$ D_{3h}
T_0 = 4440(480) gas PE[1]

$\tilde{X}$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	3	BCl stretch	1090	Ar	IR	2

[a] From vertical ionization potential.

References

[1]P. J. Bassett and D. R. Lloyd, J. Chem. Soc. A 1551 (1971).
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BBr_3^+

$\tilde{F}$
$T \cong$ 53500(480) gas PE[1]

$\tilde{E}\ ^2A_1'$ D_{3h}
T_0 = 49380(560) gas PE[1]

$\tilde{D}\ ^2E'$ D_{3h}
T_0^a = 25500(400) gas PE[1]

A broad absorption with maximum at 355 nm (28200) which appears on argon-resonance photolysis of BBr_3 isolated in an argon matrix and which can be destroyed by prolonged exposure of the sample to 340–600 nm radiation has been assigned[2] to the $\tilde{D}$–$\tilde{X}$ transition of BBr_3^+.
A = 2180(160) gas PE[1]

$\tilde{C}\ ^2A_2''$ D_{3h}
T_0 = 19200(480) gas PE[1]

$\tilde{B}\ ^2E''$ D_{3h}
T^b = 9680(480) gas PE[1]

$\tilde{A}\ ^2E'$ D_{3h}
T_0^a = 5000(400) gas PE[1]
A = 1130 gas PE[1]

$\tilde{X}\ ^2A_2'$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	3	BBr stretch	930	Ar	IR	2

[a] Onset of transition.
[b] From vertical ionization potential.

References

[1]P. J. Bassett and D. R. Lloyd, J. Chem. Soc. A 1551 (1971).
[2]J. H. Miller and L. Andrews, J. Am. Chem. Soc. **102**, 4900 (1980).

BI_3^+

$\tilde{E}\ ^2A_1'$ D_{3h}
T_0 = 47200(400) gas PE[1]

$\tilde{D}\ ^2E'$ D_{3h}
T_0^a = 24450(480) gas PE[1]
A = 4030(80) gas PE[1]

$\tilde{C}\ ^2A_2''$ D_{3h}
T_0 = 18640(400) gas PE[1]

$\tilde{B}\ ^2E''$ D_{3h}
T_0^a = 8310(400) gas PE[1]
A = 810(160) gas PE[1]

$\tilde{A}\ ^2E'$ D_{3h}
T_0^a = 4840(400) gas PE[1]
A = 1450(160) gas PE[1]

$\tilde{X}\ ^2A_2'$ D_{3h}

[a] Onset of transition.

References

[1]P. J. Bassett and D. R. Lloyd, J. Chem. Soc. A 1551 (1971).

AlF_3^+

$\tilde{E}\ ^2A_1'$ D_{3h}
T^a = 37440(320) gas PE[1]

$\tilde{C},\tilde{D}\ ^2A_2'',^2E'$ D_{3h}
T^a = 13070(320) gas PE[1]

$\tilde{B}\ ^2E'$ D_{3h}
T^a = 5240(320) gas PE[1]

$\tilde{X}\ ^2A_2'$ D_{3h}

[a] From vertical ionization potentials.

References

[1]J. M. Dyke, C. Kirby, A. Morris, B. W. J. Gravenor, R. Klein, and P. Rosmus, Chem. Phys. **88**, 289 (1984).

$AlCl_3^+$

$\tilde{E}\ ^2A_1'$ D_{3h}
T^a = 31950(320) gas PE[1,2]

$\tilde{D}\ ^2E'$ D_{3h}
T^a = 16380(320) gas PE[1,2]

$\tilde{C}\ ^2A_2''$ D_{3h}
T^a = 10650(320) gas PE[1,2]

$\tilde{B}\ ^2E''$ D_{3h}
T^a = 5810(320) gas PE[1,2]

$\tilde{A}\ ^2E'$ D_{3h}
$T^a \cong 3700$ gas PE[1,2]

$\tilde{X}\ ^2A_2''$ D_{3h}

[a] From vertical ionization potentials.

References

[1]M. F. Lappert, J. B. Pedley, G. J. Sharp, and N. P. C. Westwood, J. Electron Spectrosc. Relat. Phenom. **3**, 237 (1974).
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$AlBr_3^+$

$\tilde{E}\ ^2A_1'$ D_{3h}
T^a = 34860(320) gas PE[1,2]

$\tilde{D}\ ^2E'$ D_{3h}
T^a = 18190(320) gas PE[1,2]
A = 2500(320) gas PE[1,2]

$\tilde{C}\ ^2A_2''$ D_{3h}
T^a = 11780(320) gas PE[1,2]

$\tilde{B}\ ^2E''$ [b] D_{3h}
T^a = 6700(320) gas PE[1,2]

$\tilde{A}\ ^2E'$ [b] D_{3h}
T^a = 5000(320) gas PE[1,2]

$\tilde{X}\ ^2A_2'$ D_{3h}

[a] From vertical ionization potentials.
[b] $\tilde{A}$ and $\tilde{B}$ levels mixed by spin–orbit interaction.

References

[1]M. F. Lappert, J. B. Pedley, G. J. Sharp, and N. P. C. Westwood, J. Electron Spectrosc. Relat. Phenom. **3**, 237 (1974).
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CO_3^-

$\tilde{X}\ ^2B_1$ C_{2v} Structure: MO^2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	OCO s–stretch	1314[a] Cs	Ar	IR	1
			1308[a] K	Ar	IR	1
			1308[a] Na	Ar	IR	1
b_2	5	OCO a–stretch	1480[a] Cs	Ar	IR	1
			1494[a] K	Ar	IR	1
			1513[a] Na	Ar	IR	1

[a] Assignment given for structure obtained in *ab initio* calculation of Ref. 2. D_{3h} structure cannot be excluded on the basis of the infrared observations; NO_3^-, known to have a D_{3h} structure, exhibits a similar splitting for its NO–stretching fundamentals in an argon matrix, due to the electric field of the cation.

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[2]S. P. So, J. Chem. Soc., Faraday Trans. 2 **72**, 646 (1976).

FC(O)O

$\tilde{B}\ ^2A_1$ C_{2v}
T_0 = 13150 gas AB[1,2] $\tilde{B}$–$\tilde{X}$ 500–795 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF stretch	1110	gas	AB	1
	3	OCO bend	610	gas	AB	1
b_1	4	OPLA	840	gas	AB	1
b_2	5	OCO a–stretch	2820	gas	AB	1

$\tilde{X}\ ^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	OCO bend	520	gas	AB	1

References

[1]M. M. Maricq, J. J. Szente, Z. Li, and J. S. Francisco, J. Chem. Phys. **98**, 784 (1993).
[2]M. M. Maricq, J. J. Szente, G. A. Khitrov, and J. S. Francisco, J. Chem. Phys. **98**, 9522 (1993).

$F_2C{=}C{:}^-$

Threshold for electron detachment from ground-state $F_2C{=}C{:}^-$ = 18190(50) gas PE[1]

$\tilde{X}\ ^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF_2 s–stretch	800(35)	gas	PE	1
	3	CF_2 scissors	505(25)	gas	PE	1

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[1]M. K. Gilles, W. C. Lineberger, and K. M. Ervin, J. Am. Chem. Soc. **115**, 1031 (1993).

F_2CN

$\tilde{C}\ ^2A_1$ C_{2v} Structure: AB^1

T_0 = 27639.8 gas AB^1 $\tilde{C}-\tilde{X}$ 338–362 nm
27650(40) Ar AB^2 $\tilde{C}-\tilde{X}$ 338–362 nm
27660(40) N_2 AB^2 $\tilde{C}-\tilde{X}$ 338–362 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CN stretch	1884	gas	AB	1
			1808(80)	Ar	AB	2
			1879(80)	N_2	AB	2
	2	CF stretch	900	gas	AB	1
	3	CF_2 scissors	568	gas	AB	1
			586(80)	Ar	AB	2
			641(80)	N_2	AB	2

C_0 = 0.196 AB^1

$\tilde{X}\ ^2B_2$ C_{2v} Structure: AB^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	C=N stretch	1734vs[a]	Ar	IR	2
			1771vs			
	2	CF stretch	955ms	Ar	IR	2
b_1	4	OPLA	660m	Ar	IR	2
b_2	5	CF stretch	1257vs	Ar	IR	2
	6	CF_2 rock	497ms	N_2	IR	2

C_0 = 0.195 AB^1

[a] Strong Fermi resonance interaction with $(\nu_5 + \nu_6)$ (A_1).

References

[1]R. N. Dixon, G. Duxbury, R. C. Mitchell, and J. P. Simons, Proc. Roy. Soc. (London) **A300**, 405 (1967).
[2]M. E. Jacox and D. E. Milligan, J. Chem. Phys. **48**, 4040 (1968).

F_2CO^+

$\tilde{F}\ ^2B_1$ C_{2v}

T^a = 54700(900) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF stretch	760(40)	gas	PE	1,2

$\tilde{E}\ ^2A_1$ C_{2v}

T_0 = 49000(500) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			490(40)	gas	PE	2

$\tilde{C},\tilde{D}\ ^2B_2,^2A_2$ C_{2v}

T_0 = 31390(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO stretch	1500(40)	gas	PE	2
	3	CF_2 scissors	555(40)	gas	PE	2

$\tilde{B}\ ^2A_1$ C_{2v}

T_0 = 24850(900) gas PE[1,2]

$\tilde{A}\ ^2B_1$ C_{2v}

T_0 = 8630(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO stretch	1430(40)	gas	PE	1,2
	2	CF_2 stretch	920(40)	gas	PE	2
	3	CF_2 scissors	505(40)	gas	PE	2

$\tilde{X}\ ^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO stretch	1550(40)	gas	PE	1,2
	3	CF_2 scissors	530(40)	gas	PE	1,2

[a] From vertical ionization potential.

References

[1]C. R. Brundle, M. B. Robin, N. A. Kuebler, and H. Basch, J. Am. Chem. Soc. **94**, 1451 (1972).
[2]R. K. Thomas and H. Thompson, Proc. Roy. Soc. (London) **A327**, 13 (1972).

Cl_2CO^+

$\tilde{H}\ ^2A_1$ C_{2v}

T_0^a = 62450(320) gas PE[1,2]

$\tilde{G}\ ^2B_2$ C_{2v}

T^{ab} = 44860(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO stretch	1000T	gas	PE	1

$\tilde{F}\ ^2B_1$ C_{2v}

T_0^a = 41230(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CCl_2 scissors	280(40)	gas	PE	1,2

$\tilde{E}\ ^2A_1$ C_{2v}

T_0[a] = 34290(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO stretch	1460(20)	gas	PE	2
	2	CCl_2 stretch	560(60)	gas	PE	1,2
	3	CCl_2 scissors	270(50)	gas	PE	1,2

$\tilde{D}\ ^2A_1$ C_{2v}

T_0[a] = 14850(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CCl_2 scissors	290(40)	gas	PE	1,2

$\tilde{C}\ ^2A_2$ C_{2v}

T^{ab} = 12100(560) gas PE[1,2]

$\tilde{A},\tilde{B}\ ^2B_1,^2B_2$ C_{2v}

T^{ab} = 8500(1000) gas PE[1,2]

$\tilde{X}\ ^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CCl_2 scissors	285(40)	gas	PE	1,2

[a] The first ionization potential is taken as 11.55(2) eV, the value given by Ref. 1. Ref. 2 estimates an adiabatic ionization potential of 11.2 eV.
[b] From vertical ionization potential.

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F_2CS^+

$\tilde{D}\ ^2A_2$ C_{2v}

T_0 = 57690(320) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF_2 stretch	700(40)	gas	PE	1-3
	3	CF_2 scissors	500(40)	gas	PE	1,3

$\tilde{C}\ ^2B_2$ C_{2v}

$T^a \cong$ 48200 gas PE[1,3]

$\tilde{B}\ ^2A_1$ C_{2v}

T_0 = 35420(320) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CS stretch	1160(60)	gas	PE	1-3
	2	CF_2 stretch	694(40)	gas	PE	3
	3	CF_2 scissors	462(40)	gas	PE	3

$\tilde{A}\ ^2B_1$ C_{2v}

T_0 = 7020(320) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CS stretch	1360(60)	gas	PE	1-3
	2	CF_2 stretch	730(40)	gas	PE	1-3
	3	CF_2 scissors	480(40)	gas	PE	1,3

$\tilde{X}\ ^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CS stretch	1350(40)	gas	PE	1-3
	2	CF_2 stretch	758(40)	gas	PE	3
	3	CF_2 scissors	460(40)	gas	PE	1-3

[a] From vertical ionization potential.

References

[1]K. Wittel, A. Haas, and H. Bock, Chem. Ber. **105**, 3865 (1972).
[2]H. W. Kroto and R. J. Suffolk, Chem. Phys. Lett. **17**, 213 (1972).
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$FCICS^+$

$\tilde{F}\ ^2A'$ C_s

T^a = 62930(400) gas PE[1]

$\tilde{E}\ ^2A'$ C_s

T^a = 51640(400) gas PE[1]

$\tilde{D}\ ^2A''$ C_s

T^a = 32110(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CS stretch	1130(40)	gas	PE	1

$\tilde{C}\ ^2A'$ C_s

T^a = 27270(320) gas PE[1]

$\tilde{B}\ ^2A'$ C_s

T^a = 21380(320) gas PE[1]

$\tilde{A}\ ^2A''$ C_s
T_0 = 8070(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CS stretch	1080(40)	gas	PE	1

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CS stretch	1130(40)	gas	PE	1

[a] From vertical ionization potentials.

References

[1]K. Wittel, A. Haas, and H. Bock, Chem. Ber. **105**, 3865 (1972).

Cl_2CS^+

$\tilde{H}\ ^2A_1$ C_{2v}
T_0 = 68420(320) gas PE[1-3]

$\tilde{G}\ ^2B_2$ C_{2v}
T_0 = 51480(320) gas PE[1-3]

$\tilde{F}\ ^2B_1$ C_{2v}
T_0 = 43410(320) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CCl_2 scissors	270(80)	gas	PE	3

$\tilde{E}\ ^2A_1$ C_{2v}
T_0 = 37280(320) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCl_2 stretch	380(60)	gas	PE	1,3

$\tilde{D}\ ^2A_2$ C_{2v}
T_0 = 24850(320) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CCl_2 scissors	260(40)	gas	PE	1,3

$\tilde{C}\ ^2B_2$ C_{2v}
T_0 = 22350(320) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CCl_2 scissors	255(80)	gas	PE	3

$\tilde{B}\ ^2A_1$ C_{2v}
T_0 = 16620(320) gas PE[1-3]

$\tilde{A}\ ^2B_1$ C_{2v}
T_0 = 8390(320) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CS stretch	900(60)	gas	PE	1-3

$\tilde{X}\ ^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CS stretch	1060(40)T	gas	PE	1,3
	3	CCl_2 scissors	265(40)	gas	PE	1,3

[a] From vertical ionization potential.

References

[1]D. Chadwick, Can. J. Chem. **50**, 737 (1972).
[2]K. Wittel, A. Haas, and H. Bock, Chem. Ber. **105**, 3865 (1972).
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F_2CSe^+

$\tilde{C}\ ^2B_2$ C_{2v}
T_0 = 50800(1600) gas PE[1]

$\tilde{B}\ ^2A_1$ C_{2v}
T_0 = 37900(1600) gas PE[1]

$\tilde{A}\ ^2B_1$ C_{2v}
T_0 = 9700(1600) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1380(100)	gas	PE	1
			650(100)	gas	PE	1

$\tilde{X}\ ^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1380(50)	gas	PE	1
	3	CF_2 scissors	400(50)	gas	PE	1

[a] From vertical ionization potentials.

References

[1]H. Bock, S. Aygen, P. Rosmus, B. Solouki, and E. Weissflog, Chem. Ber. **117**, 187 (1984).

NNO_2^-

Photoelectron spectra[2] of NNO_2^- indicate that at both 532 and 355 nm dissociation into $N_2O + O^-$ occurs.

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NN stretch	1359.6wm	Ne	IR	4
			1355w	Ar	IR	1,3,4
	2	NO_2 s-stretch	1004.5wm	Ne	IR	4
			1008w	Ar	IR	1,3,4
b_2	5	NO_2 a-stretch	1199.3m	Ne	IR	4
			1205.5m	Ar	IR	1,3

References

[1]D. E. Milligan and M. E. Jacox, J. Chem. Phys. **55**, 3404 (1971).
[2]L. A. Posey and M. A. Johnson, J. Chem. Phys. **88**, 5383 (1988).
[3]J. Hacaloglu, S. Suzer, and L. Andrews, J. Phys. Chem. **94**, 1759 (1990).
[4]M. E. Jacox, J. Chem. Phys. **93**, 7622 (1990).

$c\text{-}(NO)_2^-$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	5	Asym. stretch	1424.1T	Ne	IR	1

References

[1]M. E. Jacox and W. E. Thompson, J. Chem. Phys. **93**, 7609 (1990).

$t\text{-}(NO)_2^-$

In gas-phase photoelectron spectra[2] taken at 532 nm, evidence was obtained for both electron detachment and photodissociation into $NO + NO^-$.

$\tilde{X}$ C_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	NO s-stretch	2064.7[a]	Ne	IR	4
b_u	5	NO a-stretch	1619.2	Ne	IR	4
			1593.3	Ar	IR	1,3,4

[a] $(\nu_1 + \nu_5) - \nu_5$.

References

[1]M. E. Jacox and D. E. Milligan, J. Mol. Spectrosc. **48**, 536 (1973).
[2]L. A. Posey and M. A. Johnson, J. Chem. Phys. **88**, 5383 (1988).
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[4]M. E. Jacox and W. E. Thompson, J. Chem. Phys. **93**, 7609 (1990).

$t\text{-}N_2F_2^+$

T_0 = 42000(1600) gas PE[1]

$\tilde{A}\ ^2A_u$ C_{2h}

T_0 = 6860(1200) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g			980(80)	gas	PE	1

$\tilde{X}\ ^2A_g$ C_{2h}

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[1]C. R. Brundle, M. B. Robin, N. A. Kuebler, and H. Basch, J. Am. Chem. Soc. **94**, 1451 (1972).

NO_3

$\tilde{B}\ ^2E'$ D_{3h}

T_0 = 15089 gas $AB^{1,2,4-7}LF^{8,9,17}$ $\tilde{B}\text{-}\tilde{X}$ 450–795 nm
All bands are diffuse.[2,7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	930	gas	AB	2,6
			1450	gas	AB	6
			850	gas	AB	6

τ_0 = 340(20) μs gas LF^{10}

$\tilde{A}\ ^2E''$ D_{3h}

T_0 = 7000(110) gas PE[14]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	804(4)T	gas	PE	14
e'	4	Deformation	541(8)T	gas	PE	14

$\tilde{X}\ ^2A_2'$ D_{3h} Structure: DL[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	1050	gas	LF,PE	8,9,14,17
a_2''	2	OPLA	762.33	gas	IR,LF	12,17
e'	3	NO stretch[a]	1492.39	gas	LF,DL	8,9,11,17
					IR	12
	4	Deformation[b]	360	gas	LF,PE	8,9,14,17

B_0 = 0.459 $DL^{11,13}IR^{12}$

[a] Anomalous structure appears in the high resolution spectrum of this band because of vibronic coupling with the $\tilde{B}\ ^2E'$ state.[16] Coupling with this state and with the $\tilde{A}\ ^2E''$ state leads to the appearance of infrared absorptions of several prominent overtone and combination bands between 1900 and 2600.[15,18] Among these bands, also observed in fluorescence,[8,17] is one near 2020, attributed by Ref. 17 to the occurrence of pseudorotation on the ground-state potential surface but by Ref. 15 to intensification of the fourth overtone of ν_4, which has appreciable "negative" anharmonicity, as a result of vibronic interaction with the $\tilde{A}$ and $\tilde{B}$ states.
[b] Coupled to the $\tilde{B}\ ^2E'$ state through this mode.[14]

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[2]D. A. Ramsay, Proc. Xth Colloq. Spectroscopicum Internationale, E. R. Lippincott and M. Margoshes, Eds., (Spartan Books, Washington, D. C., 1963) pp. 593–596.
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[17]B. Kim, P. L. Hunter, and H. S. Johnston, J. Chem. Phys. **96**, 4057 (1992).
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NSSS [a]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NS stretch	1309.5s	Ar	IR	1
		SS stretch	624.2m	Ar	IR	1

[a] Alternatively, peaks may have been contributed by SSNS.

References

[1]P. Hassanzadeh and L. Andrews, J. Am. Chem. Soc. **114**, 83 (1992).

FNO_2^+

$\tilde{G}\ ^2B_2$ C_{2v}
T_a = 52520(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1000(80)	gas	PE	1

$\tilde{F}\ ^2A_1$ C_{2v}
T_a = 46900(1000) gas PE[1]

$\tilde{E}\ ^2B_1$ C_{2v}
T_0 = 39600(1000) gas PE[1]

$\tilde{C},\tilde{D}\ ^2B_2,^2B_1$ C_{2v}
Transitions between approximately 15400 and 32400.[1]

$\tilde{B}\ ^2B_2$ C_{2v}
T_0 = 8960(1000) gas PE[1]

$\tilde{A}\ ^2A_1$ C_{2v}
T_a = 6620(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1170(80)	gas	PE	1

$\tilde{X}\ ^2A_2$ C_{2v}

[a] From vertical ionization potential.

References

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$ClNO_2^+$

$\tilde{E},\tilde{F},\tilde{G}$ C_{2v}
Transitions between approximately 50500 and 62600.[1]

$\tilde{D}\ ^2B_2$ C_{2v}
T_a = 14360(160) gas PE[1]

$\tilde{C}\ ^2A_1$ C_{2v}
T_0 = 9440(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			850(80)	gas	PE	1

$\tilde{B}\ ^2A_2$ C_{2v}
T_0 = 4520(160) gas PE[1]

$\tilde{X}\ ^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	NO_2 scissors	420(80)[b]	gas	PE	1

[a] From vertical ionization potential.
[b] Weak structure in first photoelectron band, possibly contributed by low-lying $\tilde{A}\ ^2B_1$ state.

References

[1]D. C. Frost, S. T. Lee, C. A. McDowell, and N. P. C. Westwood, J. Electron Spectrosc. Relat. Phenom. **7**, 331 (1975).

PO_3

$\tilde{B}\ ^2E'$ [a] D_{3h}

T_0 = 14378 Ar AB^2 $\tilde{B}$–$\tilde{X}$ 589–696 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	PO_3 s–stretch	913(10)	Ar	IR	2
e'	4	Deformation	525(10)	Ar	IR	2

$\tilde{X}$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	480.3	Ar	IR	1
e'	3	PO stretch	1273.3	Ar	IR	1
	4	Deformation	435.2	Ar	IR	1

[a] Tentative assignment, by analogy with NO_3.

References

[1]R. Withnall and L. Andrews, J. Phys. Chem. **92**, 4610 (1988).
[2]R. Withnall, M. McCluskey, and L. Andrews, J. Phys. Chem. **93**, 126 (1989).

t–O_4^+

In the gas phase, the high frequency tail of a photodissociation continuum, resulting in the formation of $O_2^+ + O_2$, has been observed[1–3] between 450 and 680 nm.

$\tilde{X}$ C_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	O=O s–stretch	1644.1[a]	Ne	IR	4
b_u	5	O=O a–stretch	1164.4	Ne	IR	4

[a] $(\nu_1 + \nu_5) - \nu_5$.

References

[1]R. A. Beyer and J. A. Vanderhoff, J. Chem. Phys. **65**, 2313 (1976).
[2]M. L. Vestal and G. H. Mauclaire, J. Chem. Phys. **67**, 3767 (1977).
[3]G. P. Smith, P. C. Cosby, and J. T. Moseley, J. Chem. Phys. **67**, 3767 (1977).
[4]W. E. Thompson and M. E. Jacox, J. Chem. Phys. **91**, 3826 (1989).

cyc–O_4^+

$\tilde{X}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		O=O s–stretch	1628.3[a]	Ne	IR	1,2
		O=O a–stretch	1320.3	Ne	IR	1,2

[a] $(\nu_1 + \nu_5) - \nu_5$.

References

[1]W. E. Thompson and M. E. Jacox, J. Chem. Phys. **91**, 3826 (1989).
[2]M. E. Jacox and W. E. Thompson, J. Chem. Phys. **100** (Jan. 1, 1994)

SO_3^+ [a]

$\tilde{E}\ ^2A_1'$ D_{3h}

T[b] = 62770(320) gas PE[3]

$\tilde{D}\ ^2E'$ D_{3h}

T_0 = 40990(160) gas PE[1–3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	SO_3 stretch	890(20)	gas	PE	1–4
e'	3	SO_3 stretch	1390	gas	PE	4
	4	Deformation	420(50)	gas	PE	2,4

$\tilde{C}\ ^2A_2''$ D_{3h}

T_0 = 16470(120) gas PE[1–3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	SO_3 stretch	890(50)	gas	PE	1–3

$\tilde{A},\tilde{B}\ ^2E',^2E''$ D_{3h}

T_0 = 7930(120) gas PE[1–3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	SO_3 stretch	730(50)	gas	PE	1–3
e'	4	Deformation	480(50)	gas	PE	1,3

$\tilde{X}\ ^2A_2'$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	SO_3 stretch	920(50)	gas	PE	1,2
e'	4	Deformation	440(50)	gas	PE	1–3

[a] Refs. 1–3 disagree on the assignment of the spectrum. The assignment given here is that of Ref. 2; the calculations of both Ref. 2 and Ref. 3 indicate that the ground state possesses A_2' symmetry, and the detailed analysis of the effect of Jahn–Teller perturbation given by Ref. 4 has provided a good fit to the structure of the 17.86 eV photoelectron band for the $\tilde{D}\ ^2E'$ assignment of Ref. 2.
[b] From vertical ionization potential.

References

[1]G. W. Mines and R. K. Thomas, Proc. Roy. Soc. (London) **A336**, 355 (1974).
[2]D. S. Alderdice and R. N. Dixon, J. Chem. Soc., Faraday Trans. 2 **72**, 372 (1976).
[3]D. R. Lloyd, P. J. Roberts, I. H. Hillier, and I. C. Shenton, Mol. Phys. **31**, 1549 (1976).
[4]F. T. Chau and L. Karlsson, Phys. Scripta **16**, 248 (1977).

CF_3^+

$\tilde{X}$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	3	CF stretch	1667	Ar	IR	1

References

[1]F. T. Prochaska and L. Andrews, J. Am. Chem. Soc. **100**, 2102 (1978).

CF_2Cl^+

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF stretch	1507s	Ar	IR	1–3
b_2	5	CF stretch	1406vs	Ar	IR	1–3

References

[1]M. E. Jacox, Chem. Phys. Lett. **54**, 176 (1978).
[2]F. T. Prochaska and L. Andrews, J. Am. Chem. Soc. **100**, 2102 (1978).
[3]F. T. Prochaska and L. Andrews, J. Chem. Phys. **68**, 5577 (1978).

CF_2Br^+

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF stretch	1480m	Ar	IR	1–3
b_2	5	CF stretch	1362s	Ar	IR	1–3

References

[1]M. E. Jacox, Chem. Phys. Lett. **54**, 176 (1978).
[2]F. T. Prochaska and L. Andrews, J. Am. Chem. Soc. **100**, 2102 (1978).
[3]F. T. Prochaska and L. Andrews, J. Phys. Chem. **82**, 1731 (1978).

CF_2I^+

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF stretch	1433	Ar	IR	1
b_2	5	CF stretch	1321	Ar	IR	1

References

[1]F. T. Prochaska and L. Andrews, J. Am. Chem. Soc. **100**, 2102 (1978).

$CFCl_2^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1352vs	Ar	IR	1
		CCl a–stretch	1142vs	Ar	IR	1

References

[1]F. T. Prochaska and L. Andrews, J. Chem. Phys. **68**, 5568 (1978).

$CFBr_2^+$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1322vs	Ar	IR	1
			1311vs	Ar	IR	1,2
		CBr stretch	991vs	Ar	IR	1,2

References

[1]F. T. Prochaska and L. Andrews, J. Phys. Chem. **82**, 1731 (1978).
[2]B. W. Keelan and L. Andrews, J. Phys. Chem. **83**, 2488 (1979).

CFI_2^+

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1270s	Ar	IR	1
		CI a–stretch	914m	Ar	IR	1

References

[1]B. W. Keelan and L. Andrews, J. Phys. Chem. **83**, 2488 (1979).

CCl_3^+

$\tilde{X}$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	3	CCl stretch	1037	Ar	IR	1–3

References

[1]M. E. Jacox and D. E. Milligan, J. Chem. Phys. **54**, 3935 (1971).
[2]M. E. Jacox, Chem. Phys. **12**, 51 (1976).
[3]F. T. Prochaska and L. Andrews, J. Chem. Phys. **67**, 1091 (1977).

CCl_2Br^+

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1020	Ar	IR	1
			954	Ar	IR	1

References

[1]L. Andrews, C. A. Wight, F. T. Prochaska, S. A. McDonald, and B. S. Ault, J. Mol. Spectrosc. **73**, 120 (1978).

$CClBr_2^+$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			976	Ar	IR	1,2
			892	Ar	IR	1,2

References

[1]L. Andrews, J. M. Grzybowski, and R. O. Allen, J. Phys. Chem. **79**, 904 (1975).
[2]L. Andrews, C. A. Wight, F. T. Prochaska, S. A. McDonald, and B. S. Ault, J. Mol. Spectrosc. **73**, 120 (1978).

CBr_3^+

$\tilde{X}$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'		CBr stretch	874	Ar	IR	1–3

References

[1]L. Andrews, J. M. Grzybowski, and R. O. Allen, J. Phys. Chem. **79**, 904 (1975).
[2]F. T. Prochaska and L. Andrews, J. Chem. Phys. **67**, 1091 (1977).
[3]L. Andrews, C. A. Wight, F. T. Prochaska, S. A. McDonald, and B. S. Ault, J. Mol. Spectrosc. **73**, 120 (1978).

F_2SiO

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Si=O stretch	1309vs	Ar	IR	1
	2	SiF s–stretch	835m	Ar	IR	1
	3	SiF_2 deform.	423wm	Ar	IR	1
b_1	4	OPLA	344s	Ar	IR	1
b_2	5	SiF a–stretch	996s	Ar	IR	1
	6	SiF_2 rock	333m	Ar	IR	1

References

[1]H. Schnöckel, J. Mol. Struct. **65**, 115 (1980).

Cl_2SiO

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Si=O stretch	1240s	Ar	IR	1
	2	SiCl s–stretch	501m	Ar	IR	1
b_1	4	OPLA	280ms	Ar	IR	1
b_2	5	SiCl a–stretch	638vs	Ar	IR	1
	6	$SiCl_2$ rock	269m	Ar	IR	1

References

[1]H. Schnöckel, Z. Anorg. Allg. Chem. **460**, 37 (1980).

Cl_2SiS

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiS stretch	805.6s	Ar	IR	1
b_1	4	OPLA	231.9br	Ar	IR	1
b_2	5	$SiCl_2$ a–stretch	609.9vs	Ar	IR	1

References

[1]H. Schnöckel, H. J. Göcke, and R. Köppe, Z. Anorg. Allg. Chem. **578**, 159 (1989).

Cl_2GeS

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Ge=S stretch	580.3m	Ar	IR	1
	2	$GeCl_2$ s–stretch	404.0m	Ar	IR	1
b_2	5	$GeCl_2$ a–stretch	439.9s	Ar	IR	1

References

[1]R. Köppe and H. Schnöckel, Z. Anorg. Allg. Chem. **592**, 179 (1991).

$SiCl_3^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SiCl stretch	742	Ar	IR	1

References

[1]J. H. Miller and L. Andrews, J. Mol. Struct. 77, 65 (1981).

F_2GeO

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	GeO stretch	989.9	Ar	IR	1
	2	GeF s-stretch	731.7	Ar	IR	1
b_1	4	OPLA	209.4	Ar	IR	1
b_2	5	GeF a-stretch	746.7	Ar	IR	1
	6	FGeO bend	226.9	Ar	IR	1

References

[1]H. Schnöckel, J. Mol. Struct. **70**, 183 (1981).

FCO_2^-

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO stretch	1316 Cs	Ar	IR	1
	2	CF stretch	883 Cs	Ar	IR	1
b_2	4	CO stretch	1749 Cs	Ar	IR	1

References

[1]B. S. Ault, Inorg. Chem. **21**, 756 (1982).

Cl_2CSe

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CSe stretch	991vs	Ne	IR	1
			984vs	Ar	IR,Ra	1
	2	CCl_2 s-stretch	437m	Ne	IR	1
			434m	Ar	IR,Ra	1
	3	CCl_2 deform.	260m	Ar	Ra	1
b_2	5	CCl_2 a-stretch	821vs	Ne	IR	1
			809vs	Ar	IR	1
	6	SeCCl deform.	248w	Ar	Ra	1

References

[1]A. Darmadi, A. Haas, H. Willner, and H. Schnöckel, Z. Naturforsch. **86b**, 1261 (1981).

FONO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO_2 a-stretch	1716s	N_2	IR	1
			1200m[a]	N_2	IR	1
			702wm	N_2	IR	1
			412m	N_2	IR	1

[a] Possibly a combination band[2].

References

[1]R. R. Smardzewski and W. B. Fox, J. Chem. Phys. **60**, 2980 (1974).
[2]T. J. Lee and J. E. Rice, J. Chem. Phys. **97**, 4223 (1992).

$ClNO_2$

The onset of continuous absorption by gas-phase $ClNO_2$ occurs near 25000 (400 nm).[3] The maximum in this absorption is beyond the 185 nm limit of the observations.

$\tilde{X}$ $^1A_1$ C_{2v} Structure: MW[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NO_2 s-stretch	1267.1vs	gas	IR	1
			1264.3	Ar	IR	4
	2	NCl stretch	792.6vs	gas	IR	1
			787.0	Ar	IR	4
	3	NO_2 scissors	369.6vs	gas	IR	1
			365.0	Ar	IR	4
b_1	4	OPLA	652.3m	gas	IR	1
b_2	5	NO_2 a-stretch	1684.6	gas	IR	1
			1674.8	Ar	IR	4
	6	NO_2 rock	408.1vw	gas	IR	1

$A_0 = 0.443$; $B_0 = 0.173$; $C_0 = 0.124$ MW[2,5]

References

[1]D. L. Bernitt, R. H. Miller, and I. C. Hisatsune, Spectrochim. Acta **23A**, 237 (1967).
[2]R. R. Filgueira, P. Forti, and G. Corbelli, J. Mol. Spectrosc. **57**, 97 (1975).
[3]A. J. Illies and G. A. Takacs, J. Photochem. **6**, 35 (1976/77).
[4]D. E. Tevault and R. R. Smardzewski, J. Chem. Phys. **67**, 3777 (1977).
[5]K. Endo, Nippon Kagaku Kaishi 1129 (1979).

ClONO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	N=O stretch	1715vs	gas	IR	2,3
			1714s	Ar	IR	1
			1717	N_2	IR	4
	2	O–N stretch	858w	gas	IR	2
			856m	Ar	IR	1
	3	ONO bend	644m	gas	IR	2
	4	ClO stretch	406vs	gas	IR	2
			398m	Ar	IR	1
			390ms			
	5	ClON bend	270T	gas	IR	2

References

[1]D. E. Tevault and R. R. Smardzewski, J. Chem. Phys. **67**, 3777 (1977).
[2]B. Janowski, N.–D. Knauth, and H. Martin, Ber. Bunsenges. Phys. Chem. **81**, 1262 (1977).
[3]H. Niki, P. D. Maker, C. M. Savage, and L. P. Breitenbach, Chem. Phys. Lett. **59**, 78 (1978).
[4]J. P. Burrows, G. S. Tyndall, and G. K. Moortgat, J. Phys. Chem. **92**, 4340 (1988).

OClNO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		N=O stretch	1752ms	Ar	IR	1

References

[1]D. E. Tevault and R. R. Smardzewski, J. Chem. Phys. **37**, 3777 (1977).

$BrNO_2$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NO_2 s–stretch	1292	gas	IR	3
			1289s	Ar	IR	1,2
	2	NO_2 deform.	787	gas	IR	3
			784s[a]	Ar	IR	2
	3	NBr stretch	496m	Ar	IR	1
b_1	4	OPLA	574s	Ar	IR	2
b_2	5	NO_2 a–stretch	1660T	gas	IR	3
			1660m[a]	Ar	IR	2
	6	NO_2 wag	402w[b]	Ar	IR	2

[a] Partially obscured by nearby N_2O_4 absorption.
[b] This fundamental assigned to a moderately intense 360–cm^{-1} absorption by Ref. 1.

References

[1]M. Feuerhahn, R. Minkwitz, and U. Engelhardt, J. Mol. Spectrosc. **77**, 429 (1979).
[2]D. E. Tevault, J. Phys. Chem. **83**, 2217 (1979).
[3]B. J. Finlayson–Pitts, F. E. Livingston, and H. N. Berko, J. Phys. Chem. **93**, 4397 (1989).

BrONO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		N=O stretch	1725vs[a]	Ar	IR	1,2
			837s	Ar	IR	2
			588vs[a]	Ar	IR	1,2
			392m	Ar	IR	2

[a] Attributed by Ref. 1 to $BrNO_2$.

References

[1]M. Feuerhahn, R. Minkwitz, and U. Engelhardt, J. Mol. Spectrosc. **77**, 429 (1979).
[2]D. E. Tevault, J. Phys. Chem. **83**, 2217 (1979).

INO_2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NO_2 s–stretch	1282.5	gas	IR	2
			1279s	Ar	IR	1
	2	NO_2 deform.	569vs[a]	Ar	IR	1
	3	NI stretch	468w	Ar	IR	1
b_1	4	OPLA	650w	Ar	IR	1
b_2	5	NO_2 a–stretch	1700s	Ar	IR	1
	6	NO_2 rock	305m	Ar	IR	1

[a] Ref. 2 attributed an absorption at 778 cm^{-1} to this fundamental, but did not observe the spectral region below 700 cm^{-1}. Their absorption may, alternatively, have been contributed by $\nu_3 + \nu_6$.

References

[1]M. Feuerhahn, R. Minkwitz, and U. Engelhardt, J. Mol. Spectrosc. **77**, 429 (1979).
[2]I. Barnes, K. H. Becker, and J. Starcke, J. Phys. Chem. **95**, 9736 (1991).

PO_2Cl

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PO_2 s–stretch	1122	Ar	IR	1
	2	PCl stretch	586	Ar	IR	1
b_2	5	PO_2 a–stretch	1429	Ar	IR	1

References

[1]R. Ahlrichs, C. Ehrhard, M. Lakenbrink, S. Schunck, and H. Schnöckel, J. Am. Chem. Soc. **108**, 3596 (1986).

PO_2Br

$\tilde{X}$ C_{2v} Structure: IR[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PO_2 s-stretch	1146.5	Ar	IR	1
	2	PO_2 scissors	513.5	Ar	IR	1
	3	PBr stretch	363.2	Ar	IR	1
b_2	5	PO_2 a-stretch	1440.1	Ar	IR	1

References

[1]S. Schunck, H.-J. Göcke, R. Köppe, and H. Schnöckel, Z. Anorg. Allg. Chem. **579**, 66 (1989).

BrP(O)S

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	PO stretch	1284m	Ar	IR	1
	2	PS stretch	723.9wm	Ar	IR	1
			722.9			
			715.0			
	3	PBr stretch	430m	Ar	IR	1
a''	6	OPLA	299.6w	Ar	IR	1

References

[1]S. Schunck, H.-J. Göcke, and H. Schnöckel, Z. Anorg. Allg. Chem. **583**, 78 (1990).

c-S_4

$\tilde{A}$ gas AB[1,2,4] $\tilde{A}$–$\tilde{X}$ 425–575 nm
Unstructured absorption maximum at 19300 (518 nm) in an Ar matrix.[6]
Unstructured absorption maximum at 18870 (530 nm) in a Kr matrix.[1,2]

$\tilde{X}$ C_{2v} Structure: MO,IR[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			661.6	Ar	IR	3,5,6
			660s	Kr	IR	3
			660	Xe	IR	3
			483wmT	Kr	IR	3
			320mT	Kr	IR	3
			270wmT	Kr	IR	3

References

[1]B. Meyer, T. V. Oommen, and D. Jensen, J. Phys. Chem. **75**, 912 (1971).
[2]B. Meyer, T. Stroyer-Hansen, and T. V. Oommen, J. Mol. Spectrosc. **42**, 335 (1972).
[3]B. Meyer and T. Stroyer-Hansen, J. Phys. Chem. **76**, 3968 (1972).
[4]R. I. Billmers and A. L. Smith, J. Phys. Chem. **95**, 4242 (1991).
[5]G. D. Brabson, Z. Mielke, and L. Andrews, J. Phys. Chem. **95**, 79 (1991).
[6]P. Hassanzadeh and L. Andrews, J. Phys. Chem. **96**, 6579 (1992).

SS_3

$\tilde{A}$

Ar AB[3] 575–645 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			590	Ar	AB	3
			320	Ar	AB	3

$\tilde{X}$ Structure: MO,IR[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			642.4	Ar	IR	2,3
			636s	Kr	IR	1
			483wmT	Kr	IR	1
			320mT	Kr	IR	1
			270wmT	Kr	IR	1

References

[1]B. Meyer and T. Stroyer-Hansen, J. Phys. Chem. **76**, 3968 (1972).
[2]G. D. Brabson, Z. Mielke, and L. Andrews, J. Phys. Chem. **95**, 79 (1991).
[3]P. Hassanzadeh and L. Andrews, J. Phys. Chem. **96**, 6579 (1992).

SeO_3

$\tilde{X}$ D_{3h} Structure: Ra[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	Deform.	356	Ar	IR	2
			358	N_2	IR	2
e'	3	SeO stretch	995	Ar	IR	2
			1005.5	N_2	IR	2

References

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[2]A. K. Brisdon and J. S. Ogden, J. Mol. Struct. **157**, 141 (1987).

c-Se_4 [a]

$\tilde{A}$

Unstructured absorption maximum at 15820 (632 nm) in an Ar matrix.[1]

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			370	Ar	IR	1

[a] Tentative identification, by analogy with that of c-S_4.

References

[1]G. D. Brabson and L. Andrews, J. Phys. Chem. **96**, 9172 (1992).

$SeSe_3$ [a]

$\tilde{A}$

Ar AB[1] $\tilde{A}$–$\tilde{X}$ 710–850 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			310(5)	Ar	AB	1

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			345	Ar	IR	1

[a] Tentative identification, by analogy with that of SS_3.

References

[1]G. D. Brabson and L. Andrews, J. Phys. Chem. **96**, 9172 (1992).

c–Te_4 [a]

$\tilde{A}$

Unstructured absorption maximum at 13160 (760 nm) in an Ar matrix.[1]

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			243	Ar	IR	1

[a] Tentative identification, by analogy with that of c–S_4.

References

[1]P. Hassanzadeh, C. Thompson, and L. Andrews, J. Phys. Chem. **96**, 8246 (1992).

$TeTe_3$ [a]

$\tilde{A}$

Ar AB[1] $\tilde{A}$–$\tilde{X}$ 900–1000 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			150(5)	Ar	AB	1

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			224	Ar	IR	1

[a] Tentative identification, by analogy with that of SS_3.

References

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CF_3

Rydberg state D_{3h}

gas AB[6]MPI[10] 139–165 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	820	gas	AB,MPI	6,10

$4s\ ^2A_1'$ D_{3h}

$T_0 \cong 51665$ gas AB[7]EM[11–14,16,20] $4s^2A_1'$–$\tilde{X}$ 180–300 nm

Calculations[14] suggest that this state is of mixed valence–Rydberg character, with increasing Rydberg contribution at large C–F distances.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	804T	gas	EM	12

τ = 12(3) ns gas EM[17,18]

Ref. 22 obtained a lifetime of 17.3(4) ns for this state, suggesting that it is identical to the upper state for the 450–750 nm emission bands of CF_3.

$3p\ ^2A_2'', ^2E'$ D_{3h}

$T_0 \cong 51600$ gas EM[8,11,13,14] $3p$–$3s^2A_1'$ 450–750 nm

τ = 17.5(5) ns gas EM[17,18,22]EF[21]

The lower state of the visible emission of CF_3, calculated[14] to be the $3s\ ^2A_1$ state, which assumes increasing valence character at large C-F distances, is both observed and calculated to be dissociative.

$\tilde{X}\ ^2A_1$ C_{3v} Structure: ESR[1]MW[9]DL[15]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF stretch	1089	gas	IR,EM	2,12
					CARS	19
			1083	Ne	IR	5
			1087s	Ar	IR	3,4
	2	Umbrella	701(3)	gas	IR,EM	2,12
			700	Ne	IR	5
			703m	Ar	IR	3,4
e	3	CF stretch	1260.16	gas	IR,DL	2,15
			1252	Ne	IR	5
			1251vs	Ar	IR	3,4
	4	Deformation	508	Ne	IR	5
			512w	Ar	IR	4

B_0 = 0.364 MW[9]; C_0 = 0.189 DL[15]

References

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[2]G. A. Carlson and G. C. Pimentel, J. Chem. Phys. **44**, 4053 (1966).
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[4]D. E. Milligan and M. E. Jacox, J. Chem. Phys. **48**, 2265 (1968).
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CF_2Cl

3p Rydberg state C_{2v}
$T_0 \leq 49220$ gas MPI[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_1	4	OPLA	745(25)	gas	MPI	3

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CF stretch	1148vs	Ar	IR	1,2
	2	CCl stretch	761s	Ar	IR	1,2
	3	CF_2 scissors	599m	Ar	IR	1,2
a''	5	CF stretch	1208vs	Ar	IR	1,2

References

[1]D. E. Milligan, M. E. Jacox, J. H. McAuley, and C. E. Smith, J. Mol. Spectrosc. **45**, 377 (1973).
[2]F. T. Prochaska and L. Andrews, J. Chem. Phys. **68**, 5577 (1978).
[3]B. P. Tsai, R. D. Johnson, III, and J. W. Hudgens, J. Phys. Chem. **93**, 5334 (1989).

CF_2Br

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1198	Ar	IR	1,2
		CF stretch	1138	Ar	IR	1,2
		CBr stretch	684	Ar	IR	1,2

References

[1]M. E. Jacox, Chem. Phys. Lett. **53**, 192 (1978).
[2]F. T. Prochaska and L. Andrews, J. Am. Chem. Soc. **100**, 2102 (1978).

CF_2I

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1126	Ar	IR	1
		CI stretch	627	Ar	IR	1

References

[1]F. T. Prochaska and L. Andrews, J. Am. Chem. Soc. **100**, 2102 (1978).

$CFCl_2$

3p Rydberg state C_{2v}
$T_0 \leq 49850$ gas MPI[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CCl_2 scissors	270(30)	gas	MPI	3
b_1	4	OPLA	590(20)	gas	MPI	3

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CF stretch	1143vs	Ar	IR	1,2
	2	CCl stretch	747m	Ar	IR	1,2
a''	5	CCl stretch	919vs	Ar	IR	1,2

References

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[2]F. T. Prochaska and L. Andrews, J. Chem. Phys. **68**, 5568 (1978).
[3]B. P. Tsai, R. D. Johnson, III, and J. W. Hudgens, J. Phys. Chem. **93**, 5334 (1989).

$CFBr_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1136vs	Ar	IR	1,2
			782s	Ar	IR	1

References

[1]F. T. Prochaska and L. Andrews, J. Phys. Chem. **82**, 1731 (1978).
[2]B. W. Keelan and L. Andrews, J. Phys. Chem. **83**, 2488 (1979).

CFI_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1149vs	Ar	IR	1
			735ms	Ar	IR	1

References

[1]B. W. Keelan and L. Andrews, J. Phys. Chem. **83**, 2488 (1979).

CCl_3

$\tilde{M}\ ^2E''$ (4d)[a] D_{3h}

T_0 = 57733(10) gas MPI[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	542(3)	gas	MPI	9

$\tilde{L}\ ^2A_2''$ (4p) D_{3h}

T_0 = 56409(10) gas MPI[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	533(15)	gas	MPI	9

$\tilde{K}\ ^2E'$ (4p) D_{3h}

T_0 = 56236(10) gas MPI[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	526(16)	gas	MPI	9

$\tilde{J}\ ^2A_1'$ (4s) D_{3h}

T_0 = 53471(10) gas MPI[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	530(20)	gas	MPI	9

$\tilde{G}\ ^2E'$ (3d)[a] D_{3h}

T_0 = 51218(10) gas MPI[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	520(17)	gas	MPI	9

$\tilde{F}\ ^2A_2''$ (3p) D_{3h}

T_0 = 47868(10) gas MPI[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	528(3)	gas	MPI	9

$\tilde{E}\ ^2E'$ (3p) D_{3h}

T_0 = 47170(10) gas MPI[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	544(6)	gas	MPI	9
a_2''	2	OPLA	509(21)	gas	MPI	9

A = 33(5) gas MPI[9]

$\tilde{C}\ ^2A_1'$ (3s) D_{3h}

gas AB[8,11] $\tilde{C}$–$\tilde{X}$ 265–195 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	569(63)	gas	AB	11

Photodissociation of CCl_3 in a pulsed supersonic beam to produce CCl_2 + Cl has been observed[10] at 308 nm.

A broad emission observed in radiofrequency discharges between 420 and 700 nm, with a maximum near 490 nm, has been attributed[7] to a transition between two electronically excited states of CCl_3.

$\tilde{X}\ ^2A_1$ C_{3v} Structure: ESR[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	Umbrella	290[b]	gas	MPI	9
			251			
e	3	CCl stretch	898vs	Ar	IR	1–4,6

[a] Tentative symmetry assignment.
[b] Inversion doublet. Barrier to inversion = 460(40) gas MPI[9]

References

[1]L. Andrews, J. Phys. Chem. **71**, 2761 (1967).
[2]L. Andrews, J. Chem. Phys. **48**, 972 (1968).
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CCl_2Br

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CCl stretch	888vs	Ar	IR	1–3
		CCl stretch	835vs	Ar	IR	1–3

References

[1]L. Andrews, J. Chem. Phys. **48**, 972 (1968).
[2]J. H. Current and J. K. Burdett, J. Phys. Chem. **73**, 3504 (1969).
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CCl_2I

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CCl stretch	871	Ar	IR	1
		CCl stretch	810	Ar	IR	1

References

[1]L. Andrews, J. Chem. Phys. **48**, 972 (1968).

$CClBr_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CCl stretch	856vs	Ar	IR	1,2
		CBr stretch	783vs	Ar	IR	1,2

References

[1]L. Andrews, J. Chem. Phys. **48**, 972 (1968).
[2]A. K. Maltsev, O. M. Nefedov, R. H. Hauge, J. L. Margrave, and D. Seyferth, J. Phys. Chem. **75**, 3984 (1971).

CBr_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	CBr stretch	773vs	Ar	IR	1–3

References

[1]L. Andrews, J. Chem. Phys. **48**, 972 (1968).
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Cl_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	Cl stretch	693	Ar	IR	1

References

[1]D. W. Smith and L. Andrews, J. Phys. Chem. **76**, 2718 (1972).

SiF_3

Unstructured emission bands between 290 and 340 nm and between 350 and 800 nm which appear with varying relative intensities on photoexcitation of SiF_4 by radiation at 99.1, 95.5, or 92.2 nm have been attributed[4] to SiF_3. The 350–800 nm band may correspond to the unstructured emission centered at 632 nm which has been observed[3,5] in the flowing afterglow of an SiF_4 discharge and in the reaction of F atoms with Si and which has been tentatively assigned to SiF_3. A third emission band, between 240 and 280 nm, becomes more prominent at higher excitation energies. This latter band occurs in the same spectral region as the 210–260 nm emission band system observed in a discharge through SiF_4. Although that band system was initially assigned[2] to SiF_3, subsequent studies[6] have demonstrated that it is entirely contributed by SiF_2.

$\tilde{X}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiF stretch	832s	Ar	IR	1
	2	Umbrella	406s	Ar	IR	1
e	3	SiF stretch	954vs	Ar	IR	1
	4	Deformation	290wm	Ar	IR	1

References

[1]D. E. Milligan, M. E. Jacox, and W. A. Guillory, J. Chem. Phys. **49**, 5330 (1968).
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[3]V. M. Donnelly and D. L. Flamm, J. Appl. Phys. **51**, 5273 (1980).
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[5]S. Vanhaelemeersch, J. Van Hoeymissen, D. Vermeylen, and J. Peeters, J. Appl. Phys. **70**, 3892 (1991).
[6]W. B. Griffith, Jr., and C. W. Mathews, private communication.

$SiCl_3$

$\tilde{A}$ (3d or 5s Rydberg state?)

$T_0 \cong 43700$ gas MPI[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	Umbrella	282(30)	gas	MPI	4

$\tilde{G}$ (4p Rydberg state?)

$T_0 \cong 43700$ gas MPI[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	Umbrella	261(15)	gas	MPI	4

$\tilde{F}$ (4p Rydberg state?)

$T_0 \cong 43700$ gas MPI[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	Umbrella	262(16)	gas	MPI	4

$\tilde{X}$ C_{3v} Structure: ESR[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiCl stretch	470m	Ar	IR	2,3
e	3	SiCl stretch	582vs	Ar	IR	2,3

References

[1]N. Leray and J. Roncin, J. Chem. Phys. **42**, 800 (1965).
[2]M. E. Jacox and D. E. Milligan, J. Chem. Phys. **49**, 3130 (1968).
[3]J. H. Miller and L. Andrews, J. Mol. Struct. **77**, 65 (1981).
[4]K. K. Irikura, R. D. Johnson III, and J. W. Hudgens, J. Phys. Chem. **96**, 4306 (1992).

$GeCl_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	$GeCl_3$ stretch	420	Ar	IR	1

References

[1]J. H. Miller and L. Andrews, J. Mol. Struct. **77**, 65 (1981).

NF_3^+

$\tilde{E}\ ^2E$ C_{3v}
T^a = 65920(900) gas PE[1]

$\tilde{D}\ ^2A_1$ C_{3v}
T_0 = 50600(560) gas PE[1]

$\tilde{C}\ ^2E$ C_{3v}
T_0 = 33800(560) gas PE[1]

$\tilde{B}\ ^2A_2$ C_{3v}
T^a = 28900(720) gas PE[1]

$\tilde{A}\ ^2E$ C_{3v}
T_0 = 20330(650) gas PE[1]

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Umbrella	565(40)	gas	PE	2

Barrier to inversion $\cong$ 6000.[2]

[a] From vertical ionization potential.

References

[1]P. J. Bassett and D. R. Lloyd, J. Chem. Soc., Dalton Trans. 248 (1972).
[2]J. Berkowitz and J. P. Greene, J. Chem. Phys. **81**, 3383 (1984).

NCl_3^+

$\tilde{E}\ ^2E$ C_{3v}
T^a = 53100(1200) gas PE[1]

$\tilde{D}\ ^2A_1$ C_{3v}
T^a = 42700(1200) gas PE[1]

$\tilde{C}\ ^2E$ C_{3v}
T^a = 23400(1000) gas PE[1]

$\tilde{B}\ ^2E$ C_{3v}
T^a = 15800(1000) gas PE[1]

$\tilde{A}\ ^2A_2$ C_{3v}
T^a = 12400(1000) gas PE[1]

$\tilde{X}\ ^2A_1$ C_{3v}

[a] From vertical ionization potential.

References

[1]D. Colbourne, D. C. Frost, C. A. McDowell, and N. P. C. Westwood, J. Chem. Phys. **69**, 1078 (1978).

PF_3^+

$\tilde{E}\ ^2E$ C_{3v}
$T_0^a \geq$ 61500(200) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PF stretch	660(30)	gas	PE	2
	2	Umbrella	360(30)	gas	PE	2

$\tilde{D}\ ^2A_1$ C_{3v}
$T_0^a \geq$ 55000(200) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PF stretch	690(30)	gas	PE	2
	2	Umbrella	395(30)	gas	PE	2

$\tilde{C}\ ^2E$ C_{3v}
$T_0^a \geq 45500(200)$ gas PE[1,2]

$\tilde{B}\ ^2E$ C_{3v}
$T^{ab} \geq 39300(600)$ gas PE[1,2]

$\tilde{A}\ ^2A_2$ C_{3v}
$T_0^a \geq 31220(500)$ gas PE[1,2]

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Umbrella	475(30)	gas	PE	1,2

[a] In accord with recent photoionization studies,[3,4] the first ionization potential of PF_3 is taken to be $\leq$ 11.44 eV.
[b] From vertical ionization potential.

References

[1]P. J. Bassett and D. R. Lloyd, J. Chem. Soc., Dalton Trans. 248 (1972).
[2]J. P. Maier and D. W. Turner, J. Chem. Soc., Faraday Trans. 2 **68**, 711 (1972).
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PF_2Cl^+

$\tilde{F}$ C_s
$T^a = 58900(1600)$ gas PE[1]

$\tilde{E}$ C_s
$T^a = 52400(1600)$ gas PE[1]

$\tilde{D}$ C_s
$T^a = 39500(1600)$ gas PE[1]

$\tilde{C}$ C_s
$T^a = 33900(1600)$ gas PE[1]

$\tilde{B}$ C_s
$T^a = 10500(1600)$ gas PE[1]

$\tilde{X},\tilde{A}$ C_s

[a] From vertical ionization potentials.

References

[1]S. Cradock and D. W. H. Rankin, J. Chem. Soc., Faraday Trans. 2 **68**, 940 (1972).

PF_2Br^+

$\tilde{F}$ C_s
$T^a = 59220(1000)$ gas PE[1]

$\tilde{E}$ C_s
$T^a = 54380(1000)$ gas PE[1]

$\tilde{D}$ C_s
$T^a = 40660(1000)$ gas PE[1]

$\tilde{C}\ ^2A'$ C_s
$T^a = 32190(320)$ gas PE[1]

$\tilde{B}\ ^2A'$ C_s
$T^a = 7580(1000)$ gas PE[1]

$\tilde{A}$ C_s
$T^a = 5240(320)$ gas PE[1]

[a] From vertical ionization potentials.

References

[1]S. Cradock and D. W. H. Rankin, J. Chem. Soc., Faraday Trans. 2 **68**, 940 (1972).

$OPCl_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		P=O stretch	1300T	Ar	IR	1
		PCl_2 a-stretch	621T	Ar	IR	1

References

[1]B. W. Moores and L. Andrews, J. Phys. Chem. **93**, 1902 (1989).

PCl_3^+

$\tilde{F}\ ^2A_1$ C_{3v}
$T^a = 67050(320)$ gas PE[1,3]

$\tilde{E}\ ^2E$ C_{3v}
$T^a = 37840(320)$ gas PE[1-3]

$\tilde{D}\ ^2A_1$ C_{3v}
$T^a = 30010(320)$ gas PE[1-3]

$\tilde{C}\ ^2E$ C_{3v}
$T^a = 19850(320)$ gas PE[1-3]

$\tilde{B}\ ^2E$ C_{3v}
$T^a = 12020(320)$ gas PE[1-3]

$\tilde{A}\ ^2A_2$ C_{3v}
$T^a = 9600(320)$ gas PE[1-3]

$\tilde{X}\ ^2A_1$ C_{3v}

[a] From vertical ionization potentials.

References

[1]P. A. Cox, S. Evans, A. F. Orchard, N. V. Richardson, and P. J. Roberts, Faraday Discuss. Chem. Soc. **54**, 26 (1972).
[2]J. L. Berkosky, F. O. Ellison, T. H. Lee, and J. W. Rabalais, J. Chem. Phys. **59**, 5342 (1973).
[3]D. G. Nicholson and P. Rademacher, Acta Chem. Scand. **A28**, 1136 (1974).

$OPBr_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			558T	Ar	IR	1

References

[1]B. W. Moores and L. Andrews, J. Phys. Chem. **93**, 1902 (1989).

PBr_3^+

$\tilde{E}\ ^2E$ C_{3v}
T^a = 33560(320) gas PE[1-3]

$\tilde{D}\ ^2A_1$ C_{3v}
T^a = 25580(320) gas PE[1-3]

$\tilde{C}\ ^2E$ C_{3v}
T^a = 14760(320) gas PE[1-3]

$\tilde{B}\ ^2E$ C_{3v}
T^a = 8390(320) gas PE[1-3]
A = 2660(320) gas PE[1-3]

$\tilde{A}\ ^2A_2$ C_{3v}
T^a = 5240(320) gas PE[1-3]

$\tilde{X}\ ^2A_1$ C_{3v}

[a] From vertical ionization potentials.

References

[1]P. A. Cox, S. Evans, A. F. Orchard, N. V. Richardson, and P. J. Roberts, Faraday Discuss. Chem. Soc. **54**, 26 (1972).
[2]J. L. Berkosky, F. O. Ellison, T. H. Lee, and J. W. Rabalais, J. Chem. Phys. **59**, 5342 (1973).
[3]D. G. Nicholson and P. Rademacher, Acta Chem. Scand. **A28**, 1136 (1974).

AsF_3^+

$\tilde{E}\ ^2E$ C_{3v}
T^a = 38890(320) gas PE[1]

$\tilde{D}\ ^2A_1$ C_{3v}
T^a = 34050(320) gas PE[1]

$\tilde{C}\ ^2E$ C_{3v}
T^a = 25900(320) gas PE[1]

$\tilde{A},\tilde{B}\ ^2E,^2A_2$ C_{3v}
T^a = 18070(320) gas PE[1]

$\tilde{X}\ ^2A_1$ C_{3v}

[a] From vertical ionization potentials.

References

[1]A. W. Potts, H. J. Lempka, D. G. Streets, and W. C. Price, Phil. Trans. Roy. Soc. (London) **A268**, 59 (1970).

$AsCl_3^+$

$\tilde{E}\ ^2E$ C_{3v}
T^a = 32760(320) gas PE[1,3]

$\tilde{D}\ ^2A_1$ C_{3v}
T^a = 25820(320) gas PE[1,3]

$\tilde{C}\ ^2E$ C_{3v}
T^a = 16460(320) gas PE[1,3]

$\tilde{B}\ ^2E$ C_{3v}
T^a = 10000(320) gas PE[1,3]

$\tilde{A}\ ^2A_2$ C_{3v}
T^a = 8470(320) gas PE[3]

$\tilde{X}\ ^2A_1$ C_{3v}

[a] From vertical ionization potential. The first ionization potential of $AsCl_3$ is taken as 10.55(2) eV, as in the photoionization and photoelectron spectroscopic studies of Ref. 2.

References

[1]A. W. Potts, H. J. Lempka, D. G. Streets, and W. C. Price, Phil. Trans. Roy. Soc. (London) **A268**, 59 (1970).
[2]R. A. W. Johnstone and F. A. Mellon, J. Chem. Soc., Faraday Trans. 2 **68**, 1209 (1972).
[3]T. H. Lee and J. W. Rabalais, J. Chem. Phys. **60**, 1172 (1974).

$AsBr_3^+$

$\tilde{E}\ ^2E$ C_{3v}
T^a = 27510(400) gas PE[1,2]

$\tilde{D}\ ^2A_1$ C_{3v}
T^a = 20650(400) gas PE[1,2]

$\tilde{C}\ ^2E$ C_{3v}
T^a = 10650(400) gas PE[1,2]

$\tilde{B}\ ^2E$ C_{3v}
T^a = 5360(320) gas PE[1,2]
A = 2500(320) gas PE[1]

$\tilde{A}\ ^2A_2$ C_{3v}
T^a = 2500(320) gas PE[1]

$\tilde{X}\ ^2A_1$ C_{3v}

[a] From vertical ionization potentials.

References

[1]T. H. Lee and J. W. Rabalais, J. Chem. Phys. **60**, 1172 (1974).
[2]J. B. Peel and G. D. Willett, J. Electron Spectrosc. Relat. Phenom. **9**, 175 (1976).

SbF_3^+

$\tilde{F}\ ^2A_1$ C_{3v}
T^a = 50350(320) gas PE[1]

$\tilde{E}\ ^2E$ C_{3v}
T^a = 32110(320) gas PE[1]

$\tilde{D}\ ^2A_1$ C_{3v}
T^a = 27750(320) gas PE[1]

$\tilde{C}\ ^2E$ C_{3v}
T^a = 22030(320) gas PE[1]

$\tilde{A},\tilde{B}\ ^2A_2,^2E$ C_{3v}
T^a = 16460(320) gas PE[1]

$\tilde{X}\ ^2A_1$ C_{3v}

[a] From vertical ionization potentials.

References

[1]I. Novak and A. W. Potts, J. Chem. Soc., Dalton Trans. 635 (1983).

$SbCl_3^+$

$\tilde{E}\ ^2E$ C_{3v}
T^a = 25660(320) gas PE[1,2]

$\tilde{D}\ ^2A_1$ C_{3v}
T^a = 19610(320) gas PE[1,2]

$\tilde{C}\ ^2E$ C_{3v}
T^a = 12590(320) gas PE[1,2]

$\tilde{A},\tilde{B}\ ^2A_2,^2E$ C_{3v}
T^a = 7020(320) gas PE[1,2]

$\tilde{X}\ ^2A_1$ C_{3v}

[a] From vertical ionization potentials.

References

[1]T. H. Lee and J. W. Rabalais, J. Chem. Phys. **60**, 1172 (1974).
[2]D. G. Nicholson and P. Rademacher, Acta Chem. Scand. **A28**, 1136 (1974).

$SbBr_3^+$

$\tilde{E}\ ^2E$ C_{3v}
T^a = 24120(320) gas PE[1,2]

$\tilde{D}\ ^2A_1$ C_{3v}
T^a = 17670(320) gas PE[1,2]

$\tilde{C}\ ^2E$ C_{3v}
T^a = 10090(320) gas PE[1,2]

$\tilde{B}\ ^2E$ C_{3v}
T^a = 5890(320) gas PE[1,2]
A = 2340(320) gas PE[1]

$\tilde{A}\ ^2A_2$ C_{3v}
T^a = 2740(320) gas PE[1,2]

$\tilde{X}\ ^2A_1$ C_{3v}

[a] From vertical ionization potential. The first ionization potential of $SbBr_3$ is taken as 10.07 eV, as in Ref. 1, and values from the photoelectron spectrum of that study, run at a somewhat lower temperature than that of Ref. 2, were used for the table.

References

[1]T. H. Lee and J. W. Rabalais, J. Chem. Phys. **60**, 1172 (1974).
[2]D. G. Nicholson and P. Rademacher, Acta Chem. Scand. **A28**, 1136 (1974).

$t\text{–}O_4^-$

An unstructured absorption which appears near 270 nm in $Ar:O_2$ samples in which an alkali metal is also present and which grows on controlled warmup of the sample has been attributed[7] to $M^+O_4^-$.

Threshold for photodestruction near 900 nm, and increasing cross section for photodestruction, probably by photodetachment, in the 850–400 nm spectral region.[8] Photoelectron studies[9] suggest that both photodetachment and photodissociation occur at 532 and 355 nm.

$\tilde{X}$ C_{2h} Structure: MO^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	O=O stretch	1292 K	Ar	IR	10
	2	O···O stretch	287 Cs	Ar	Ra	6
			298 Rb	Ar	Ra	6
			305 K	Ar	Ra	5
b_u	5	O=O a–stretch	973.1	Ne	IR	11
			1001 Cs	Ar	IR	4
			992 Rb	Ar	IR	3
			993 K	Ar	IR	3,10
			1001 Na	Ar	IR	2,4
			991 Na			
	6	Asym. bend	131 K	Ar	IR	10

References

[1]D. C. Conway, J. Chem. Phys. **50**, 3864 (1969).
[2]L. Andrews, J. Phys. Chem. **73**, 3922 (1969).
[3]L. Andrews, J. Chem. Phys. **54**, 4935 (1971).
[4]M. E. Jacox and D. E. Milligan, Chem. Phys. Lett. **14**, 518 (1972).
[5]R. R. Smardzewski and L. Andrews, J. Chem. Phys. **57**, 1327 (1972).
[6]R. R. Smardzewski and L. Andrews, J. Phys. Chem. **77**, 801 (1973).
[7]L. Andrews, J. Mol. Spectrosc. **61**, 337 (1976).
[8]L. C. Lee and G. P. Smith, J. Chem. Phys. **70**, 1727 (1979).
[9]L. A. Posey, M. J. Deluca, and M. A. Johnson, Chem. Phys. Lett. **131**, 170 (1986).
[10]L. Manceron, A.–M. Le Quéré, and J.–P. Perchard, J. Phys. Chem. **93**, 2960 (1989).
[11]W. E. Thompson and M. E. Jacox, J. Chem. Phys. **91**, 3826 (1989).

SO_3^-

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		S=O stretch	1191 Cs	Ar	IR	1
		S–O stretch	1093 Cs	Ar	IR	1
			1091 Cs			
		S–O stretch	965 Cs	Ar	IR	1
			585 Cs	Ar	IR	1
			504 Cs	Ar	IR	1
			474T Cs	Ar	IR	1

References

[1]D. M. Stanbury, T. A Holme, Z. H. Kafafi, and J. L. Margrave, Chem. Phys. Lett. **129**, 181 (1986).

F_2SO^+

$\tilde{E}$ C_s

T_0 = 47120(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	SF_2 stretch	705(40)	gas	PE	1
	4	SF_2 scissors	390(40)	gas	PE	1

$\tilde{D}\ ^2A'$ C_s

T^a = 38570(320) gas PE[1,2]

$\tilde{C}\ ^2A''$ C_s

T^a = 34800(1000) gas PE[1,2]

$\tilde{B}\ ^2A''$ C_s

T_0 = 18960(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SO stretch	1180(40)	gas	PE	1,2
	2	SF_2 s-stretch	790(40)	gas	PE	1,2
	4	SF_2 scissors	350(40)	gas	PE	1,2

$\tilde{A}\ ^2A'$ C_s

T^a = 15330(500) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SO stretch	1000T	gas	PE	2

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			420(40)	gas	PE	1,2

[a] From vertical ionization potential.

References

[1]G. W. Mines, R. K. Thomas, and H. Thompson, Proc. Roy. Soc. (London) **A329**, 275 (1972).
[2]D. Chadwick, D. C. Frost, F. G. Herring, A. Katrib, C. A. McDowell, and R. A. N. McLean, Can. J. Chem. **51**, 1893 (1973).

Cl_2SO^+

$\tilde{H}\ ^2A''$ C_s

T^a = 44600(1000) gas PE[4]

$\tilde{G}\ ^2A'$ C_s

T^a = 41790(320) gas PE[1,3,4]

$\tilde{F}\ ^2A'$ C_s

T^a = 37360(320) gas PE[1,3,4]

$\tilde{D},\tilde{E}\ ^2A',^2A''$ C_s

T^a = 16400(1000) gas PE[1,3,4]

$\tilde{C}\ ^2A'$ C_s

T^a = 11780(320) gas PE[1–4]

$\tilde{B}\ ^2A''$ C_s

T^a = 8710(320) gas PE[1–4]

$\tilde{A}\ ^2A''$ C_s

T^a = 6620(320) gas PE[1–4]

$\tilde{X}\ ^2A'$ C_s

References

[1]G. W. Mines, R. K. Thomas, and H. Thompson, Proc. Roy. Soc. (London) **A329**, 275 (1972).
[2]H. Bock and B. Solouki, Angew. Chem. Intern. Ed. **11**, 436 (1972).
[3]D. Chadwick, D. C. Frost, F. G. Herring, A. Katrib, C. A. McDowell, and R. A. N. McLean, Can. J. Chem. **51**, 1893 (1973).
[4]H. Bock and B. Solouki, Chem. Ber. **107**, 2299 (1974).

F_2SS^+

$\tilde{D}$ C_s

T^a = 38900(1000) gas PE[1]

$\tilde{C}$ C_s

$T^a \cong$ 35700 gas PE[1]

$\tilde{B}$ C_s

T^a = 17180(320) gas PE[1]

$\tilde{A}$ C_s

T^a = 5240(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]G. Wagner, H. Bock, R. Budenz, and F. Seel, Chem. Ber. **106**, 1285 (1973).

$FSSF^+$

$\tilde{D}$ C_2
T^a = 38400(1000) gas PE[1]

$\tilde{C}$ C_2
T^a = 34400(1000) gas PE[1]

$\tilde{B}$ C_2
T^a = 16940(320) gas PE[1]

$\tilde{A}$ C_2
T^a = 3310(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]G. Wagner, H. Bock, R. Budenz, and F. Seel, Chem. Ber. **106**, 1285 (1973).

$S_2Cl_2^+$

$\tilde{G}\ ^2B$ C_2
T^a = 48330(400) gas PE[1,2]

$\tilde{F}\ ^2A$ C_2
T^a = 35580(400) gas PE[1,2]

$\tilde{E}\ ^2B$ C_2
$T^a \cong$ 23700 gas PE[1,2]

$\tilde{D}\ ^2A$ C_2
T^a = 23080(400) gas PE[1,2]

$\tilde{C}\ ^2B$ C_2
T^a = 20500(400) gas PE[1,2]

$\tilde{B}\ ^2A$ C_2
T^a = 14280(400) gas PE[1,2]

$\tilde{A}\ ^2B$ C_2
$T^a \cong$ 5160 gas PE[1,2]

$\tilde{X}\ ^2A$ C_2

[a] From vertical ionization potential. The first ionization potential of S_2Cl_2 is taken to equal 9.66(3) eV, from the photoionization study of Ref. 3.

References

[1]R. J. Colton and J. W. Rabalais, J. Electron Spectrosc. Relat. Phenom. **3**, 345 (1974).
[2]B. Solouki and H. Bock, Inorg. Chem. **16**, 665 (1977).
[3]R. Kaufel, G. Vahl, R. Minkwitz, and H. Baumgärtel, Z. Anorg. Allg. Chem. **481**, 207 (1981).

$S_2Br_2^+$

$\tilde{H}$ C_2
T^a = 43300(1000) gas PE[1,2]

$\tilde{G}$ C_2
T^a = 34370(400) gas PE[1,2]

$\tilde{F}$ C_2
$T^a \cong$ 31200 gas PE[1,2]

$\tilde{E}$ C_2
T^a = 20700(1000) gas PE[1,2]

$\tilde{D}$ C_2
T^a = 19100(1000) gas PE[1,2]

$\tilde{C}$ C_2
T^a = 15980(400) gas PE[1,2]

$\tilde{B}$ C_2
T^a = 12590(400) gas PE[1,2]

$\tilde{A}$ C_2
T^a = 5000(400) gas PE[1,2]

[a] From vertical ionization potential. The first ionization potential of S_2Br_2 is taken to equal 9.23(3) eV, from the photoionization study of Ref. 3.

References

[1]R. J. Colton and J. W. Rabalais, J. Electron Spectrosc. Relat. Phenom. **3**, 345 (1974).
[2]B. Solouki and H. Bock, Inorg. Chem. **16**, 665 (1977).
[3]R. Kaufel, G. Vahl, R. Minkwitz, and H. Baumgärtel, Z. Anorg. Allg. Chem. **481**, 207 (1981).

$Se_2Cl_2^+$

$\tilde{H}\ ^2A$ C_2
$T^a \cong$ 39100 gas PE[1]

$\tilde{H}\ ^2B$ C_2
$T^a \cong$ 31000 gas PE[1]

$\tilde{F}\ ^2A$ C_2
$T^a \cong$ 29000 gas PE[1]

$\tilde{E}\ ^2A$ C_2
$T^a \cong$ 21700 gas PE[1]

$\tilde{D}\ ^2B$ C_2
$T^a \cong$ 19900 gas PE[1]

$\tilde{C}\ ^2B$ C_2
$T^a \cong$ 17900 gas PE[1]

$\tilde{B}\ ^2A$ C_2
$T^a \cong$ 10000 gas PE[1]

$\tilde{X},\tilde{A}\ ^2A,^2B$ C_2

[a] From vertical ionization potentials.

References

[1]E. Nagy-Felsobuki and J. B. Peel, J. Chem. Soc., Faraday Trans. 2 **76**, 148 (1980).

CF_2Br^-

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1219mT	Ar	IR	1
			1099sT	Ar	IR	1

References

[1]F. T. Prochaska and L. Andrews, J. Phys. Chem. **82**, 1731 (1978).

FSO_2^-

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	SO_2 s–stretch	1100m Cs	Ar	IR	1
	2		598m Cs	Ar	IR	1
	3		572m Cs	Ar	IR	1
	4		360w Cs	Ar	IR	1
	5	SO_2 a–stretch	1178m Cs	Ar	IR	1

References

[1]K. Garber and B. S. Ault, Inorg. Chem. **22**, 2509 (1983).

FOOF

The onset of continuous absorption by gas–phase FOOF occurs near 17000 (590 nm).[1] The maximum in this absorption lies beyond 220 nm.

$\tilde{X}$ C_2 Structure: MW^2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	OO stretch	1210(3)	gas	IR	7
	2	OF s–stretch	630(3)	gas	IR	7
			627	Ar	IR	3,5,6
			624	O_2	IR	4
	3	Deform.	360T	gas	IR	7
			366	Ar	IR	5
			368	O_2	IR	4
	4	Torsion	202T	gas	IR	7
b	5	OF a–stretch	614(3)	gas	IR	7
			612	Ar	IR	3,5,6
			612	O_2	IR	4
	6	Deform.	466	Ar	IR	5,6
			462	O_2	IR	4

$A_0 = 0.676$; $B_0 = 0.167$; $C_0 = 0.145$ MW^2

References

[1]P. H. Broderson, P. Frisch, and H.–J. Schumacher, Z. Phys. Chem. **B37**, 25 (1937).
[2]R. H. Jackson, J. Chem. Soc. 4585 (1962).
[3]A. Arkell, J. Am. Chem. Soc. **87**, 4058 (1965).
[4]R. D. Spratley, J. J. Turner, and G. C. Pimentel, J. Chem. Phys. **44**, 2063 (1966).
[5]D. J. Gardiner, N. J. Lawrence, and J. J. Turner, J. Chem. Soc. A 400 (1971).
[6]M. E. Jacox, J. Mol. Spectrosc. **84**, 74 (1980).
[7]K. C. Kim and G. M. Campbell, J. Mol. Struct. **129**, 263 (1985).

ClOOCl

An unstructured gas–phase absorption with maximum at 40800 (245 nm) has been assigned[1,4–6] to ClOOCl. Cl atoms have been detected[6] on irradiation of ClOOCl in this band.

$\tilde{X}$ C_2 Structure: MW^3

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			750	gas	IR	4
			752.6	Ar	IR	2
			653	gas	IR	4
			649.8	Ar	IR	2
			647.6			

$A_0 = 0.437$; $B_0 = 0.080$; $C_0 = 0.071$ MW^3

References

[1]R. A. Cox and G. D. Hayman, Nature **332**, 796 (1988).
[2]B.–M. Cheng and Y.–P. Lee, J. Chem. Phys. **90**, 5930 (1989).
[3]M. Birk, R. R. Friedl, E. A. Cohen, H. M. Pickett, and S. P. Sander, J. Chem. Phys. **91**, 6588 (1989).
[4]J. B. Burkholder, J. J. Orlando, and C. J. Howard, J. Phys. Chem. **94**, 687 (1990).
[5]W. B. DeMore and E. Tschuikow–Roux, J. Phys. Chem. **94**, 5856 (1990).
[6]M. J. Molina, A. J. Colussi, L. T. Molina, R. N. Schindler, and T.–L. Tso, Chem. Phys. Lett. **173**, 310 (1990).

$ClClO_2$

In the gas phase, prominent, unstructured absorption maxima appear[2,3] at 231 and 296 nm (43300 and 33800). In a neon matrix, unstructured absorption maxima are observed[1,3] at 236 and 296 nm (42400 and 33800), with half band widths of 40 and 45 nm, respectively.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ClO_2 s–stretch	1041.5(5)s	gas	IR	2,3
			1041.2s	Ne	IR	1,3
	2	ClO_2 scissors	522.7(5)wm	gas	IR	2,3
			522.5wm	Ne	IR	1,3
	3	ClCl stretch	440.5(5)s	gas	IR	2,3
			440.4s	Ne	IR	1,3
	4	Umbrella	271.4wm	Ne	IR	1,3
a"	5	ClO_2 a–stretch	1218.2(5)vs	gas	IR	2,3
			1216.4vs	Ne	IR	1,3
	6	ClO_2 rock	251.4vw	Ne	IR	1,3

References

[1]H. S. P. Müller and H. Willner, Proc. 1st European Workshop on Polar Stratospheric Ozone, Schliersee, Germany, 1990 (Air Pollution Research Report 34, CEC and BMFT, J. A. Pyle and N. R. P. Harris, Eds.).
[2]H. S. P. Müller and H. Willner, Ber. Bunsenges. Phys. Chem. **96**, 427 (1992).
[3]H. S. P. Müller and H. Willner, Inorg. Chem. **31**, 2527 (1992).

O_2ICl

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	IO s–stretch	844.7	Ar	IR	1
			845.5	Kr	IR	1
			852.2	N_2	IR	1
	2	IO_2 scissors	421.1	Ar	IR	1
	3	ICl stretch	330.5	Ar	IR	1
			327.5	Kr	IR	1
			331.9	N_2	IR	1
b_2	5	IO a–stretch	886.5	Ar	IR	1
			879.5			
			883.5	Kr	IR	1
			879.6			
			883.7	N_2	IR	1
			879.7			

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$SSCl_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		SS stretch	699	Ar	IR	1,2
			696	N_2	IR	1
		SCl_2 s–stretch	403	Ar	IR	1,2
			403	N_2	IR	1
a''		SCl_2 stretch	377	Ar	IR	1,2
			378	N_2	IR	1,2

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$SSBr_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		SS stretch	693	Ar	IR	1
		SBr_2 stretch	317	Ar	IR	1
a''		SBr_2 stretch	311	Ar	IR	1

References

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SF_3

$\tilde{X}$ C_{2v} Structure: ESR[1,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Eq. SF_2 s–stretch	843.8	Ar	IR	5
		Ax. SF_2 a–stretch	681.8	Ar	IR	2,3,5

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ClF_3^+

$\tilde{F}\ ^2B_2$ C_{2v}
T_0 = 33640(900) gas PE[1]

$\tilde{E}\ ^2B_1$ C_{2v}
T^a = 27590(480) gas PE[1]

$\tilde{D}\ ^2A_2$ C_{2v}
T^a = 21860(720) gas PE[1]

$\tilde{C}\ ^2B_2$ C_{2v}
T^a = 17590(720) gas PE[1]

$\tilde{B}\ ^2A_1$ C_{2v}
T_0 = 8960(900) gas PE[1]

$\tilde{X},\tilde{A}\ ^2B_1,^2A_1$ C_{2v}

[a] From vertical ionization potential.

References

[1]R. L. DeKock, B. R. Higginson, D. R. Lloyd, A. Breeze, D. W. J. Cruickshank, and D. R. Armstrong, Mol. Phys. **24**, 1059 (1972).

BrF_3^+

$\tilde{I}\ ^2B_2$ C_{2v}
T^a = 53330(640) gas PE[1]

$\tilde{G},\tilde{H}\ ^2A_1,^2B_1$ C_{2v}
T^a = 43890(480) gas PE[1]

$\tilde{F}\ ^2B_2$ C_{2v}
T_0 = 33160(560) gas PE[1]

$\tilde{E}\ ^2B_1$ C_{2v}
T^a = 27920(560) gas PE[1]

$\tilde{D}\ ^2A_2$ C_{2v}
T^a = 23400(560) gas PE[1]

$\tilde{C}\ ^2B_2$ C_{2v}
T^a = 19770(640) gas PE[1]

$\tilde{B}\ ^2A_1$ C_{2v}
T_0 = 14440(400) gas PE[1]

$\tilde{X},\tilde{A}\ ^2B_1,^2A_1$ C_{2v}

[a] From vertical ionization potential.

References

[1]R. L. DeKock, B. R. Higginson, D. R. Lloyd, A. Breeze, D. W. J. Cruickshank, and D. R. Armstrong, Mol. Phys. **24**, 1059 (1972).

Cl_2F_2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	5	FClF stretch	636	Ar	IR	1

References

[1]E. S. Prochaska, L. Andrews, N. R. Smyrl, and G. Mamantov, Inorg. Chem. **17**, 970 (1978).

Br_2F_2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	5	FBrF stretch	555	Ar	IR	1

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[1]E. S. Prochaska, L. Andrews, N. R. Smyrl, and G. Mamantov, Inorg. Chem. **17**, 970 (1978).

I_2F_2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	5	FIF stretch	526	Ar	IR	1

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6.8. H_5^+ and Five-Atomic Tetra- and Trihydrides

H_5^+

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			3910	gas	VP[a]	1
			3532	gas	VP	1

[a] Vibrational predissociation of mass-selected beam. Four overtones and combination bands have also been studied[2] using vibrational predissociation.

References

[1]M. Okumura, L. I. Yeh, and Y. T. Lee, J. Chem. Phys. **83**, 3705 (1985).
[2]Y. K. Bae, Chem. Phys. Lett. **180**, 179 (1991).

TiH_4

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		TiH stretch	1665.9T	Ar	IR	1
			1657.8T	Kr	IR	1

TiD_4

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		TiD stretch	1207.0T	Ar	IR	1
			1201.1T	Kr	IR	1

References

[1]Z. L. Xiao, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **95**, 2696 (1991).

CH_4^+

$\tilde{C}\ ^2A_1$ T_d
T_0 = 78870(160)[a] gas PE[3,6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	2190(80)	gas	PE	6

$\tilde{B}$ [b] C_s ?
T[c] ≅ 19240 gas PE[1-3,5,6]

$\tilde{A}$ [b] C_s ?
$T_0 \leq$ 13350[a] gas PE[1-3,5,6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1300(100)	gas	PE	5

$\tilde{X}$ [b] C_{2v} Structure: ESR[7] MO[8,10]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1700(100)[d]	gas	PE	5
			1200(100)	gas	PE	3,5

CD_4^+

$\tilde{C}\ ^2A_1$ T_d
T_0 = 79400(200) gas PE[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD stretch	1460(80)	gas	PE	3,6

[a] Based on adiabatic ionization potential of 12.615(10) eV for CH_4[4,5] and of 12.658(15) eV for CD_4.[9]
[b] Resulting from Jahn–Teller distortion of the ground $^2T_2$ state of CH_4^+.
[c] From vertical ionization potential.
[d] Two progressions, with onset near 3670.

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SiH_4^+

$\tilde{C}\ ^2A_1$ T_d
T_0 = 56070(240)[a] gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiH stretch	1690(30)	gas	PE	2

$\tilde{A},\tilde{B}$ [b]
$T_0 \leq$ 14930(240)[a] gas PE[1,2]

$\tilde{X}$ [bc] C_s Structure: MO[3,5,6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			760(10)	gas	PE,PI	1,2,4

[a] Based on adiabatic ionization potential of 11.00(2) eV for SiH_4.[4]
[b] Resulting from Jahn–Teller distortion of the ground $^2T_2$ state of SiH_4^+.
[c] Threshold for formation of $SiH_2^+ + H_2$ = 4360(240) and for formation of $SiH_3^+ + H \leq$ 8760.[4]

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[1] B. P. Pullen, T. A. Carlson, W. E. Moddeman, G. K. Schweitzer, W. E. Bull, and F. A. Grimm, J. Chem. Phys. **53**, 768 (1970).
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GeH_4^+

$\tilde{C}\ ^2A_1$ T_d
$T_0 \geq$ 55430(160)[a] gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	GeH stretch	1534(30)	gas	PE	2

$\tilde{A},\tilde{B}$ [b]
$T_0 \geq$ 9040(160)[a] gas PE[1,2]

$\tilde{X}$ [b]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			670(20)	gas	PE	1,2

[a] Based on an adiabatic ionization potential of 11.34 eV.[2] As for CH_4 and SiH_4, the true adiabatic ionization potential is likely to be substantially lower than the value obtained by photoelectron spectroscopy.
[b] Resulting from Jahn–Teller distortion of the ground $^2T_2$ state of GeH_4^+.

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NH_4^+

$\tilde{X}$ T_d Structure: $LD^{1,4}CC^2$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
t_2	3	NH stretch	3343.14	gas	LD,CC	1–3,6
	4	Deformation	1447.22	gas	DL	5

B_0 = 5.929 $LD^{1,4}CC^2$

ND_4^+

$\tilde{X}$ T_d

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
t_2	3	ND stretch	2495.0	gas	LD	4

B_0 = 2.979(3) LD^4

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NH_4

$3p\ ^2F_2$ T_d
$T_0 \cong 15078^{ab}$ gas $EM^{1,2,4}$ $3p^2F_2$–$3s^2A_1$ 663.5 nm
Diffuse.

$3s\ ^2A_1$ T_d
gas $3p^2F_2$–$3s^2A_1$ 663.5 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NH stretch	2552T	gas	EM	1,4
e	2	Deformation	1581T	gas	EM	1,4

ND_4

$3p\ ^2F_2$ T_d
T_0^a = 14828.285(4) gas $EM^{1,2,4}AB^{3,5}$ $3p^2F_2$–$3s^2A_1$ 675 nm

Three weak bands have been observed[4] 775, 1138, and 1722 cm^{-1} above the band origin. However, the assignment of these bands has not yet been established.
B_0 = 3.122 gas AB^5

$3s\ ^2A_1$ T_d
gas $3p^2F_2$–$3s^2A_1$ 675 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ND stretch	1960T	gas	EM	1,4
e	2	Deformation	1080.25(7)	gas	EM	7

$\tau \cong 30$ μs gas AB^5
B_0 = 3.041 gas AB^5

[a] Measured with respect to the lowest Rydberg state, $3s\ ^2A_1$. The ground state is dissociative.
[b] Estimated[5] by scaling of data for ND_4.

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$NaCH_3$

$\tilde{X}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 s–stretch	2760s	N_2	IR	1
	2	CH_3 s–deform.	1092w	N_2	IR	1
	3	CNa stretch	298s	N_2	IR	1
e	4	CH_3 a–stretch	2805s	N_2	IR	1
	5	CH_3 a–deform.	1384w	N_2	IR	1
	6	HCNa bend	362s	N_2	IR	1

$NaCD_3$

$\tilde{X}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_3 s–stretch	2019m	N_2	IR	1
	2	CD_3 s–deform.	836m	N_2	IR	1
	3	CNa stretch	278m	N_2	IR	1
e	4	CD_3 a–stretch	2123m	N_2	IR	1
	5	CD_3 a–deform.	972w	N_2	IR	1
	6	DCNa bend	285s	N_2	IR	1

References

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KCH_3

$\tilde{X}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 s–stretch	2732s	N_2	IR	1
	2	CH_3 s–deform.	1053w	N_2	IR	1
	3	CK stretch	280	N_2	IR	1
e	4	CH_3 a–stretch	2775s	N_2	IR	1
	5	CH_3 a–deform.	1384w	N_2	IR	1
	6	HCK bend	307m	N_2	IR	1

KCD_3

$\tilde{X}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_3 s–stretch	1994m	N_2	IR	1
	2	CD_3 s–deform.	807m	N_2	IR	1
	3	CK stretch	259s	N_2	IR	1
e	4	CD_3 a–stretch	2101m	N_2	IR	1
	5	CD_3 a–deform.	967w	N_2	IR	1
	6	DCK bend	237m	N_2	IR	1

References

[1]K. Burczyk and A. J. Downs, J. Chem. Soc., Dalton Trans. 2351 (1990).

$CaCH_3$

$\tilde{B}\ ^2A_1$ C_{3v}
T_0 = 16003(10) gas LF[1] $\tilde{B}$–$\tilde{X}$ 620–630 nm

$\tilde{A}\ ^2E$ C_{3v}
T_0 = 14743.174[a] gas LF[1,2] $\tilde{A}$–$\tilde{X}$ 630–730 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 umbrella	1048(10)	gas	LF	1
	3	CaC stretch	413(10)	gas	LF	1
e	6	CaCH deform.	391(5)H	gas	LF	1

A = 73.13 gas LF[1,2]
A_0 = 5.384; B_0 = 0.254 LF[2]

$\tilde{X}\ ^2A_1$ C_{3v} Structure: LF[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 umbrella	1085(10)	gas	LF	1
	3	CaC stretch	419(10)	gas	LF	1
e	6	CaCH deform.	319(5)H	gas	LF	1

A_0 = 5.448; B_0 = 0.252 LF[2]

[a] Predissociated above ca. 16200.[1]

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[1]C. R. Brazier and P. F. Bernath, J. Chem. Phys. **86**, 5918 (1987).
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$SrCH_3$

$\tilde{B}\ ^2A_1$ C_{3v}
T_0 = 14777(10) gas LF[1] $\tilde{B}$–$\tilde{X}$ 670–680 nm

$\tilde{A}\ ^2E$ C_{3v}
T_0 = 13653(10)[a] gas LF[1] $\tilde{A}$–$\tilde{X}$ 670–740 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 umbrella	1054(10)	gas	LF	1
	3	SrC stretch	373(10)	gas	LF	1
e	6	SrCH deform.	342(5)H	gas	LF	1

A = 273(20) gas LF[1]

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 umbrella	1072(10)	gas	LF	1
	3	SrC stretch	362(10)	gas	LF	1
e	6	SrCH deform.	279(5)H	gas	LF	1

[a] Predissociated above ca. 15000.[1]

References

[1]C. R. Brazier and P. F. Bernath, J. Chem. Phys. **86**, 5918 (1987).

$ZnCH_3$

$\tilde{C}\ ^2A_1$ [a] C_{3v}
T_0 = 36510 gas AB[1] $\tilde{C}$–$\tilde{X}$ 260–274 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 deform.	950T	gas	AB	1

$\tilde{A}\ ^2E$ C_{3v}
T_0 = 24077 gas AB[1]EM[2]LF[5] $\tilde{A}$–$\tilde{X}$ 379–437 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 deform.	1048	gas	AB,LF	1,4,5
	3	ZnC stretch	460	gas	LF	5

τ = 40(3) ns gas EM[3]LF[4]
A = 253 gas AB[1]EM[2,3]LF[4,5]

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 deform.	1064	gas	EM,LF	3–5
	3	ZnC stretch	445	gas	LF	4,5
e	6	ZnCH deform.	315T	gas	LF	5

[a] Assignment to $\tilde{C}$ state suggested[4] by analogy with ZnH.

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$CdCH_3$

$\tilde{B}\ ^2E$ C_{3v}
T_0 = 34916 gas AB^1LF^7 $\tilde{B}$–$\tilde{X}$ 264–287 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 deform.	960T	gas	AB	1
	3	CdC stretch	339T	gas	LF	7

$\tilde{A}\ ^2E_{1/2}$ C_{3v}
T_0 = 22514 gas $AB^1EM^{2\text{-}5}LF^{6,7}$ $\tilde{A}$–$\tilde{X}$ 400–458 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 deform.	1019(3)	gas	LF	7
	3	CdC stretch	400(3)	gas	LF	6,7

τ = 70(4) ns gas $EM^{2,4}LF^7$

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 deform.	1000(3)	gas	EM,LF	5–7
	3	CdC stretch	355(3)	gas	EM,LF	5–7

References

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$HFeNH_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NH stretch	3381	Ar	IR	1
		FeH stretch	1717.4	Ar	IR	1
		NH_2 bend	1517.8	Ar	IR	1
		FeN stretch	649.8	Ar	IR	1
		FeNH bend	536.8	Ar	IR	1

$DFeND_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		FeD stretch	1236.4	Ar	IR	1
		ND_2 bend	1131.7	Ar	IR	1
		FeN stretch	614.3	Ar	IR	1

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[1]J. W. Kauffman, R. H. Hauge, and J. L. Margrave, High Temp. Sci. **17**, 237 (1984).

$HNiNH_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NH_2 stretch	3367.5	Ar	IR	1
			3358.2	Kr	IR	1
		NiH stretch	1918.1	Ar	IR	1
			1918.1	Kr	IR	1
		NH_2 scissors	1533.3	Ar	IR	1
			1531.7	Kr	IR	1
		NiN stretch	676.5	Ar	IR	1
			671.7	Kr	IR	1
		NH_2 wag	619.2	Ar	IR	1
			618.7	Kr	IR	1

$DNiND_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ND_2 stretch	2522.9	Ar	IR	1
		NiD stretch	1431.3	Ar	IR	1
		ND_2 scissors	1177.1	Ar	IR	1
		NiN stretch	653.6	Ar	IR	1

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[1]D. W. Ball, R. H. Hauge, and J. H. Margrave, High Temp. Sci. **25**, 95 (1988).

$HCuNH_2$

In an argon matrix, threshold for photodecomposition into Cu + NH_3 near 400 nm.[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NH stretch	3329.5	Ar	IR	1
		CuH stretch	1851.2	Ar	IR	1
		NH_2 deform.	1524.1	Ar	IR	1
		NH_2 wag	592.2	Ar	IR	1

$DCuND_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ND stretch	2444.1	Ar	IR	1
		CuD stretch	1334.2	Ar	IR	1
		ND_2 deform.	1133.4	Ar	IR	1

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$C_2H_3^+$

$\tilde{X}$ C_{2v} (bridged) Structure: CE[1]LD[2,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
A_{1u}^+		CH stretch	3142.2	gas	LD	3

A_0 = 13.341; B_0 = 1.142; C_0 = 1.046 LD[2,3]MW[4]

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C_2H_3

Rydberg state

T_0 = 59410 gas AB[3] 164–169 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1306	gas	AB	3

$\tilde{A}\ ^2A''$ C_s

$T_0 \leq$ 20020 gas AB[1] 500–400 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CC stretch	1200	gas	AB	1
		CCH bend	920	gas	AB	1

$\tilde{X}$ C_s[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	7	Mixed OPLA	895.16	gas	DL	4
			900	Ar	IR	2

A_0 = 7.913; B_0 = 1.083; C_0 = 0.949 DL[4]

C_2D_3

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	7	Mixed OPLA	704	Ar	IR	2

[a] Rapid tunneling, giving effective C_{2v} symmetry.[4]

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CH_2SiH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			830(15)	gas	PE	1
			490(15)	gas	PE	1

CD_2SiD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			650(15)	gas	PE	1
			370(15)	gas	PE	1

References

[1]A. A. Bengali and D. G. Leopold, J. Am. Chem. Soc. **114**, 9192 (1992).

CH_3Si

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Si–C stretch	610(15)	gas	PE	1

CD_3Si

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Si–C stretch	610(15)	gas	PE	1
		CD_3 rock	470(10)	gas	PE	1

References

[1]A. A. Bengali and D. G. Leopold, J. Am. Chem. Soc. **114**, 9192 (1992).

CH_2NH^+

$\tilde{C}\ ^2A'$ C_s
$T \cong 52400$ gas PE[1]

$\tilde{B}\ ^2A'$ C_s
$T \cong 34600$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2530(160)	gas	PE	1
			1660(160)	gas	PE	1

$\tilde{A}\ ^2A''$ C_s
$T \cong 18300$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CN stretch	1370(160)	gas	PE	1

$\tilde{X}\ ^2A'$ C_s

References

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CH_2PH^+

$\tilde{C}$
T^a = 37900(800) gas PE[1]

$\tilde{B}$
T^a = 23400(800) gas PE[1]

$\tilde{A}\ ^2A'$ C_s
T^a = 3200(800) gas PE[1]

[a] From vertical ionization potentials.

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H_2BOH

$\tilde{X}$ C_s Structure: MW[1]
A_0 = 5.758; B_0 = 1.016; C_0 = 0.861 MW[1]

D_2BOD

$\tilde{X}$ C_s
A_0 = 2.957; B_0 = 0.799; C_0 = 0.627 MW[1]

References

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H_2BSH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	BH_2 a–stretch	2614	Ar	IR	1
	2	SH stretch	2574T	Ar	IR	1
	3	BH_2 s–stretch	2539	Ar	IR	1
	4	BH_2 s–bend	1191	Ar	IR	1
	6	BH_2 wag	940	Ar	IR	1
	7	B–S stretch	804	Ar	IR	1
	8	BH_2 rock	674	Ar	IR	1
	9	Torsion	635	Ar	IR	1

References

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CH_2SiH^-

Threshold for electron detachment from ground–state CH_2SiH^- = 16220(80) gas PE[1]

References

[1]A. A. Bengali and D. G. Leopold, J. Am. Chem. Soc. **114**, 9192 (1992).

CH_3Si^-

Threshold for electron detachment from ground–state CH_3Si^- = 6870(80) gas PE[1]

References

[1]A. A. Bengali and D. G. Leopold, J. Am. Chem. Soc. **114**, 9192 (1992).

CH_2NH

Photodissociates, producing HNC, on irradiation at 254 nm.[2]

$\tilde{X}\ ^1A'$ C_s Structure: MW[3,4,6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH stretch	3262.62	gas	IR	10,12
	2	CH stretch	3024.45	gas	IR	14
			3036wm	Ar	IR	1,5
	3	CH stretch	2914.18	gas	IR	10,14
			2926m	Ar	IR	1,5
	4	C=N stretch	1638.30	gas	LS,IR	7,8,10
			1641s	Ar	IR	1,5
	5	CH_2 scissors	1452.04	gas	IR	8–10
			1453s	Ar	IR	1,5
	6	HCNH deform.	1344.27	gas	IR	8–10
			1348vs	Ar	IR	1,5
	7	HCNH deform.	1058.18	gas	IR	10,13,15
			1059s	Ar	IR	1,5
a''	8	Torsion	1126.99	gas	IR	10,11, 13,15
			1123vs	Ar	IR	1,5
	9	H_2CN OPLA	1060.76	gas	IR	10,13,15
			1063m	Ar	IR	1,5

$A_0 = 6.545$; $B_0 = 1.156$; $C_0 = 0.979$ MW[3]

CD_2ND

$\tilde{X}\ ^1A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CD stretch	2269m	Ar	IR	1,5
	3	CD stretch	2184m	Ar	IR	1,5
	4	C=N stretch	1577ms	Ar	IR	1,5
	5	DCND deform.	1089m	Ar	IR	1,5
	6	CD_2 scissors	1067w	Ar	IR	1,5
	7	DCND deform.	770s	Ar	IR	1,5
a''	9	Torsion	821s	Ar	IR	1,5

$A_0 = 3.406$; $B_0 = 0.904$; $C_0 = 0.712$ MW[6]

CH_3N

$\tilde{A}\ ^3E$ C_{3v} Structure: EM[4]

T_0 = 31830.913(12) gas AB[1],EM[1,2,4,5,7] $\tilde{A}$–$\tilde{X}$ 288–356 nm
31576(20) N_2 AB[3,6] $\tilde{A}$–$\tilde{X}$ 281–317 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 deform.	1166T	N_2	AB	6
	3	CN stretch	758(4)	gas	UV	1,2
			755(22)	N_2	AB	3,6
e	6	CH_3 rock	728(4)	gas	EM	5

$A = -22.52$ gas EM[4,7]
$A_0 = 5.423$; $B_0 = 0.845$ EM[4,7]

$\tilde{X}\ ^3A_2$ C_{3v} Structure: EM[4,7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 s–stretch	2943(4)	gas	EM	2,5
	2	CH_3 deform.	1349(4)	gas	EM	2,5
	3	CN stretch	1040(4)	gas	EM	2,5
			1029	N_2	AB	3
e	4	CH_3 a–stretch	2989(4)	gas	EM	5
	5	CH_3 deform.	1490(4)	gas	EM	5
	6	CH_3 rock	903(8)	gas	EM	2,5

$A_0 = 5.61$; $B_0 = 0.929$ EM[4,7]

CD_3N

$\tilde{A}\ ^3E$ C_{3v}

T_0 = 31774.158(2)[b] gas AB[1],EM[2,4,5] $\tilde{A}$–$\tilde{X}$ 294–365 nm
31516(30) N_2 AB[3,6] $\tilde{A}$–$\tilde{X}$ 277–318 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_3 deform.	1044T	N_2	AB	6
	3	CN stretch	759(4)	gas	UV	1,2
			695T	N_2	AB	6
e		CD_3 rock	579(4)[a]	gas	EM	2

$B_0 = 0.691$ EM[4]

$\tilde{X}\ ^3A_2$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_3 deform.	941(4)	gas	EM	5
	3	CN stretch	1110(4)	gas	EM	2,5
e	6	CD_3 rock	749(8)	gas	EM	2,5

$B_0 = 0.744$ EM[4]

[a] Observed as sequence band.
[b] Calculated assuming $A(CD_3N) = A(CH_3N)$.

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$HSiNH_2$

In an argon matrix, a prominent absorption maximum at 208 nm and a shoulder at 220 nm have been assigned[1] to $HSiNH_2$.

In an argon matrix, a weak, broad, unstructured absorption with maximum at 348 nm is associated with the photolysis of $HSiNH_2$ to produce $HNSi + H_2$.[1] *Subsequent irradiation at 254 nm reverses this photodecomposition.*

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NH_2 stretch	3494.5wm	Ar	IR	1
		NH_2 stretch	3408.7w	Ar	IR	1
		SiH stretch	1975.3vs	Ar	IR	1
		NH_2 scissors	1562.6m	Ar	IR	1
		SiN stretch	866.4s	Ar	IR	1
		NH_2 wag	570.4vs	Ar	IR	1

$DSiND_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ND_2 stretch	2611.2wm	Ar	IR	1
		ND_2 stretch	2500.8wm	Ar	IR	1
		SiD stretch	1432.4vs	Ar	IR	1
		ND_2 scissors	1179.3vs	Ar	IR	1
		SiN stretch	814.3m	Ar	IR	1
		ND_2 wag	443.6ms	Ar	IR	1

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CD_3O^+

$\tilde{X}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_3 s-stretch	2400T	gas	PI	1

References

[1]B. Ruscic and J. Berkowitz, J. Chem. Phys. **95**, 4033 (1991).

CH_2OH^+

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3422.802	gas	LD	2
		CO stretch	1650(30)	gas	PE	1
		CH_2 deform.	1370(30)	gas	PE	1

$A_0 = 6.590$; $B_0 = 1.146$; $C_0 = 0.973$ LD^2

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[1]J. M. Dyke, A. R. Ellis, N. Jonathan, N. Keddar, and A. Morris, Chem. Phys. Lett. **111**, 207 (1984).
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CH_3S^+

$\tilde{X}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CS stretch	700(60)	gas	PI	1

CD_3S^+

$\tilde{X}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CS stretch	730(60)	gas	PI	1

References

[1]B. Ruscic and J. Berkowitz, J. Chem. Phys. **97**, 1818 (1992).

CH_2SH^+

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CS stretch	1020(40)	gas	PI	1
			600(80)T	gas	PI	1

References

[1]B. Ruscic and J. Berkowitz, J. Chem. Phys. **97**, 1818 (1992).

$N_2H_3^+$

$\tilde{X}\ ^1A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	4	N=N stretch	1570(80)	gas	PI	1

References

[1]B. Ruscic and J. Berkowitz, J. Chem. Phys. **95**, 4378 (1991).

CH_3O

$\tilde{A}\ ^2A_1$ C_{3v} Structure: LF[22,23]
T_0 = 31614.51(4) gas EM[1,2,11,12]AB[5]LF[6,8,18,19,22-24] $\tilde{A}-\tilde{X}$ 271–421 nm
31291(3) Ar LF[21] $\tilde{A}-\tilde{X}$ 270–420 nm
Evidence for predissociation above 36800.[13]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 stretch	3079	gas	LF	19
	2	Umbrella	1315	gas	LF	19
			1308(4)	Ar	LF	21
	3	CO stretch	660	gas	AB,EM LF	5,12,19
			657(2)	Ar	LF	21
e	4	CH_3 stretch	2962	gas	LF	19
	5	CH_2 scissors	1407	gas	LF	19
			1410(3)	Ar	LF	21
	6	HCO deform.	595	gas	LF	19

τ = 2.2(2)μs gas EM[2,9]LF[4,14,15,16,18,20]
A_0 = 4.981(3); B_0 = 0.743 LF[22-24]

$\tilde{X}\ ^2E$ C_{3v}[a] Structure: LMR[3,7]MW[10,17]LF[22]
High vibrational levels have been studied using SEP.[25]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 stretch	2840	gas	LF	19
	2	CH_3 umbrella	1362	gas	LF	19
			1356(2)	Ar	LF	21
	3	CO stretch	1047	gas	LF,EM	6,9,12 19
			1044(2)	Ar	LF	21
e	4	CH_3 stretch	2774T	gas	LF	19
			2758(3)	Ar	LF	21
	5	CH_2 scissors	1487	gas	LF	19
			1406(2)	Ar	LF	21
	6	HCO deform.	651.5	gas	LF,SEP	19,26

A = −61.97(7) gas LMR[7]MW[10]EM[11,12]LF[19,22,23]
A_0 = 5.206(4); B_0 = 0.932 LMR[7]MW[10,17]LF[22,23]

CD_3O

$\tilde{A}\ ^2A_1$ C_{3v}
T_0 = 31554 gas LF[6,19]EM[12] $\tilde{A}-\tilde{X}$ 282–410 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_3 stretch	2015	gas	LF	19
	2	CD_3 umbrella	971	gas	LF	19
	3	CO stretch	663	gas	EM,LF	12,19
e	5	CD_2 scissors	1047	gas	LF	19

$\tilde{X}\ ^2E$ C_{3v}[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CO stretch	1000T	gas	LF	19
	3	CD_3 umbrella	893T	gas	LF	19
e	5	CD_2 scissors	1174	gas	LF,EM	6,12,19
	6	DCO deform.	496	gas	LF	19

A = −56(2) gas EM[12]
B_0 = 0.740 MW[17]

[a] Somewhat distorted by Jahn–Teller coupling.

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CH_2OH

3p Rydberg state C_s
T_0 = 41064 gas MPI[3,4]AB[5] $3p$–$\tilde{X}$ 217–244 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	4	CH_2 scissors	1459	gas	MPI	3
	5	COH bend + CH_2 rock	1091	gas	MPI	3
	6	CO stretch	1623	gas	MPI	3,4
	7	CH_2 rock + COH bend	1351	gas	MPI	3
a''	8	CH_2 wag	950	gas	MPI	3
	9	Torsion	573	gas	MPI	3

3s Rydberg state C_s
T_0 = 35050 gas AB[5] $3s$–$\tilde{X}$ 243–285 nm
Threshold for photodecomposition into H_2CO + H near 280 nm.[1,2]

$\tilde{A}$
Threshold for photodecomposition into H_2CO + H near 280 nm.[1,2]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OH stretch	3650m	Ar	IR	1,2
			3637m	N_2	IR	1
	4	CH_2 scissors	1459w	Ar	IR	2
	5	OH deform.	1334m	Ar	IR	1,2
	6	CO stretch	1183vs	Ar	IR	1,2
			1183s	N_2	IR	1
	7	HCOH deform.	1048s	Ar	IR	1,2
			1056m	N_2	IR	1
	8	CH_2 rock	607(15)	gas	MPI	4
	9	Torsion	420m	Ar	IR	1,2
			482m	N_2	IR	1

CD_2OD

3p Rydberg state C_s
T_0 = 40913 gas MPI[3,4]AB[6] $3p$–$\tilde{X}$ 216–244 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	4	CD_2 scissors	1109	gas	MPI,AB	3,6
	5	COD bend + CD_2 rock	803	gas	MPI	3
	6	CO stretch	1565	gas	MPI,AB	3,4,6
a''	9	Torsion	440	gas	MPI	3

3s Rydberg state C_s
T_0 = 35124 gas AB[6]

$\tilde{A}$
Threshold for photodecomposition into D_2CO + D near 280 nm.[1,2]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OD stretch	2694wm	Ar	IR	2
			2682m	N_2	IR	1
	4	CO stretch	1223m	Ar	IR	2
			1222m	N_2	IR	1
	5		1041m	Ar	IR	2
	7		765wm	Ar	IR	2
	8	CD_2 rock	498(15)	gas	MPI	4

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CH_3S

A diffuse, unstructured absorption at 218.5 nm, observed on flash photolysis[1] of a number of sulfur–containing compounds or on pulse radiolysis[12] of CH_3SH in the presence of an F–atom source, has been attributed to CH_3S.

$\tilde{A}$ $^2A_1$ C_{3v} Structure: LF[9]
T_0 = 26396.8 gas EM^{2}LF[6,9,11] $\tilde{A}$–$\tilde{X}$ 350–530 nm
Predissociation threshold ≥ 27885.[11] In an argon matrix, CH_2SH is formed.[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 umbrella	1098(2)	gas	LF	11
	3	CS stretch	401(2)	gas	EM,LF	2,6,9,11
e	6	HCS deform.	635(10)	gas	LF	11

τ_0 = 760(60) ns gas LF[8]; 1130(70) ns gas LF[10,11]
A_0 = 5.343(47); B_0 = 0.346 LF[9]

$\tilde{X}$ ^2E C_{3v} Structure: MW^{7}LF[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 stretch	2776T	gas	LF	11
	2	CH_3 umbrella	1313(5)	gas	PD,LF	4,6,11
	3	CS stretch	727(3)	gas	EM,PE	2–4,6
					PD,LF	11
e	4	CH_3 stretch	2706T	gas	LF	11
	5	CH_3 deform.	1496(6)	gas	LF	11
	6	HCS deform.	586T	gas	LF	11

A = −259.1 gas LF[9,11]
A_0 = 5.68(4); B_0 = 0.450 MW^{7}LF[9]

CD_3S

$\tilde{A}\ ^2A_1$ C_{3v}
T_0 = 26574 gas LF[6] $\tilde{A}-\tilde{X}$ 352–378 nm
Predissociation threshold ≤ 27728.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_3 umbrella	837(1)	gas	LF	6
	3	CS stretch	395(1)	gas	LF	6

τ_0 = 0.45(11) μs gas LF[6]

$\tilde{X}\ ^2E$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_3 umbrella	1100(50)	gas	PD	4
	3	CS stretch	667(1)	gas	PD,LF	4,6
e	5	DCS deform.	780(30)H	gas	PD	4

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CH_2SH

An unstructured absorption between 250 and 300 nm, with a maximum near 260 nm, which appears on pulse radiolysis of CH_3SH in the presence of an F-atom source has been attributed[3] to CH_2SH.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		H_2CS umbrella	425s	Ar	IR	1,2

CD_2SD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		D_2CS umbrella	322(5)	Ar	IR	2

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CH_3Te

$\tilde{B}$ C_{3v}
T_0 = 41068 gas AB[1,2] $\tilde{B}-\tilde{X}$ 225–245 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 deform.	1100T	gas	AB	2

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CH_3F^+

$\tilde{C}\ ^2A_1$ C_{3v}
$T_0 \cong$ 87700 gas PE[2,4]

$\tilde{A},\tilde{B}\ ^2A_1,^2E$ C_{3v}
$T_0 \cong$ 30400 gas PE[1–5]
A weak, broad absorption maximum at 255 nm (39200) which appears on argon-resonance photolysis of CH_3F isolated in solid argon and which can be destroyed by mercury-arc photolysis has been attributed[6] to the $\tilde{A},\tilde{B}-\tilde{X}$ transition of CH_3F^+.

$\tilde{X}\ ^2E$ [a] C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CF stretch	695(80)	gas	PE	5
e	5	CH_3 deform.	1315(80)	gas	PE	5
	6	HCF deform.	880(80)	gas	PE	5

[a] The high resolution PE spectrum[5] suggests a Jahn-Teller splitting of ca. 4800, with excitation of a progression in ν_5 (ca. 1050) in the higher energy component.

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CH_3Cl^+

$\tilde{C}\ ^2A_1$ C_{3v}
T^a = 82400(900) gas PE[2]

$\tilde{B}\ ^2E$ C_{3v}
T^a = 33170(900) gas PE[1-4,7]
Position of first maximum is given. A Jahn–Teller splitting of ca. 5000 is observed.[4,7]

A weak, broad absorption with onset near 400 nm (25000) and maximum at 335 nm (29800) which appears on argon–resonance photolysis of CH_3Cl isolated in an argon matrix and which is destroyed by exposure of the sample to 290–1000 nm radiation has been attributed[6] to the $\tilde{B}$–$\tilde{X}$ and $\tilde{A}$–$\tilde{X}$ transitions of CH_3Cl^+.

$\tilde{A}\ ^2A_1$ C_{3v}
T_0 = 20260(900) gas PE[1-4,7]

$\tilde{X}\ ^2E$ C_{3v}
Analysis of Ref. 5 suggests that the observed splitting of 218(50) is predominantly due to the Jahn–Teller effect and that the structure is distorted to C_s or C_1 symmetry. Small differences between the vibrational spacings observed for the two components of the overall transition are within the experimental error.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 umbrella	1073(50)	gas	PE	2,4
	3	CCl stretch	654(50)	gas	PE	3,4
e	5	CH_3 deform.	1550(50)	gas	PE	3,4
	6	CH_3 rock	870(50)	gas	PE	3,4

[a] From vertical ionization potential.

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CH_3Br^+

$\tilde{C}\ ^2A_1$ C_{3v}
T^a = 75500(900) gas PE[1]

$\tilde{B}\ ^2E$ C_{3v}
T_0 = 31930(900) gas PE[1,3]
A Jahn–Teller splitting of ca. 5600 is observed.[1-3] (Onset of the transition is given.)

A broad absorption with maximum at 267 nm (37400) which appears on argon–resonance photolysis of CH_3Br isolated in an argon matrix and which has a photodecomposition threshold at a wavelength longer than 500 nm has been assigned[5] to the $\tilde{B}$–$\tilde{X}$ transi tion of CH_3Br^+.

$\tilde{A}\ ^2A_1$ C_{3v}
T_0 = 19820(900) gas PE[1-3]
A broad absorption with maximum at 348 nm (28700) which appears on argon–resonance photolysis of CH_3Br isolated in an argon matrix and which has a photodecomposition threshold at a wavelength longer than 500 nm has been assigned[5] to the $\tilde{A}$–$\tilde{X}$ transition of CH_3Br^+.

$\tilde{X}\ ^2E_{3/2}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 stretch[b]	2930(120)	gas	PE	3
	2	CH_3 umbrella	1290(80)	gas	PE	1–3
	3	CBr stretch	468(80)	gas	PE	3
e	4	CH_3 stretch	3130(100)	gas	PE	2,3
	6	CH_3 rock	850(80)	gas	PE	1–3

A = 2570(100) gas PE[2-4]

CD_3Br^+

$\tilde{X}\ ^2E_{3/2}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_3 umbrella	947(80)	gas	PE	2
e	4	CD_3 stretch	2165(80)	gas	PE	2

A = 2730(100) gas PE[2]

[a] From vertical ionization potential.
[b] Identified for $^2E_{1/2}$, but not for $^2E_{3/2}$.

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CH_3I^+

$\tilde{C}\ ^2A_2$ C_{3v}
T^a = 81200(900) gas PE[1]

$\tilde{B}\ ^2E$ C_{3v}
T_0 = 35180(900) gas PE[1-3]
A Jahn–Teller splitting of ca. 5600 is observed.[1-3] (Onset of the transition is given.)

$\tilde{A}\ ^2A_1$ C_{3v}
T_0 = 16884 gas PE[1-3]PF[6-11]
A broad, unstructured absorption with onset near 420 nm (23800) and with maximum at 373 nm (26800) which appears on argon-resonance photolysis of CH_3I isolated in solid argon and which has a photodecomposition threshold between 500 and 650 nm has been assigned[5] to the $\tilde{A}$–$\tilde{X}$ transition of CH_3I^+.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 stretch	2810	gas	PF	7
	2	CH_3 umbrella	1192	gas	PF	9–11
	3	CI stretch	294.2	gas	PE,PF	3,9–11

A^b = 5.07(5); B^b = 0.185 PF[6,8]

$\tilde{X}\ ^2E$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 stretch[c]	2970(50)	gas	PE	2,3
	2	CH_3 umbrella	1254	gas	PE,PF	1–3,9
	3	CI stretch	492(50)	gas	PE	1,3
e	4	CH_3 stretch	3060(50)	gas	PE	3,4
	6	CH_3 rock	920(50)	gas	PE	3

A = 5050 gas PE[1-4]PF[9,11]

CD_3I^+

$\tilde{A}\ ^2A_1$ C_{3v}
T_0 = 16982 gas PE,PF[7,9-11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_3 stretch	2100	gas	PF	9
	2	CD_3 umbrella	918	gas	PF	10,11
	3	CI stretch	276.3	gas	PF	10,11

$\tilde{X}\ ^2E$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_3 stretch	2125	gas	PF	11
	2	CD_3 umbrella	952	gas	PF	7
	3	CI stretch	442	gas	PF	11

A = 5036 gas PF[11]

[a] From vertical ionization potential.
[b] From study of band at 16978 in $\tilde{A}$–$\tilde{X}$ $^2E_{1/2}$ transition.
[c] Identified for $^2E_{1/2}$ but not for $^2E_{3/2}$.

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SiH_3F^+

$\tilde{C}\ ^2A_1$ C_{3v}
T^a = 52400(400) gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			800T	gas	PE	2

$\tilde{B}\ ^2E$ C_{3v}
$T^a \cong$ 28900 gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiH_3 stretch	1470(80)	gas	PE	2

$\tilde{A}\ ^2A_1$ C_{3v}
$T^a \cong$ 26900 gas PE[1,2]

$\tilde{X}\ ^2E$ C_{3v}
Jahn–Teller splitting = 3550(160).[2]

[a] From vertical ionization potentials. Transitions are measured from first maximum in the photoelectron spectrum.

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SiH_3Cl^+

$\tilde{C}\ ^2A_1$ C_{3v}
T^a = 51900(500) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiH_3 stretch	1760(80)[b]	gas	PE	1,2

$\tilde{B}\ ^2E$ C_{3v}
$T^a \cong$ 18000 gas PE[1,2]

$\tilde{A}\ ^2A_1$ C_{3v}
T^a = 14400(1000) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	SiCl stretch	480(40)	gas	PE	1

$\tilde{X}\ ^2E$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	SiCl stretch	520(40)	gas	PE	1,2

[a] From vertical ionization potentials.
[b] ca. 1320 for SiD_3Cl^+.[2]

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SiH_3Br^+

$\tilde{D}\ ^2A_1$ C_{3v}
T^a = 68900(1000) gas PE[1]

$\tilde{C}\ ^2A_1$ C_{3v}
T^a = 57120(320) gas PE[1,2]

$\tilde{B}\ ^2E$ C_{3v}
T^a = 20500(1000) gas PE[1,2]
Jahn–Teller splitting = 3200(320) gas PE[2]

$\tilde{A}\ ^2A_1$ C_{3v}
T^a = 15250(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	SiBr stretch	400(80)	gas	PE	2

$\tilde{X}\ ^2E_{3/2}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			320T	gas	PE	2

A = 1600(320) gas PE[2]

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. **67**, 3425 (1971).
[2]D. C. Frost, F. G. Herring, A. Katrib, R. A. N. McLean, J. E. Drake, and N. P. C. Westwood, Can. J. Chem. **49**, 4033 (1971).

SiH_3I^+

$\tilde{B}\ ^2E$ C_{3v}
T^a = 24400(1000) gas PE[1]

$\tilde{A}\ ^2A_1$ C_{3v}
T^a = 18230(320) gas PE[1]

$\tilde{X}\ ^2E_{3/2}$ C_{3v}
A = 4440(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. **67**, 3425 (1971).

GeH_3F^+

$\tilde{A},\tilde{B}\ ^2A_1,^2E$ C_{3v}
$T^a \cong$ 22000 gas PE[1]

$\tilde{X}\ ^2E$ C_{3v}

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. **67**, 3425 (1971).

GeH_3Cl^+

$\tilde{B}\ ^2E$ C_{3v}
T^a = 16100(1000) gas PE[1]

$\tilde{A}\ ^2A_1$ C_{3v}
T^a = 14120(320) gas PE[1]

$\tilde{X}\ ^2E$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	GeCl stretch	400T	gas	PE	1

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. **67**, 3425 (1971).

GeH_3Br^+

$\tilde{B}\ ^2E$ C_{3v}
T^a = 1850(1000) gas PE[1]

$\tilde{A}\ ^2A_1$ C_{3v}
T^a = 15330(320) gas PE[1]

$\tilde{X}\ ^2E_{3/2}$ C_{3v}
A = 1775(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. **67**, 3425 (1971).

GeH_3I^+

$\tilde{B}\ ^2E$ C_{3v}
T^a = 24300(1000) gas PE[1]

$\tilde{A}\ ^2A_1$ C_{3v}
T^a = 17100(320) gas PE[1]

$\tilde{X}\ ^2E_{3/2}$ C_{3v}
A = 4440(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. **67**, 3425 (1971).

NH_2OH^+

$\tilde{D}\ ^2A''$ C_s
T^a = 54500(1000) gas PE[2]

$\tilde{C}\ ^2A'$ C_s
T^a = 50100(1000) gas PE[1,2]

$\tilde{B}\ ^2A'$ C_s
T^a = 39620(320) gas PE[1,2]

$\tilde{A}\ ^2A''$ C_s
T^a = 8960(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3100(160)	gas	PE	1,2

$\tilde{X}\ ^2A'$ C_s

[a] From vertical ionization potentials.

References

[1]K. Kimura and S. Katsumata, J. Chem. Phys. **67**, 1225 (1977).
[2]P. Rademacher and B. Freckmann, J. Electron Spectrosc. Relat. Phenom. **19**, 251 (1980).

CH_3O^-

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 umbrella	1075(100)	gas	PE	1

CD_3O^-

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_3 umbrella	915(100)	gas	PE	1

References

[1]P. C. Engelking, G. B. Ellison, and W. C. Lineberger, J. Chem. Phys. **69**, 1826 (1978).

CH_3S^-

Threshold for electron detachment from ground-state CH_3S^- = 15020(30) gas PD[2]PE[1,3]

$\tilde{X}$ C_{3v} Structure: MO[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CS stretch	770(190)	gas	PE	3

References

[1]P. C. Engelking, G. B. Ellison, and W. C. Lineberger, J. Chem. Phys. **69**, 1826 (1978).
[2]B. K. Janousek and J. I. Brauman, J. Chem. Phys. **72**, 694 (1980).
[3]S. Moran and G. B. Ellison, J. Phys. Chem. **92**, 1794 (1988).

PH_3O

$\tilde{X}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PH_3 stretch	2359.0[a]	Ar	IR	1
	2	PO stretch	1240.2	Ar	IR	1
	3	PH_3 umbrella	1143.5	Ar	IR	1
e	4	PH_3 stretch	2371.5	Ar	IR	1
	5	PH_3 deform.	1114.3	Ar	IR	1
	6	HPO deform.	853.0	Ar	IR	1

PD_3O

$\tilde{X}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PD_3 stretch	1721.1	Ar	IR	1
	2	PO stretch	1217.3	Ar	IR	1
	3	PD_3 umbrella	843.6	Ar	IR	1
e	6	DPO deform.	655.9	Ar	IR	1

[a] In Fermi resonance with $\nu_2 + \nu_3$.

References

[1]R. Withnall and L. Andrews, J. Phys. Chem. **91**, 784 (1987).

c–H_2POH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3643.6	Ar	IR	1
	2	PH_2 s–stretch	2304.8	Ar	IR	1
	3	PH_2 scissors	1123.9	Ar	IR	1
	4	POH deform.	1074.8	Ar	IR	1
	5	PH_2 wag	915.0	Ar	IR	1
	6	PO stretch	797.1	Ar	IR	1
a''	7	PH_2 a–stretch	2278.1	Ar	IR	1
	8	PH_2 rock	848.1	Ar	IR	1
	9	Torsion	375.3	Ar	IR	1

c–D_2POD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2688.5	Ar	IR	1
	2	PD_2 s–stretch	1679.1	Ar	IR	1
	3	POD deform.	828.5	Ar	IR	1
	4	PD_2 scissors	813.6	Ar	IR	1
	5	PO stretch	796.1	Ar	IR	1
	6	PD_2 wag	681.6	Ar	IR	1
a''	7	PD_2 a–stretch	1658.5	Ar	IR	1
	8	PD_2 rock	622.6	Ar	IR	1

References

[1]R. Withnall and L. Andrews, J. Phys. Chem. **91**, 784 (1987).

H_3AsO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		AsH stretch	2173.5s	Ar	IR	1
		AsH stretch	2170.1s	Ar	IR	1
		AsH_3 deform.	983.4s	Ar	IR	1
		AsH_3 deform.	979.8s	Ar	IR	1
		As=O stretch	937.9vs	Ar	IR	1
		HAsO deform.	817.1m	Ar	IR	1

D_3AsO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		AsD stretch	1568.2	Ar	IR	1
		AsD stretch	1559.8	Ar	IR	1
		As=O stretch	938.2vs	Ar	IR	1
		AsD_3 deform.	707.8	Ar	IR	1
		AsD_3 deform.	704.9	Ar	IR	1
		DAsO deform.	576.3	Ar	IR	1

References

[1]L. Andrews, R. Withnall, and B. W. Moores, J. Phys. Chem. **93**, 1279 (1989).

H_2AsOH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3652.2	Ar	IR	1
		AsH stretch	2092[a]	Ar	IR	1
		AsH stretch	2086.3	Ar	IR	1
		AsH stretch	2080.7	Ar	IR	1
		AsH_2 scissors	976[a]	Ar	IR	1
		AsH_2 scissors	974.5	Ar	IR	1
		HAsO deform.	813[a]	Ar	IR	1
		HAsO deform.	806.7	Ar	IR	1
		AsH_2 rock	687.2	Ar	IR	1
		AsO stretch	647.9s	Ar	IR	1
		Torsion	366[a]	Ar	IR	1
		Torsion	297.5	Ar	IR	1

D_2AsOD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OD stretch	2694.6	Ar	IR	1
		AsD stretch	1504.2	Ar	IR	1
		AsD stretch	1498.9	Ar	IR	1
		AsOD deform.	762.0	Ar	IR	1
		AsD_2 scissors	697.7	Ar	IR	1
		AsO stretch	647.8	Ar	IR	1
		AsD_2 rock	516.1	Ar	IR	1

[a] Believed to be contributed by the other rotamer of the *cis–trans* pair.

References

[1]L. Andrews, R. Withnall, and B. W. Moores, J. Phys. Chem. **93**, 1279 (1989).

H_3SbO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	SbH_3 deform.	791.8	Ar	IR	1
e	4	SbH_3 stretch	1970	Ar	IR	1

D_3SbO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Sb=O stretch	824.6	Ar	IR	1
	3	SbD_3 deform.	568	Ar	IR	1
e	4	SbD_3 stretch	1413	Ar	IR	1
	6	DSbO a–deform.	402.0	Ar	IR	1

References

[1]L. Andrews, B. W. Moores, and K. K. Fonda, Inorg. Chem. **28**, 290 (1989).

H_2SbOH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3654	Ar	IR	1
		SbH_2 stretch	1836.8	Ar	IR	1
		SbO stretch	583.5	Ar	IR	1

D_2SbOD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OD stretch	2697	Ar	IR	1
		SbD_2 stretch	1320.6	Ar	IR	1
		SbO stretch	598	Ar	IR	1

References

[1]L. Andrews, B. W. Moores, and K. K. Fonda, Inorg. Chem. **28**, 290 (1989).

6.9. Five–Atomic Dihydrides

Ca_3H_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1099.7	Kr	IR	1
			970.7	Kr	IR	1

Ca_3D_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			789.9	Kr	IR	1
			707.7	Kr	IR	1

References

[1]Z. L. Xiao, R. H. Hauge, and J. L. Margrave, High Temp. Sci. **31**, 59 (1991).

Cu_3H_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1082.1	Ar	IR	1
			1039.7	Ar	IR	1
			537.1	Ar	IR	1

Cu_3D_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			781	Ar	IR	1
			755.7	Ar	IR	1

References

[1]R. H. Hauge, Z. H. Kafafi, and J. L. Margrave, in *Physics and Chemistry of Small Clusters*, P. Jena, B. K. Rao, and S. N. Khanna, Eds., p. 787 (Plenum, New York, 1987).

LiC_2H_2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH s–stretch	2952	Ar	IR	1
	2	C=C stretch	1655	Ar	IR	1
	4	CLi s–stretch	600	Ar	IR	1
b_1	6	CH deform.	479	Ar	IR	1
b_2	7	CH a–stretch	2908	Ar	IR	1
	8	CH a–deform.	714	Ar	IR	1

LiC_2D_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD s-stretch	2272	Ar	IR	1
	2	C=C stretch	1561	Ar	IR	1
b_1	6	CD deform.	366	Ar	IR	1
b_2	7	CD a-stretch	2161	Ar	IR	1
	8	CD deform.	576	Ar	IR	1

References

[1]L. Manceron and L. Andrews, J. Am. Chem. Soc. **107**, 563 (1985).

HBCBH

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	4	BCB a-stretch	1872.0	Ar	IR	1

DBCBD

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	BD a-stretch	2190.9	Ar	IR	1
	4	BCB a-stretch	1727.4	Ar	IR	1

References

[1]P. Hassanzadeh and L. Andrews, J. Am. Chem. Soc. **114**, 9239 (1992).

HFeCCH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3276.2	Ar	IR	1
		C≡C stretch	1976.4	Ar	IR	1
			1974.8			
		FeH stretch	1765.0	Ar	IR	1
			1762.6			

DFeCCD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD stretch	2432.8	Ar	IR	1
		C≡C stretch	1862.7	Ar	IR	1
			1861.0			
		FeD stretch	1269.4	Ar	IR	1
			1267.2			

References

[1]E. S. Kline, Z. H. Kafafi, R. H. Hauge, and J. L. Margrave, J. Am. Chem. Soc. **107**, 7559 (1985).

$(C_2H_2)Ni$

Exposure of the sample isolated in solid argon to radiation of wavelength longer than 400 nm results in isomerization to $NiC=CH_2$.[1]

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		C=C stretch	1647.4	Ar	IR	1
		CH bend	847.3	Ar	IR	1
b_1		CH bend	730.9	Ar	IR	1
b_2		CH bend	658.1	Ar	IR	1
?		CNi stretch	548.6	Ar	IR	1

$(C_2D_2)Ni$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		C=C stretch	1540.6	Ar	IR	1
		CD bend	718.6	Ar	IR	1
b_1		CD bend	548.4	Ar	IR	1
b_2		CD bend	506.2	Ar	IR	1
?		CNi stretch	507.4	Ar	IR	1

References

[1]E. S. Kline, Z. H. Kafafi, R. H. Hauge, and J. L. Margrave, J. Am. Chem. Soc. **109**, 2402 (1987).

$NiC=CH_2$

In an argon matrix, isomerizes to $(C_2H_2)Ni$ on exposure to radiation of wavelength between 280 and 360 nm.[1]

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s–stretch	2889.1	Ar	IR	1
	2	C=C stretch	1635.0	Ar	IR	1
b_1	6	H_2CC OPLA	758.6	Ar	IR	1
b_2	8	CH_2 a–stretch	2983.5	Ar	IR	1
	9	CH_2 rock	833.6	Ar	IR	1

$NiC{=}CD_2$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C=C stretch	1626.2	Ar	IR	1
b_1	6	H_2CC OPLA	606.3	Ar	IR	1

References

[1]E. S. Kline, Z. H. Kafafi, R. H. Hauge, and J. L. Margrave, J. Am. Chem. Soc. **109**, 2402 (1987).

HMgOMgH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		MgH stretch	1561.3	Ar	IR	1
		MgO stretch	936.7	Ar	IR	1

DMgOMgD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		MgD stretch	1145.1	Ar	IR	1
		MgO stretch	925.6	Ar	IR	1

References

[1]J. W. Kauffman, R. H. Hauge, and J. L. Margrave, High Temp. Sci. **18**, 97 (1984).

HMg_2OH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		MgH stretch	1524.4	Ar	IR	1
		MgO stretch	736.2	Ar	IR	1
		MgOH bend	692	Ar	IR	1
		MgMg stretch	544.2	Ar	IR	1

DMg_2OD [a]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		MgD stretch	1109.6	Ar	IR	1
		MgO stretch	704.4	Ar	IR	1
		MgOD bend	569	Ar	IR	1
		MgMg stretch	536.6	Ar	IR	1

[a] ^{18}O–substituted species.

References

[1]J. W. Kauffman, R. H. Hauge, and J. L. Margrave, High Temp. Sci. **18**, 97 (1984).

HCaOCaH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CaH stretch	1179.0	Ar	IR	1
		CaO stretch	726.1	Ar	IR	1
		HCaO bend	515.1	Ar	IR	1

DCaOCaD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CaD stretch	851.6	Ar	IR	1
		CaO stretch	715.0	Ar	IR	1

References

[1]J. W. Kauffman, R. H. Hauge, and J. L. Margrave, High Temp. Sci. **18**, 97 (1984).

HCa_2OH

$\tilde{X}$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CaH stretch	1239.2	Ar	IR	1
	CaO stretch	588.6	Ar	IR	1

References

[1]J. W. Kauffman, R. H. Hauge, and J. L. Margrave, High Temp. Sci. **18**, 97 (1984).

HMnOMnH

$\tilde{X}$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	MnH stretch	1648.7[a]	Ar	IR	1
		1643.2[a]			
		1637.7			
	MnOMn stretch	874.5[a]	Ar	IR	1
		872.3[a]			
		870.4			

DMnOMnD

$\tilde{X}$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	MnD stretch	1174.5	Ar	IR	1
	MnOMn stretch	870.3	Ar	IR	1

[a] Diminished in intensity when matrix was annealed.

References

[1]J. W. Kauffman, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **89**, 3541 (1985).

HMn_2OH

$\tilde{X}$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	MnH stretch	1562.0	Ar	IR	1
		1556.4			
	MnO stretch	640.1	Ar	IR	1

References

[1]J. W. Kauffman, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **89**, 3541 (1985).

HFeOFeH

$\tilde{X}$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	FeH stretch	1724.0[a]	Ar	IR	1
		1708.2			
	FeO stretch	914.5[a]	Ar	IR	1
		911.8			

DFeOFeD

$\tilde{X}$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	FeD stretch	1239.2[a]	Ar	IR	1
		1231.8[a]			
		1228.7			
	FeO stretch	914.3[a]	Ar	IR	1
		911.7			

[a] Diminished in intensity when matrix was annealed.

References

[1]J. W. Kauffman, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **89**, 3541 (1985).

HFe_2OH

$\tilde{X}$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	FeH stretch	1713.1	Ar	IR	1
	FeO stretch	649.9	Ar	IR	1
		522.4	Ar	IR	1

DFe_2OD

$\tilde{X}$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	FeD stretch	1215.8	Ar	IR	1
	FeO stretch	630.4	Ar	IR	1
		521.7	Ar	IR	1

References

[1]J. W. Kauffman, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **89**, 3541 (1985).

HNi_2OH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3660.5	Ar	IR	1
		NiHNi stretch	1187.0	Ar	IR	1
			1134.2	Ar	IR	1
		NiONi stretch	662.7	Ar	IR	1
		Deformation	593.2	Ar	IR	1

DNi_2OD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OD stretch	2717.5	Ar	IR	1
		NiDNi stretch	868.5	Ar	IR	1
			830.9	Ar	IR	1

References

[1]M. Park, R. H. Hauge, and J. L. Margrave, High Temp. Sci. **25**, 1 (1988).

$cyc\text{-}C_3H_2^+$

$\tilde{X}$ C_{2v} Structure: PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		C=C stretch	1170(150)	gas	PE	1,2

References

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$cyc\text{-}C_3H_2$

Photodecomposition threshold in an argon matrix near 360 nm; linear C_3H_2 formed.[1,6,7]

$\tilde{X}$ C_{2v} Structure: MW[4,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3		1277.37	gas	IR	8
			1278.6	Ar	IR	1,6,7
			1277.7			
			1063.6[a]	Ar	IR	1,6,7
			887.1[a]	Ar	IR	1,6,7
			787.8[a]	Ar	IR	1,6,7

A_0 = 1.171; B_0 = 1.075; C_0 = 0.559 MW[2-5,9]

$cyc\text{-}C_3D_2$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1261.8	Ar	IR	7

[a] Did not diminish in intensity on mercury–arc irradiation at wavelengths longer than 345 nm,[7] calling into question the assignment to $cyc\text{-}C_3H_2$.

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$H_2C{=}C{=}C{:}$

Photoisomerization to HCCCH occurs at 254 nm.[1,2]

$\tilde{X}$[a] C_{2v} Structure: MW[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s-stretch	3059.6	Ar	IR	1,2
			3049.5			
	2	C_3 a-stretch	1963.2	Ar	IR	1,2
			1952.2			
	3	CH_2 scissors	1449.3	Ar	IR	1,2
			1446.9			
b_1	5	H_2CC OPLA	1003.0	Ar	IR	1,2
			999.2			
b_2	8	CH_2 rock	1025.0	Ar	IR	1

A_0 = 9.633; B_0 = 0.353; C_0 = 0.340 MW[3,5]

$D_2C=C=C$:

$\tilde{X}$ [a] C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_2 s–stretch	2212.5	Ar	IR	1
			2200.5			
	2	C_3 a–stretch	1944.4	Ar	IR	1
			1933.4			
	3	CD_2 scissors + C_3 s–stretch	1208.7	Ar	IR	1
	4	C_3 s–stretch + CD_2 scissors	950.8	Ar	IR	1
b_1	5	D_2CC OPLA	803.2	Ar	IR	1
			800.3			
b_2	8	CD_2 rock	832.6	Ar	IR	1
			829.2			

A_0 = 4.842; B_0 = 0.314; C_0 = 0.294 MW^4

[a] Singlet state.

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HCCCH

Prolonged 313–nm irradiation of HCCCH isolated in solid argon leads to its isomerization to $H_2C=C=C$:, which has a singlet ground state.[5]

An absorption band system of singlet HCCCH has been identified[2] in the 310–370-nm spectral region, but a detailed analysis has not been reported. Beyond 28900 the bands are diffuse, and a continuous absorption is superposed on the short wavelength end of the band system. The molecule is linear in at least one of the states of the transition. A progression involving an upper-state vibrational frequency of 1094 has been tentatively identified. The preliminary analysis found B′ = 0.310 and B″ = 0.324.

$\tilde{X}\ ^3A'$ C_s Structure: ESR[1]IR,MO[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CH stretch	3266.0s	Ar	IR	5–7
			3285	Kr	IR	3
		C_3 a–stretch	1619.4w	Ar	IR	6,7
		CCH s–bend	550.4m	Ar	IR	6
			402.6	Ar	IR	4–7
			401.5wm			
			408	Kr	IR	3
a'	7	HCC wag	248.5	Ar	IR	4–7
			245.9s			
			258	Kr	IR	3

DCCCD

$\tilde{X}\ ^3A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CD stretch	2457.9s	Ar	IR	4,6,7
			2482	Kr	IR	3
		C_3 a–stretch	1529.0w	Ar	IR	6,7
		CCD, C_3 bend	384.0m	Ar	IR	6,7
			392	Kr	IR	3
a''	7	DCC wag	171m	Ar	IR	4

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HCCH=C:

On exposure of the sample to radiation of wavelength longer than 250 nm, the 1959.5 cm^{-1} absorption decreases and the 3292.4 cm^{-1} absorption grows. This process is reversed on irradiation of the sample at wavelengths longer than 295 nm.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3292.4[a]	Ar	IR	1
		CC stretch	1959.5[b]	Ar	IR	1

DCCD=C:

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD stretch	2472.1[a]	Ar	IR	1
		CC stretch	1938.6[b]	Ar	IR	1

[a] Tentatively assigned to *cis*– isomer.
[b] Tentatively assigned to *trans*– isomer.

References

[1]J. W. Huang and W. R. M. Graham, J. Chem. Phys. **93**, 1583 (1990).

H_2CCN

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_1	5	H_2CC OPLA	680[a]	gas	PE	1

$A_0 = 9.53$; $B_0 = 0.342$; $C_0 = 0.329$ MW^2

D_2CCN

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_1	5	D_2CC OPLA	538[a]	gas	PE	1

[a] From computer fit.

References

[1]S. Moran, H. B. Ellis, Jr., D. J. DeFrees, A. D. McLean, and G. B. Ellison, J. Am. Chem. Soc. **109**, 5996 (1987).
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H_2CNC

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_1	5	H_2CN OPLA	615[a]	gas	PE	1

D_2CNC

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_1	5	D_2CN OPLA	486[a]	gas	PE	1

[a] From computer fit.

References

[1]S. Moran, H. B. Ellis, Jr., D. J. DeFrees, A. D. McLean, S. E. Paulson, and G. B. Ellison, J. Am. Chem. Soc. **109**, 6004 (1987).

H_2CCO^+

$\tilde{E}\ ^2A_1$ C_{2v}
$T_0 = 68343(11)$ gas PE[2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CH_2 scissors	1177(4)	gas	PE	2,4
			671(4)	gas	PE	4
			397(4)	gas	PE	4

$\tilde{D}\ ^2A_1$ C_{2v}
$T_0 = 53414T$ gas PE[2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1488(4)	gas	PE	4
			1164(4)	gas	PE	4
			709(4)	gas	PE	4

$\tilde{C}\ ^2B_2$ C_{2v}
$T_0 = 52037(10)$ gas PE[1-4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		1697(4)	gas	PE	4
	3	CH_2 scissors	1087(4)	gas	PE	1,2,4

$\tilde{B}\ ^2B_1$ C_{2v}
$T_0 = 40259(10)$ gas PE[1-4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCO a-stretch	2001(4)	gas	PE	4
	4	CCO s-stretch	1001(4)	gas	PE	1,2,4
			347(4)	gas	PE	4

$\tilde{A}\ ^2B_2$ C_{2v}
$T_0 = 33706(6)$ gas PE[1-4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1528(4)	gas	PE	4
			1164(4)	gas	PE	4
			690(4)	gas	PE	4
b_1		OPLA	461(4)	gas	PE	4

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCO a-stretch	2263(4)	gas	PE	2-4
	3		1379(4)	gas	PE	4
	4		1227(4)	gas	PE	4

D_2CCO^+

$\tilde{E}\ ^2A_1$ C_{2v}
T_0 = 68261(11) gas PE[2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1133(4)	gas	PE	4
			834(4)	gas	PE	2,4

$\tilde{D}\ ^2A_1$ C_{2v}
T_0 = 54117T gas PE[2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1267(4)	gas	PE	4
			1204(4)	gas	PE	4
			1169(4)	gas	PE	4

$\tilde{C}\ ^2B_2$ C_{2v}
T_0 = 52222(3) gas PE[1-4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1102(4)	gas	PE	4
			800(4)	gas	PE	2,4

$\tilde{B}\ ^2B_1$ C_{2v}
T_0 = 39383(8) gas PE[2-4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1732(4)	gas	PE	4
			1056(4)	gas	PE	4
			848(4)	gas	PE	4

$\tilde{A}\ ^2B_2$ C_{2v}
T_0 = 34077(9) gas PE[2-4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			2140(4)	gas	PE	4
			1007(4)	gas	PE	4
			106(4)	gas	PE	4
b_1		OPLA	299(4)	gas	PE	4

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			2286(4)	gas	PE	2-4
			1091(4)	gas	PE	2-4
			925(4)	gas	PE	4

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$Ca(OH)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CaO a-stretch	591.9	Ar	IR	1

$Ca(OD)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CaO a-stretch	594.6	Ar	IR	1

References

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$Ba(OH)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BaO a-stretch	482.1	Ar	IR	1

$Ba(OD)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BaO a-stretch	472.0	Ar	IR	1

References

[1]J. W. Kauffman, R. H. Hauge, and J. L. Margrave, High Temp. Sci. **18**, 97 (1984).

$Fe(OH)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OFeO stretch	735.5	Ar	IR	1

$Fe(OD)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OFeO stretch	721.7	Ar	IR	1

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$Ni(OH)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ONiO stretch	800.8 795.5	Ar	IR	1

$Ni(OD)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ONiO stretch	777.4 770.4	Ar	IR	1

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H_2CCN^-

Threshold for electron detachment from ground-state $H_2CCN^- \cong$ 12500 gas $PD^{1,3}PE^2$

Dipole–Bound State C_{2v}
T_0 = 12428.665(2) gas $PD^{3,4}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			951(10)	gas	PD	4
	5	H_2CC deform.	692(10)	gas	PD	4

A_0 = 9.510; B_0 = 0.341; C_0 = 0.329 PD^3

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	5	H_2CC deform.	424.77[a]	gas	PD,PE	1–3

Barrier to inversion = 100(50) gas PE^2
A_0 = 9.294; B_0 = 0.338; C_0 = 0.327 $PD^{1,3}PE^2$

D_2CCN^-

Threshold for electron detachment from ground-state $D_2CCN^- \cong$ 12430 gas $PD^{1,3}PE^2$

Dipole–Bound State C_{2v}
T_0 = 12360.434 gas PD^3
A_0 = 4.771; B_0 = 0.302; C_0 = 0.284 PD^3

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	5	D_2CC deform.	289.13[b]	gas	PD,PE	1–3

A_0 = 4.695; B_0 = 0.300; C_0 = 0.283 $PD^{1,3}PE^2$

[a] $1^+ - 0^+$ band separation.[3] $0^\pm$ inversion splitting = 152.[2]
[b] $1^+ - 0^+$ band separation.[3] $0^\pm$ inversion splitting = 101.[2]

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H_2CNC^-

Threshold for electron detachment from ground-state H_2CNC^- = 8540(190) gas PE^1

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	5	H_2CN deform.	374[a]	gas	PE	1

Barrier to inversion = 650(50) gas PE^1
A = 8.07(28); B = 0.366(10); C = 0.357 PE^1

D_2CNC^-

Threshold for electron detachment from ground-state D_2CNC^- = 8630(190) gas PE^1

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	5	D_2CN deform.	335[b]	gas	PE	1

A = 4.18(17); B = 0.327; C = 0.312 PE^1

[a] From computer fit. $0^\pm$ inversion splitting = 5 PE^1
[b] From computer fit. $0^\pm$ inversion splitting = 1 PE^1

References

[1]S. Moran, H. B. Ellis, Jr., D. J. DeFrees, A. D. McLean, S. E. Paulson, and G. B. Ellison, J. Am. Chem. Soc. **109**, 6004 (1987).

H_2CCS^+

$\tilde{E}\ ^2A_1$ C_{2v}
$T^a \cong 67000$ gas PE[1,2]

$\tilde{D}\ ^2B_2$ C_{2v}
$T^a \cong 53300$ gas PE[1,2]

$\tilde{C}\ ^2A_1$ C_{2v}
$T^a = 45670(160)$ gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			950(80)	gas	PE	1,2

$\tilde{B}\ ^2B_1$ C_{2v}
$T^a = 26220(160)$ gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			710(80)	gas	PE	1,2

$\tilde{A}\ ^2B_2$ C_{2v}
$T^a = 19610(160)$ gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCS a-stretch	1660(80)	gas	PE	1,2
			680(80)	gas	PE	1,2

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCS a-stretch	1450(80)	gas	PE	1,2
			700(80)	gas	PE	1,2

[a] From vertical ionization potentials.

References

[1]H. Bock, B. Solouki, G. Bert, and P. Rosmus, J. Am. Chem. Soc. **99**, 1663 (1977).
[2]P. Rosmus, B. Solouki, and H. Bock, Chem. Phys. **22**, 453 (1977).

NH_2CN^+

$\tilde{D}\ ^2A''$ C_s
$T^a = 65760(900)$ gas PE[1]

$\tilde{C}\ ^2A'$ C_s
$T^a = 28880(160)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		C–N stretch	1040(80)	gas	PE	1
		NCN deform.	480(80)	gas	PE	1

$\tilde{B}\ ^2A'$ C_s
$T^a = 18800(160)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		C–N stretch	800(80)	gas	PE	1
		NCN deform.	400(80)	gas	PE	1

$\tilde{A}\ ^2A''$ C_s
$T^a = 14930(160)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	C≡N stretch	2080(80)	gas	PE	1

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	C≡N stretch	2000(80)	gas	PE	1
	3	C–N stretch	1600(80)	gas	PE	1
	4	Inversion	720(80)	gas	PE	1

[a] From vertical ionization potentials.

References

[1]H. Stafast and H. Bock, Chem. Ber. **107**, 1882 (1974).

$CH_2N_2^+$

$\tilde{E}\ ^2A_1$ C_{2v}
$T^a = 85520(1000)$ gas PE[1]

$\tilde{D}\ ^2B_2$ C_{2v}
$T^a = 76650(1000)$ gas PE[1]

$\tilde{C}\ ^2B_1$ C_{2v}
$T^a = 63980(320)$ gas PE[1]

$\tilde{B}\ ^2A_1$ C_{2v}
$T_0 = 49460(320)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	NN stretch	2180(80)	gas	PE	1
	3	CH_2 scissors	1360(80)	gas	PE	1

$\tilde{A}\ ^2B_2$ C_{2v}
$T_0 = 38490(320)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s-stretch	2780(80)	gas	PE	1
	2	NN stretch	2040(80)	gas	PE	1
	3	CH_2 scissors	1200(80)	gas	PE	1

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	NN stretch	2180(80)	gas	PE	1
	4	CN stretch	970(80)	gas	PE	1

$CD_2N_2^+$

$\tilde{E}\ ^2A_1$ C_{2v}
T^a = 85520(1000) gas PE[1]

$\tilde{D}\ ^2B_2$ C_{2v}
T^a = 76650(1000) gas PE[1]

$\tilde{C}\ ^2B_1$ C_{2v}
T^a = 63980(320) gas PE[1]

$\tilde{B}\ ^2A_1$ C_{2v}
T_0 = 49460(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	NN stretch	2250(80)	gas	PE	1
	3	CD_2 scissors	1020(80)	gas	PE	1

$\tilde{A}\ ^2B_2$ C_{2v}
T_0 = 38490(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_2 s–stretch	2170(80)	gas	PE	1
	2	NN stretch	1930(80)	gas	PE	1
	4	CD_2 scissors	800(80)	gas	PE	1

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	NN stretch	2180(80)	gas	PE	1
	4	CN stretch	970(80)	gas	PE	1

[a] From vertical ionization potential.

References

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cyc–$CH_2N_2^+$

$\tilde{D}\ ^2B_1$ C_{2v}
T^a = 58090(1600) gas PE[1]

$\tilde{C}\ ^2A_1$ C_{2v}
$T_0 \cong$ 46000 gas PE[1]

$\tilde{B}\ ^2A_1$ C_{2v}
T_0 = 31060(1000) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1330(80)	gas	PE	1

$\tilde{A}\ ^2B_1$ C_{2v}
T_0 = 20170(1600) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			2200(80)[b]	gas	PE	1
			890(80)	gas	PE	1

$\tilde{X}\ ^2B_2$ C_{2v}

[a] From vertical ionization potential.
[b] Comparison with the spectrum of the neutral molecule suggests that this relatively prominent progression may be contributed by (890 + 1300) combinations.

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HN=C=NH

$\tilde{X}$ C_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	2	NCN s–stretch	1285(20)[a]	gas	IR	2
			1275[a]	Ar	IR	1
	5	NCN deform.	537m	Ar	IR	1
b	7	NCN a–stretch	2104.7	gas	IR	2
			2097s	Ar	IR	1
	8	NH deform.	890(10)	gas	IR	2
			886vs	Ar	IR	1

A_0 = 12.650; B_0 = 0.346; C_0 = 0.346 IR,MW[3,4]

DN=C=ND

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	ND stretch	2545s[b]	Ar	IR	1
	5	NCN deform.	471m	Ar	IR	1
b	6	ND stretch	2545s[b]	Ar	IR	1
	7	NCN a–stretch	2107vs	Ar	IR	1
	8	ND deform.	752s	Ar	IR	1

[a] Calculated from (ν_2 + ν_8) combination band.
[b] Both ND–stretching frequencies presumed equal.

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HCCOH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3501.3s	Ar	IR	1
	2	CH stretch	3339.6m	Ar	IR	1
	3	C≡C stretch	2198.3vs	Ar	IR	1
	4	COH bend	1232.1m	Ar	IR	1
	5	CO stretch	1072.1m	Ar	IR	1
	6	Bend	599T	Ar	IR	1
	7	Bend	523T	Ar	IR	1
	8	Bend	383T	Ar	IR	1
	9	Bend	346T	Ar	IR	1

DCCOD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD,CD stretch	2620.4vs	Ar	IR	1
	2	OD,CD stretch	2586.8vs	Ar	IR	1
	3	C≡C stretch	2035.1s	Ar	IR	1
	4	CO stretch	1046.9wm	Ar	IR	1
	5	COD bend	944.5m	Ar	IR	1

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H_2CCS

$\tilde{A}$ $^1A''$ C_s
$T_0 \cong 17995$ gas AB[10] $\tilde{A}$–$\tilde{X}$ 450–550 nm
Diffuse bands.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	C=C stretch	1402	gas	AB	10
	8	CCS bend	284T	gas	AB	10

$\tilde{X}$ $^1A_1$ C_{2v} Structure: MW[2–5]IR[9,11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s-stretch	3020	gas	IR	9
			3012w	Ar	IR	1,6,7
	2	C=C stretch	1757	gas	IR	9
			1755vs	Ar	IR	1,6–8
	3	CH_2 scissors	1331.67	gas	IR	9,11
			1323m	Ar	IR	1,6,7
	4	C=S stretch	850	gas	IR	9
			858	Ar	IR	7
b_1	5	H_2C=C OPLA	698.09	gas	IR	11
			692s	Ar	IR	1,6–8
	6	CCS bend	404vw	Ar	IR	1,7
b_2	7	CH_2 a-stretch	3107.33	gas	IR	9,11
			3097	Ar	IR	7
			3068			
	8	CH_2 rock	921.60	gas	IR	9,11
			918	Ar	IR	7
	9	CCS bend	356	Ar	IR	7

$A_0 = 9.554$; $B_0 = 0.189$; $C_0 = 0.185$ MW[2–5]IR[9,11]

D_2CCS

$\tilde{A}$ $^1A''$ C_s
$T_0 \cong 18002$ gas AB[10] $\tilde{A}$–$\tilde{X}$ 450–550 nm
Diffuse bands.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	C=C stretch	1400	gas	AB	10
	8	CCS bend	256T	gas	AB	10

$\tilde{X}$ $^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_2 s-stretch	2237.48	gas	IR	11
			2229	Ar	IR	1,7
	2	C=C stretch	1740	gas	IR	11
			1738vs	Ar	IR	1,7
	3	CD_2 scissors	1030	Ar	IR	7
	4	C=S stretch	755	Ar	IR	7
b_1	5	D_2C=C OPLA	558.04	gas	IR	11
			555s	Ar	IR	1,7
	6	CCS bend	375	Ar	IR	7
b_2	7	CD_2 a-stretch	2330T	Ar	IR	7
	8	CD_2 rock	775	Ar	IR	7
	9	CCS bend	308	Ar	IR	7

$A_0 = 4.784$; $B_0 = 0.168$; $C_0 = 0.162$ IR[11]

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HC≡CSH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3315s	Ar	IR	1–3
		SH stretch	2575vw	Ar	IR	2
		C≡C stretch	2065w	Ar	IR	1,2
			1112m	Ar	IR	2
			959w	Ar	IR	2,3
		CCH bend (⊥ plane)	558w	Ar	IR	1–3

DC≡CSD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD stretch	2580s	Ar	IR	1
		C≡C stretch	1925vw	Ar	IR	1
		SD stretch	1835vw	Ar	IR	1
		CCD bend (⊥ plane)	430m	Ar	IR	1

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cyc-C_2H_2S

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	3207w	Ar	IR	2–4
			3202	N_2	IR	6
	2	C=C stretch	1663w	Ar	IR	1–4
			1660	N_2	IR	6
	4	C–S stretch	657mT	Ar	IR	3,4,7
b_1	6	OPLA	563m	Ar	IR	1–4,7
			570	N_2	IR	6
b_2	7	CH stretch	3169m	Ar	IR	1–4
			3166m			
			3161	N_2	IR	6
	8	CH deform.	912m	Ar	IR	1–4,7
			910	N_2	IR	6

cyc-C_2D_2S

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD stretch	2485w	Ar	IR	2,4,6
	2	C=C stretch	1567w	Ar	IR	2,4,6
	3	C–S stretch	681m	Ar	IR	4
b_1	6	OPLA	423m	Ar	IR	2,4,6
b_2	7	CD stretch	2355m	Ar	IR	4
	8	CD deform.	716s	Ar	IR	4,6

[a] For assignment, see Ref. 8.

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HGe_2OH

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			784.8	Ar	IR	1
			710.8	Ar	IR	1
			683.0	Ar	IR	1

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HSn_2OH

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1100	Ar	IR	1
			748.9	Ar	IR	1
			690.0	Ar	IR	1
			620.3	Ar	IR	1

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t–CHF=CH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	C=C stretch	1623vs	Ar	IR	1
	4	HCF scissors	1211wm	Ar	IR	1
	5	CF stretch	1066vs	Ar	IR	1
	6	C=CH deform.	678s	Ar	IR	1
	7	C=CF deform.	462m	Ar	IR	1
a''	8	HFC=C OPLA	785s	Ar	IR	1
	9	Torsion	631vs	Ar	IR	1

t–DCF=CD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	C=C stretch	1564s	Ar	IR	1
	4	CF stretch	1070m	Ar	IR	1
a''	8	DFC=C OPLA	624m	Ar	IR	1
	9	Torsion	485m	Ar	IR	1

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CHBr=CH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CH stretch	3094wm	Ar	IR	1
		C=C stretch	1564wm	Ar	IR	1
		H deform.	1120w	Ar	IR	1
		CBr stretch	495m	Ar	IR	1
a''		H deform.	794vs	Ar	IR	1

CDBr=CD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CD stretch	2288vw	Ar	IR	1
		C=C stretch	1506wm	Ar	IR	1
		D deform.	828w	Ar	IR	1
		CBr stretch	480wm	Ar	IR	1
a''			600wm	Ar	IR	1
			573m	Ar	IR	1

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$HCOOH^+$

$\tilde{E}\ ^2A'$ C_s
T^a = 49700(320) gas PE[1,3]

$\tilde{D}\ ^2A'$ C_s
T_0 = 45500(320) gas PE[1,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CO stretch	1300(40)	gas	PE	1,2

$\tilde{C}\ ^2A''$ C_s
$T_0 \cong$ 32800 gas PE[1,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			940	gas	PE	1

$\tilde{B}\ ^2A'$ C_s
$T_0 \cong$ 23200 gas PE[1,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			940	gas	PE	1

$\tilde{A}\ ^2A''$ C_s
T_0 = 8390(320) gas PE[1,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		C=O stretch	2340(40)	gas	PE	2
		C–O stretch	1080(60)	gas	PE	1,2

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CO stretch	1460(30)	gas	PE	1,2

$DCOOD^+$

$\tilde{D}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CO stretch	1210(40)	gas	PE	2
		COD bend ?	880(40)	gas	PE	2

$\tilde{A}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		C=O stretch	2280(40)	gas	PE	2
		C–O stretch	1090(40)	gas	PE	2

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CO stretch	1494(40)	gas	PE	2
		COD bend	970(40)	gas	PE	2

[a] From vertical ionization potential.

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H_2CSO^+

$\tilde{E}\ ^2A'$ C_s
T^a = 64550(320) gas PE[1]

$\tilde{D}\ ^2A'$ C_s
T^a = 55910(320) gas PE[1]

$\tilde{C}\ ^2A''$ C_s
T^a = 43650(320) gas PE[1]

$\tilde{B}\ ^2A'$ C_s
T^a = 36230(320) gas PE[1]

$\tilde{A}\ ^2A'$ C_s
T^a = 11620(320) gas PE[1]

$\tilde{X}\ ^2A''$ C_s

[a] From vertical ionization potentials.

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$CH_2=NCl$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	C=N stretch	1611w	gas	IR	1
	4	CH_2 scissors	1420w	gas	IR	1
	5	CH_2 rock	1150m	gas	IR	1
	6	NCl stretch	619s	gas	IR	1
a''	8	OPLA	1006s	gas	IR	1

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$CH_2=PCl$

$\tilde{X}$ C_s Structure: MW[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH_2 a–stretch	3095.6vw	gas	IR	3
	2	CH_2 s–stretch	2974.3vw	gas	IR	3
	3	CH_2 scissors	1372.3m	gas	IR	3
	4	C=P stretch	979.7w	gas	IR	3
	5	CH_2 rock	792.4s	gas	IR	3
	6	PCl stretch	499.7vs	gas	IR	3
	7	PCCl deform.	340.2w	gas	IR	3
a''	8	CH_2 wag	804.7vs	gas	IR	3
	9	Torsion	609.4vw	gas	IR	3

A_0 = 0.758; B_0 = 0.156; C_0 = 0.108 MW[1,2,4]

$CD_2=PCl$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CP stretch + CD_2 scissors	1120.8m	gas	IR	3
	4	CP stretch + CD_2 scissors	847.9w	gas	IR	3
	5	CD_2 rock	642.9s	gas	IR	3
	6	PCl stretch	490.0vs	gas	IR	3
a''	8	CD_2 wag	634.5s	gas	IR	3
	9	Torsion	431.6vw	gas	IR	3

A_0 = 0.655; B_0 = 0.144; C_0 = 0.118 gas MW[1,2,4]

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H_2CSO

$\tilde{X}$ C_s Structure: MW^2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH_2 a–stretch	3013w	Ar	IR	3
	2	CH_2 s–stretch	2960m	Ar	IR	3
	3	CH_2 scissors	1395w	Ar	IR	3
	4	CSO a–stretch	1357s	Ar	IR	3
	5	CSO s–stretch	1170	gas	IR	1
			1165vs	Ar	IR	3
	6	CH_2 rock	1055m	Ar	IR	3
	7	CSO bend	394m	Ar	IR	3
a''	8	Torsion	972m	Ar	IR	3
	9	H_2CS OPLA	760	gas	IR	1
			767vs	Ar	IR	3

A_0 = 1.348; B_0 = 0.313; C_0 = 0.254 $MW^{1,2}$

D_2CSO

$\tilde{X}$ C_s

A_0 = 1.148; B_0 = 0.277; C_0 = 0.223 MW^2

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t–HCSSH

$\tilde{X}$ C_s Structure: MW^2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	2988.8	gas	IR	3
	3	HCS deform.	1283.0	gas	IR	3
			1290.5	Ar	IR	4
	4	C=S stretch	1057.2	gas	IR	3
			1059.8	Ar	IR	4
	5	CSH deform.	935.5	gas	IR	3
			933.4	Ar	IR	4
	6	C–S stretch	682.5	gas	IR	3
			682.6	Ar	IR	4
a''	8	C=S OPLA	824.0	gas	IR	3
			836.8	Ar	IR	4

A_0 = 1.642(3); B_0 = 0.115; C_0 = 0.107 $MW^{1,2}$

t–DCSSD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1133.5	Ar	IR	4
			867	Ar	IR	4
			764.5	Ar	IR	4
			670.0	Ar	IR	4
			622.0	Ar	IR	4

References

[1]B. Bak, O. J. Nielsen, and H. Svanholt, J. Mol. Spectrosc. **69**, 401 (1978).
[2]B. Bak, O. Nielsen, H. Svanholt, and J. J. Christiansen, J. Mol. Spectrosc. **75**, 134 (1979).
[3]F. Ioannoni, D. C. Moule, J. D. Goddard, and D. J. Clouthier, J. Mol. Struct. **197**, 159 (1989).
[4]R. B. Bohn, G. D. Brabson, and L. Andrews, J. Phys. Chem. **96**, 1582 (1992).

c–HCSSH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	HCS deform.	1255.5	gas	IR	3
			1265.4	Ar	IR	4
	4	C=S stretch	1080.8	gas	IR	3
			1082.2	Ar	IR	4
	5		925.5	Ar	IR	4
	6	C–S stretch	710.0	gas	IR	3
			725.8	Ar	IR	4
a''	8	C=S OPLA	794.5	gas	IR	3
			807.2	Ar	IR	4

A_0 = 1.633(13); B_0 = 0.117; C_0 = 0.109 $MW^{1,2}$

c–DCSSD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1123.4	Ar	IR	4
			776.7	Ar	IR	4
			655.8	Ar	IR	4
			613.3	Ar	IR	4

References

[1]B. Bak, O. J. Nielsen, and H. Svanholt, J. Mol. Spectrosc. **69**, 401 (1978).
[2]B. Bak, O. Nielsen, H. Svanholt, and J. J. Christiansen, J. Mol. Spectrosc. **75**, 134 (1979).
[3]F. Ioannoni, D. C. Moule, J. D. Goddard, and D. J. Clouthier, J. Mol. Struct. **197**, 159 (1989).
[4]R. B. Bohn, G. D. Brabson, and L. Andrews, J. Phys. Chem. **96**, 1582 (1992).

HSiOOH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Si=O stretch	1249	Ar	IR	1,2

DSiOOD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Si=O stretch	1245	Ar	IR	1,2
		Si–O stretch	891	Ar	IR	2

References

[1]R. Withnall and L. Andrews, J. Am. Chem. Soc. **107**, 2567 (1985).
[2]R. Withnall and L. Andrews, J. Phys. Chem. **89**, 3261 (1985).

NH_2NO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	4	NH_2 scissors	1521.2 1514.5	Ar	IR	1
	5	NNH deform.	1207.3[a]	Ar	IR	1
			1223	N_2	IR	1

ND_2NO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ND_2 stretch	2627.3 2616.7	Ar	IR	1
			1257.5	Ar	IR	1
			1232.4	Ar	IR	1

[a] Most prominent of four bands between 1200 and 1210.

References

[1]J. N. Crowley and J. R. Sodeau, J. Phys. Chem. **94**, 8103 (1990).

$CH_2F_2^+$

$\tilde{G}\ ^2A_1$ C_{2v}
T_0 = 83900(1000) gas PE[1,3]

$\tilde{D}, \tilde{E}, \tilde{F}\ ^2B_1, ^2A_1, ^2B_2$ C_{2v}
T_0 = 44380(400) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CF_2 stretch	700(100)	gas	PE	1–3

$\tilde{C}\ ^2A_2$ C_{2v}
T^a = 24300(400) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CF_2 stretch	970(80)	gas	PE	1–3
	4	CF_2 scissors	500(80)	gas	PE	1,3

$\tilde{A}, \tilde{B}\ ^2A_1, ^2B_1$ C_{2v}
T_0 = 14760(400) gas PE[1-3]

$\tilde{X}\ ^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	2744m	Ar	IR	4
	2	CH_2 scissors	1120(80)	gas	PE	1–3
b_1	6	CH stretch	2854wm	Ar	IR	4
b_2	8	CH_2 wag	1408s	Ar	IR	4
	9	CF stretch	1255vs	Ar	IR	4

$CD_2F_2^+$

$\tilde{C}\ ^2A_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CF_2 stretch	970(80)	gas	PE	3
	4	CF_2 scissors	500(80)	gas	PE	3

$\tilde{X}\ ^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD stretch	2062m	Ar	IR	4
b_1	7		980w	Ar	IR	4
b_2	8	CD_2 wag	1063s	Ar	IR	4
	9	CF stretch	1262vs	Ar	IR	4

[a] From vertical ionization potential.

References

[1]A. W. Potts, H. J. Lempka, D. G. Streets, and W. C. Price, Phil. Trans. Roy. Soc. (London) **A268**, 59 (1970).
[2]B. P. Pullen, T. A. Carlson, W. E. Moddeman, G. K. Schweitzer, W. E. Bull, and F. A. Grimm, J. Chem. Phys. **53**, 768 (1970).
[3]C. R. Brundle, M. B. Robin, and H. Basch, J. Chem. Phys. **53**, 2196 (1970).
[4]L. Andrews and F. T. Prochaska, J. Chem. Phys. **70**, 4714 (1979).

CH_2FCl^+

T^a = 62610(1000) gas PE[1]

T^a = 50510(1000) gas PE[1]

T^a = 41230(400) gas PE[1]

T^a = 23080(1000) gas PE[1]

T^a = 21060(400) gas PE[1]

T^a = 19040(1000) gas PE[1]

T^a = 17020(1000) gas PE[1]

T^a = 4520(1000) gas PE[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_2 stretch	2902m	Ar	IR	2
		CH_2 scissors	1200(80)	gas	PE	1
		CCl stretch	874s	Ar	IR	2

CD_2FCl^+

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD_2 stretch	2162mT	Ar	IR	2
		CCl stretch	843vs	Ar	IR	2

[a] From vertical ionization potential.

References

[1]J. Doucet, P. Sauvageau, and C. Sandorfy, J. Chem. Phys. **58**, 3708 (1973).
[2]F. T. Prochaska and L. Andrews, J. Chem. Phys. **73**, 2651 (1980).

CH_2FBr^+

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_2 stretch	2913m	Ar	IR	1
		CBr stretch	735s	Ar	IR	1

References

[1]F. T. Prochaska and L. Andrews, J. Chem. Phys. **73**, 2651 (1980).

CH_2FI^+

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_2 stretch	2914m	Ar	IR	1
		CI stretch	653m	Ar	IR	1

References

[1]F. T. Prochaska and L. Andrews, J. Chem. Phys. **73**, 2651 (1980).

$CH_2Cl_2^+$

$\tilde{G}\ ^2A_1$ C_{2v}
T^a = 72500(1000) gas PE[1]

$\tilde{F}\ ^2B_1$ C_{2v}
T^a = 43970(240) gas PE[1]

$\tilde{E}\ ^2A_1$ C_{2v}
T^a = 37280(240) gas PE[1]

$\tilde{D}\ ^2B_2$ C_{2v}
T^a = 32110(240) gas PE[1]

$\tilde{B},\tilde{C}\ ^2A_2, ^2A_1$ [b] C_{2v}
T^a = 7260(240) gas PE[1]

$\tilde{X},\tilde{A}\ ^2B_2, ^2B_1$ [b] C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CCl_2 stretch	640(80)	gas	PE	1

[a] From vertical ionization potential. The first ionization potential of CH_2Cl_2 is taken as 11.32(1) eV, as in the photoionization study of Ref. 3.
[b] The order of these states is uncertain.[2,4]

References

[1]A. W. Potts, H. J. Lempka, D. G. Streets, and W. C. Price, Phil. Trans. Roy Soc. (London) **A268**, 59 (1970).
[2]R. N. Dixon, J. N. Murrell, and B. Narayan, Mol. Phys. **20**, 611 (1971).
[3]A. S. Werner, B. P. Tsai, and T. Baer, J. Chem. Phys. **60**, 3650 (1974).
[4]J. C. Bünzli, D. C. Frost, F. G. Herring, and C. A. McDowell, J. Electron Spectrosc. Relat. Phenom. **9**, 289 (1976).

$CH_2Br_2^+$

$\tilde{G}\ ^2A_1$ C_{2v}
T^a = 74070(800) gas PE[1]

$\tilde{F}\ ^2B_1$ C_{2v}
T^a = 46230(560) gas PE[1]

$\tilde{E}\ ^2A_1$ C_{2v}
T^a = 34130(560) gas PE[1]

$\tilde{D}\ ^2B_2$ C_{2v}
T^a = 29040(560) gas PE[1]

$\tilde{B},\tilde{C}\ ^2A_2,^2A_1$ [b] C_{2v}
T^a = 6130(560) gas PE[1]

$\tilde{A}\ ^2B_1$ [b] C_{2v}
T^a = 2420(560) gas PE[1]

$\tilde{X}\ ^2B_2$ C_{2v}

[a] From vertical ionization potential. The first ionization potential of CH_2Br_2 has been taken as 10.52(5) eV, as determined in the photoelectron–photoion coincidence study of Ref. 3.
[b] For assignment, see Ref. 2.

References

[1]A. W. Potts, H. J. Lempka, D. G. Streets, and W. C. Price, Phil. Trans. Roy. Soc. (London) **A268**, 59 (1970).
[2]R. N. Dixon, J. N. Murrell, and B. Narayan, Mol. Phys. **20**, 611 (1971).
[3]B. P. Tsai, T. Baer, A. S. Werner, and S. F. Lin, J. Phys. Chem. **79**, 570 (1975).

$CH_2I_2^+$

$\tilde{G}\ ^2A_1$ C_{2v}
T^a = 81000(1000) gas PE[1]

$\tilde{F}\ ^2B_1$ C_{2v}
T^a = 48410(320) gas PE[1]

$\tilde{E}\ ^2A_1$ C_{2v}
T^a = 33970(320) gas PE[1]

$\tilde{D}\ ^2B_2$ C_{2v}
T^a = 26540(320) gas PE[1]

$\tilde{C}\ ^2A_1$ C_{2v}
T^a = 8880(320) gas PE[1]

$\tilde{B}\ ^2B_1$ C_{2v}
T^a = 6050(320) gas PE[1]

$\tilde{A}\ ^2A_2$ C_{2v}
T^a = 2420(320) gas PE[1]

$\tilde{X}\ ^2B_2$ C_{2v}

[a] From vertical ionization potential. The first ionization potential of CH_2I_2 has been taken as 9.46(2) eV, as determined in the photoelectron–photoion coincidence study of Ref. 2.

References

[1]A. W. Potts, H. J. Lempka, D. G. Streets, and W. C. Price, Phil. Trans. Roy. Soc. (London) **A268**, 59 (1970).
[2]B. P. Tsai, T. Baer, A. S. Werner, and S. F. Lin, J. Phys. Chem. **79**, 570 (1975).

$SiH_2F_2^+$

$\tilde{G}\ ^2A_1$ C_{2v}
T^a = 59220(480) gas PE[2]

$\tilde{F}\ ^2A_1$ C_{2v}
T^a = 44000(1200) gas PE[2]

$\tilde{E}\ ^2B_2$ C_{2v}
T^a = 41000(1200) gas PE[2]

$\tilde{D}\ ^2B_1$ C_{2v}
T^a = 38300(1200) gas PE[1,2]

$\tilde{C}\ ^2A_2$ C_{2v}
T^a = 28400(900) gas PE[2]

$\tilde{B}\ ^2B_2$ C_{2v}
T^a = 26000(900) gas PE[1,2]

$\tilde{A}\ ^2A_1$ C_{2v}
T^a = 18960(560) gas PE[1,2]

$\tilde{X}\ ^2B_1$ C_{2v}

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. **67**, 3425 (1971).
[2]D. C. Frost, F. G. Herring, A. Katrib, R. A. N. McLean, J. E. Drake, and N. P. C. Westwood, Can. J. Chem. **49**, 4033 (1971).

$SiH_2Cl_2^+$

$\tilde{G}\ ^2A_1$ C_{2v}
$T^a \cong$ 53400 gas PE[1,2]

$\tilde{F}\ ^2B_1$ C_{2v}
T^a = 23400(720) gas PE[2]

$\tilde{E}\ ^2A_1$ C_{2v}
T^a = 22180(720) gas PE[2]

$\tilde{D}\ ^2B_2$ C_{2v}
T^a = 20170(720) gas PE[1,2]

$\tilde{C}\ ^2A_1$ C_{2v}
T^a = 8550(480) gas PE[2]

$\tilde{B}\ ^2A_2$ C_{2v}
T^a = 6700(480) gas PE[1,2]

$\tilde{A}\ ^2B_1$ C_{2v}
T^a = 3150(320) gas PE[1,2]

$\tilde{X}\ ^2B_2$ C_{2v}

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. **67**, 3425 (1971).
[2]D. C. Frost, F. G. Herring, A. Katrib, R. A. N. McLean, J. E. Drake, and N. P. C. Westwood, Can. J. Chem. **49**, 4033 (1971).

$SiH_2Br_2^+$

$\tilde{D}$ C_{2v}
T^a = 22400(1000) gas PE[1]

$\tilde{C}$ C_{2v}
T^a = 19600(320) gas PE[1]

$\tilde{B}$ C_{2v}
T^a = 5570(320) gas PE[1]

$\tilde{A}$ C_{2v}
T^a = 1610(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. **67**, 3425 (1971).

$SiH_2I_2^+$

$\tilde{F}$ C_{2v}
T^a = 28640(320) gas PE[1]

$\tilde{E}$ C_{2v}
T^a = 23720(320) gas PE[1]

$\tilde{D}$ C_{2v}
T^a = 19690(320) gas PE[1]

$\tilde{C}$ C_{2v}
T^a = 8390(320) gas PE[1]

$\tilde{B}$ C_{2v}
T^a = 5320(320) gas PE[1]

$\tilde{A}$ C_{2v}
T^a = 2420(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. **67**, 3425 (1971).

$GeH_2F_2^+$

$\tilde{B}$ C_{2v}
T^a = 26600(1600) gas PE[1]

$\tilde{A}$ C_{2v}
T^a = 12900(1600) gas PE[1]

$\tilde{X}\ ^2B_1$ C_{2v}

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. **67**, 3425 (1971).

$GeH_2Cl_2^+$

$\tilde{C}$ C_{2v}
T^a = 18880(320) gas PE[1]

$\tilde{B}$ C_{2v}
T^a = 5320(320) gas PE[1]

$\tilde{A}$ C_{2v}
T^a = 2420(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. **67**, 3425 (1971).

$GeH_2Br_2^+$

$\tilde{E}$ C_{2v}
T^a = 24370(320) gas PE[1]

$\tilde{D}$ C_{2v}
T^a = 20010(320) gas PE[1]

$\tilde{C}$ C_{2v}
T^a = 18070(320) gas PE[1]

$\tilde{B}$ C_{2v}
T^a = 4760(320) gas PE[1]

$\tilde{A}$ C_{2v}
T^a = 1290(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. **67**, 3425 (1971).

$GeH_2I_2^+$

$\tilde{F}$ C_{2v}
T^a = 27920(320) gas PE[1]

$\tilde{E}$ C_{2v}
T^a = 22270(320) gas PE[1]

$\tilde{D}$ C_{2v}
T^a = 18800(320) gas PE[1]

$\tilde{C}$ C_{2v}
T^a = 7830(320) gas PE[1]

$\tilde{B}$ C_{2v}
T^a = 5000(320) gas PE[1]

$\tilde{A}$ C_{2v}
T^a = 2100(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. **67**, 3425 (1971).

$H_2CCl–Cl$

A broad absorption with maximum near 360 nm (28000) which appears[1-3] on vacuum ultraviolet photolysis of CH_2Cl_2 isolated in solid argon and a much weaker absorption near 620 nm (16000) have been attributed[3] to this product. Exposure of the sample to radiation in the spectral region of either of these absorptions leads to destruction of $H_2Cl–Cl$ and to re-formation of CH_2Cl_2.

$\tilde{X}$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CH_2 stretch	3143.3w	Ar	IR	3
	CH_2 stretch	3023.5wm	Ar	IR	3
	CH_2 scissors	1404.9wm	Ar	IR	3
		1193sT	Ar	IR	1,2
	CCl stretch	958.5wm	Ar	IR	3
		763.2vs	Ar	IR	1–3

D_2CCl–Cl

$\tilde{X}$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CD_2 stretch	2375.5vw	Ar	IR	3
	CD_2 stretch	2220.7wm	Ar	IR	3
	CD_2 scissors	1083.4ms	Ar	IR	2,3
	CCl stretch	886.1m	Ar	IR	3
	CD_2 wag	603.1vs	Ar	IR	1–3

References

[1]L. Andrews, F. T. Prochaska, and B. S. Ault, J. Am. Chem. Soc. **101**, 9 (1979).
[2]B. J. Kelsall and L. Andrews, J. Mol. Spectrosc. **97**, 362 (1983).
[3]G. Maier, H. P. Reisenauer, J. Hu, L. J. Schaad, and B. A. Hess, Jr., J. Am. Chem. Soc. **112**, 5117 (1990).

H_2CCl–Br

A broad absorption with maximum near 382 nm (26200) which appears[1] on 230– or 240–nm irradiation of CH_2ClBr isolated in solid argon has been attributed[1] to this product. Exposure of the sample to 360 nm radiation or to radiation of wavelength longer than 570 nm leads to destruction of H_2CCl–Br and to re–formation of CH_2ClBr.

$\tilde{X}$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CH_2 stretch	3038.6w	Ar	IR	1
	CH_2 scissors	1388.3wm	Ar	IR	1
	CCl stretch	931.2wm	Ar	IR	1
	CH_2 wag	726.6vs	Ar	IR	1

D_2CCl–Br

$\tilde{X}$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CD_2 stretch	2232.3wm	Ar	IR	1
	CD_2 scissors	1069.6s	Ar	IR	1
	CCl stretch	868.8m	Ar	IR	1
	CD_2 wag	573.3vs	Ar	IR	1

References

[1]G. Maier, H. P. Reisenauer, J. Hu, L. J. Schaad, and B. A. Hess, Jr., J. Am. Chem. Soc. **112**, 5117 (1990).

H_2CCl–I

In a nitrogen matrix, this species contributes a very strong absorption maximum at 438 nm and a much weaker absorption maximum at 745 nm. Irradiation in either of these absorption regions results in re–formation of the more stable CH_2ClI structure in which both halogen atoms are bonded to the carbon atom.[1,2]

$\tilde{X}$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CH_2 stretch	3168.8vw	Ar	IR	1,2
	CH_2 stretch	3042.3m	Ar	IR	1,2
		3039.4wm			
	CCl stretch	886.2s	Ar	IR	1,2
	CH_2 wag	639.0ms	Ar	IR	1,2
		633.5vs			

D_2CCl–I

$\tilde{X}$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CD_2 stretch	2395.2vw	Ar	IR	1,2
	CD_2 stretch	2228.2m	Ar	IR	1,2
	CD_2 scissors	1072.5wm	Ar	IR	1,2
	CCl stretch	836.5vs	Ar	IR	1,2
	CD_2 wag	502.9ms	Ar	IR	1,2
		498.8vs			

References

[1]G. Maier and H. P. Reisenauer, Angew. Chem. **98**, 829 (1986); Angew. Chem. Int. Ed. Engl. **25**, 819 (1986).
[2]G. Maier, H. P. Reisenauer, J. Hu, L. J. Schaad, and B. A. Hess, Jr., J. Am. Chem. Soc. **112**, 5117 (1990).

H_2CBr–Br

A broad absorption with maximum near 360nm (28000) which appears[1–3] on ultraviolet or vacuum ultraviolet photolysis of CH_2Br_2 isolated in solid argon has been attributed[3] to this product. Exposure of the sample to 360 nm radiation or to radiation of wavelength longer than 570 nm leads to destruction of H_2CBr–Br and to re–formation of CH_2Br_2.

$\tilde{X}$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CH_2 stretch	3156.3vw	Ar	IR	3
	CH_2 stretch	3030.4w	Ar	IR	3
	CH_2 scissors	1333.6w	Ar	IR	3
		1129mT	Ar	IR	1
		695.2wm	Ar	IR	1,3
	CBr stretch	684.4vs	Ar	IR	1–3

$D_2CBr–Br$

$\tilde{X}$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CD_2 stretch	2384.1vw	Ar	IR	3
	CD_2 stretch	2213.2w	Ar	IR	3
	CD_2 scissors	1029.8wm	Ar	IR	3
	CBr stretch	732.4w	Ar	IR	3
	CD_2 wag	545.5vs	Ar	IR	1–3

References

[1]L. Andrews, F. T. Prochaska, and B. S. Ault, J. Am. Chem. Soc. **101**, 9 (1979).
[2]B. J. Kelsall and L. Andrews, J. Mol. Spectrosc. **97**, 362 (1983).
[3]G. Maier, H. P. Reisenauer, J. Hu, L. J. Schaad, and B. A. Hess, Jr., J. Am. Chem. Soc. **112**, 5117 (1990).

$H_2CBr–I$

In a nitrogen matrix, this species contributes a very strong absorption maximum at 403 nm and a much weaker absorption maximum at 660 nm. Irradiation in either of these absorption regions results in reformation of the more stable CH_2BrI structure in which both halogen atoms are bonded to the carbon atom.[1,2]

$\tilde{X}$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CH_2 stretch	3165.2vw	Ar	IR	1,2
	CH_2 stretch	3035.7w	Ar	IR	1,2
	CH_2 wag	638.1s	Ar	IR	1,2
		630.6vs			

$D_2CBr–I$

$\tilde{X}$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CD_2 stretch	2390.4vw	Ar	IR	2
	CD_2 stretch	2222.6wm	Ar	IR	2
	CD_2 scissors	1054.9vw	Ar	IR	2
	CBr stretch	713.6w	Ar	IR	2
		707.5wm			
	CD_2 wag	505.3vs	Ar	IR	2
		500.0s			

References

[1]G. Maier and H. P. Reisenauer, Angew. Chem. **98**, 829 (1986); Angew. Chem. Int. Ed. Engl. **25**, 819 (1986).
[2]G. Maier, H. P. Reisenauer, J. Hu, L. J. Schaad, and B. A. Hess, Jr., J. Am. Chem. Soc. **112**, 5117 (1990).

$H_2CI–I$

In a nitrogen matrix, this species contributes a very strong absorption maximum at 370 nm and a much weaker absorption maximum at 545 nm. Irradiation in either of these absorption regions results in reformation of the more stable CH_2I_2 structure in which both iodine atoms are bonded to the carbon atom.[1,2]

$\tilde{X}$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CH_2 stretch	3151.2vw	Ar	IR	1,2
	CH_2 stretch	3028.0vw	Ar	IR	1,2
	CH_2 scissors	1372.8w	Ar	IR	1,2
	CI stretch	713.6w	Ar	IR	1,2
		704.6wm			
	CH_2 wag	622.7s	Ar	IR	1,2
		618.3s			
		611.1vs			

$D_2CI–I$

$\tilde{X}$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CD_2 stretch	2377.6vw	Ar	IR	1,2
	CD_2 stretch	2213.0w	Ar	IR	1,2
	CD_2 scissors	1032.7w	Ar	IR	1,2
	CI stretch	645.3w	Ar	IR	1,2
	CD_2 wag	498.0ms	Ar	IR	1,2
		488.6vs			

References

[1]G. Maier and H. P. Reisenauer, Angew. Chem. **98**, 829 (1986); Angew. Chem. Int. Ed. Engl. **25**, 819 (1986).
[2]G. Maier, H. P. Reisenauer, J. Hu, L. J. Schaad, and B. A. Hess, Jr., J. Am. Chem. Soc. **112**, 5117 (1990).

HSO_2H

$\tilde{X}$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	SH stretch	2591w	Ar	IR	1
	S=O stretch	1209s	Ar	IR	1
	SOH bend	1093m	Ar	IR	1
	S–O stretch	762s	Ar	IR	1
	HSOH deform.	476ms	Ar	IR	1
	OSOH deform.	450wm	Ar	IR	1
	SO wag	340wm	Ar	IR	1
	Torsion	270	Ar	IR	1

DSO_2D

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		S=O stretch	1202s	Ar	IR	1
		SOD bend	849	Ar	IR	1
		S–O stretch	758s	Ar	IR	1
		DSOD deform.	471s	Ar	IR	1
		OSOH deform.	425wm	Ar	IR	1
		SO wag	319w	Ar	IR	1
		Torsion	260	Ar	IR	1

References

[1]M. A. Fender, Y. M. Sayed, and F. T. Prochaska, J. Phys. Chem. **95**, 2811 (1991).

6.10. Five-Atomic Monohydrides

C_4H

$^2\Pi$ $C_{\infty v}$

T_0 = 33740 Ne AB[1] 259–296 nm

33797 Ar AB[1] 248–295 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3100(10)	Ar	AB	1
	2	C≡C stretch	2130(10)	Ar	AB	1
	3	C≡C stretch	2028(10)	Ne	AB	1
			2060(10)	Ar	AB	1
	4	C–C stretch	800(10)	Ne	AB	1
			760(10)	Ar	AB	1
Π	5	HCC bend	570H	Ar	AB	1

Groups of absorptions observed in an argon matrix[1] between 13408 and 13906, 17629 and 17939, 21972 and 25667, and 26867 and 32104 have also tentatively been attributed to C_4H.

$\tilde{X}$ $^2\Sigma$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3307.4w	Ar	IR	7
	2	C≡C stretch	2083.9wm	Ar	IR	7
	3	C≡C stretch	2060.6ms	Ar	IR	1,7
Π	7	Skel. bend	131T	gas	MW	6

B_0 = 0.165 MW^{2-5}

C_4D

$^2\Pi$ $C_{\infty v}$

T_0 = 33900 Ar AB[1] 258–294 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2640(10)	Ar	AB	1
	2	C≡C s–stretch	2140(10)	Ar	AB	1
	4	C–C stretch	760(10)	Ar	AB	1
Π	5	DCC bend	485H	Ar	AB	1

An absorption at 17685 and a group of bands between 26925 and 30883 in the argon–matrix observations[1] have also tentatively been assigned to C_4D.

$\tilde{X}$ $^2\Sigma$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2579.3w	Ar	IR	7
	2	C≡C stretch	2056.5wm	Ar	IR	7
	3	C≡C stretch	2049.6ms	Ar	IR	1,7

References

[1]K. I. Dismuke, W. R. M. Graham, and W. Weltner, Jr., J. Mol. Spectrosc. **57**, 127 (1975).
[2]M. Guélin, S. Green, and P. Thaddeus, Astrophys. J. **224**, L27 (1978).
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$HC\equiv C\text{-}C\equiv N^+$

$\tilde{C}$

T_0 = 48570(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1320(40)	gas	PE	1

$\tilde{B}$ $^2\Pi$ $C_{\infty v}$

T_0 = 19600(160) gas PE[1]

19374(43) Ne AB[2] $\tilde{B}$–$\tilde{X}$ 474–516 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+			1940(40)	gas	PE	1
	4	C–C stretch	810(40)	gas	PE	1
			820(60)	Ne	AB	2

$\tilde{A}\ ^2\Sigma^+$ $C_{\infty v}$
T_0 = 15650(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	4	C–C stretch	860(40)	gas	PE	1

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2180(40)	gas	PE	1

References

[1]C. Baker and D. W. Turner, Proc. Roy. Soc. (London) **A308**, 19 (1968).
[2]J. Fulara, S. Leutwyler, J. P. Maier, and U. Spittel, J. Phys. Chem. **89**, 3190 (1985).

$HC\equiv C\text{-}N\equiv C^+$

$\tilde{B}\ ^2\Pi$ $C_{\infty v}$
T^a = 32600(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+			740(80)	gas	PE	1

$\tilde{A}\ ^2\Sigma^+$ $C_{\infty v}$
T_0 = 5400(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2		2340(80)	gas	PE	1
	3		2180(80)	gas	PE	1
	4		890(80)	gas	PE	1

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2		2180(80)	gas	PE	1

[a] From vertical ionization potential.

References

[1]L. Zanathy, H. Bock, D. Lentz, D. Preugschat, and P. Botschwina, J. Chem. Soc., Chem. Commun. 403 (1992).

$HC\equiv C\text{-}N\equiv C$

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3338.96s	gas	IR	1,3
	2	N≡C stretch	2218.64s	gas	IR	1,3
	3	C≡C stretch	2036.66s	gas	IR	1,3
	4	C–C stretch	938.09w[a]	gas	IR	3
Π	5	HCC bend	620.63vs	gas	IR	1,3
	6		430T	gas	IR	3
	7		207T	gas	IR	3

B_0 = 0.166 $MW^{1,2}$

$DC\equiv C\text{-}N\equiv C$

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2617.39s	gas	IR	3
	2	N≡C stretch	2157.58s	gas	IR	3
	3	C≡C stretch	1965.48s	gas	IR	3
	4	C–C stretch	923.58w[a]	gas	IR	3
Π	5	DCC bend	480.17	gas	IR	3
	6		425T	gas	IR	3

B_0 = 0.153 MW^1IR^3

[a] Deperturbed value.

References

[1]M. Krüger, H. Dreizler, D. Preugschat, and D. Lentz, Angew. Chem. **103**, 1674 (1991); Angew. Chem. Int. Ed. Engl. **30**, 1644 (1991).
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HNCCC

$\tilde{X}$ C_s
B_0 = 0.156 MW^1

DNCCC

$\tilde{X}$ C_s
B_0 = 0.147 MW^1

References

[1]Y. Hirahara, Y. Ohshima, and Y. Endo, Astrophys. J. **403**, L83 (1993).

$HNCCN^+$

$\tilde{X}$ $D_{\infty h}$ Structure: MW[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NH stretch	3448.27	gas	LD	1

B_0 = 0.148 LD[1]MW[2]

$DNCCN^+$

$\tilde{X}$ $D_{\infty h}$
B_0 = 0.139 MW[3]

References

[1]H. E. Warner and T. Amano, J. Mol. Spectrosc. **145**, 66 (1991).
[2]T. Amano and F. Scappini, J. Chem. Phys. **95**, 2280 (1991).
[3]G. Cazzoli, C. Degli Esposti, and F. Scappini, Chem. Phys. Lett. **194**, 297 (1992).
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HCOOCa

$\tilde{B},\tilde{C}\ ^2B_2,^2B_1$ C_{2v}
T_0 = 15913(20) gas LF[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Ca stretch	354(10)	gas	LF	1

$\tilde{A}\ ^2A_1$ C_{2v}
T_0 = 14715(20) gas LF[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Ca stretch	356(10)	gas	LF	1

$\tilde{X}\ ^2A_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Ca stretch	349(10)	gas	LF	1

References

[1]L. C. O'Brien, C. R. Brazier, S. Kinsey-Nielsen, and P. F. Bernath, J. Phys. Chem. **94**, 3543 (1990).

HCOOSr

$\tilde{C}\ ^2B_1$ C_{2v}
T_0 = 14903(20) gas LF[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Sr stretch	285(10)	gas	LF	1

$\tilde{B}\ ^2B_2$ C_{2v}
T_0 = 14749(20) gas LF[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Sr stretch	291(10)	gas	LF	1

$\tilde{A}\ ^2A_1$ C_{2v}
T_0 = 13624(20) gas LF[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Sr stretch	307(10)	gas	LF	1

$\tilde{X}\ ^2A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Sr stretch	275(10)	gas	LF	1

References

[1]L. C. O'Brien, C. R. Brazier, S. Kinsey-Nielsen, and P. F. Bernath, J. Phys. Chem. **94**, 3543 (1990).

HCCCO

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2		2308.6	Ar	IR	3

A_0 = 8.709(2); B_0 = 0.153; C_0 = 0.150 MW[1,2]

DCCCO

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2		2287.4	Ar	IR	3

A_0 = 8.488(3); B_0 = 0.142; C_0 = 0.139 MW[2]

References

[1]A. L. Cooksy, J. K. G. Watson, C. A. Gottlieb, and P. Thaddeus, Astrophys. J. **386**, L27 (1992).
[2]A. L. Cooksy, J. K. G. Watson, C. A. Gottlieb, and P. Thaddeus, J. Mol. Spectrosc. **153**, 610 (1992).
[3]Q. Jiang and W. R. M. Graham, J. Chem. Phys. **98**, 9251 (1993).

HCOCN

$\tilde{A}\ ^1A''$ C_s
T_0 = 26283.396 gas LF[1,4,6]AB[4] $\tilde{A}$–$\tilde{X}$ 345–385 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CO stretch	1308	gas	LF	1,6
	4	HCO bend	1121	gas	LF	1,6
	5	CC stretch	943	gas	LF	1,6
	6	CCO bend	530	gas	LF	1,6
	7	CCN bend	217	gas	LF	1,6
a''	8	Bend	418	gas	LF	1,6
	9	Bend	376	gas	LF	1,6

A_0 = 1.957; B_0 = 0.169; C_0 = 0.154 AB,LF[4]

$\tilde{X}\ ^1A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	2892m	gas	IR	5
	2	C≡N stretch	2229m	gas	IR,EM	2,5,6
	3	C=O stretch	1716s	gas	IR,EM	2,5,6
	4	CH rock	1383	gas	IR	5
	5	C–C stretch	914ms	gas	IR,EM	2,5,6
	6	CCO bend	626vw	gas	IR	5
	7	CCN bend	230	gas	LF,IR	1,2,6
a''	8	CH wag	960	gas	EM	6
	9	CCN bend	278	gas	LF,EM	1,6

A_0 = 2.251; B_0 = 0.167; C_0 = 0.155 MW[3]

DCOCN

$\tilde{A}\ ^1A''$ C_s
T_0 = 26335.6 gas LF[6] $\tilde{A}$–$\tilde{X}$ 345–380 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CD stretch	2232	gas	LF	6
	3	CO stretch	1279	gas	LF	6
	4	CC stretch	931	gas	LF	6
	5	CD rock	732	gas	LF	6
	6	CCO bend	527	gas	LF	6
	7	CCN bend	214	gas	LF	6
a''	8	Bend	406	gas	LF	6
	9	Bend	315	gas	LF	6

A^a = 1.561; B^a = 0.169; C^a = 0.152 LF[6]

$\tilde{X}\ ^1A'$ C_s
A_0 = 1.737; B_0 = 0.168; C_0 = 0.152 LF[6]

[a] From analysis of 9_0^1 band.

References

[1]R. H. Judge, D. C. Moule, A. Biernacki, M. Benkel, J. M. Ross, and J. Rustenburg, J. Mol. Spectrosc. **116**, 364 (1986).
[2]D. J. Clouthier and D. C. Moule, J. Am. Chem. Soc. **109**, 6259 (1987).
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HFCCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	3025.9	Xe	IR	2
	2	CO stretch	2142.2vs	Xe	IR	2
	3		1383.0m	Xe	IR	2
	4		1168.0m	Xe	IR	2
	5		1031.5w	Xe	IR	2
a''	8	HFCC OPLA	755	Xe	IR	2
	9	CCO bend	525.5w	Xe	IR	2

A_0 = 1.795; B_0 = 0.154; C_0 = 0.142 MW[1]

References

[1]R. D. Brown, P. D. Godfrey, and B. Kleibömer, Chem. Phys. **105**, 301 (1986).
[2]G. Davidovics, M. Monnier, and A. Allouche, Chem. Phys. **150**, 395 (1991).

HClCCO

$\tilde{X}$ C_s Structure: MW[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CO stretch	2141.4vs	Xe	IR	2
	3	HCCl deform.	1293w	Xe	IR	2
	4	CC stretch	1107w	Xe	IR	2
	5	CCl stretch	842.2vw	Xe	IR	2
a''	8	HClCC OPLA	747	Xe	IR	2

A_0 = 1.206; B_0 = 0.101; C_0 = 0.093 MW[1]

DClCCO

$\tilde{X}$ C_s
A_0 = 0.974; B_0 = 0.101; C_0 = 0.091 MW[1]

References

[1]M. C. L. Gerry, W. Lewis-Bevan, and N. P. C. Westwood, J. Chem. Phys. **79**, 4655 (1983).
[2]G. Davidovics, M. Monnier, and A. Allouche, Chem. Phys. **150**, 395 (1991).

HC(O)OO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C=O stretch	1790.2	O_2	IR	1,2
		C–O stretch	1089.9	O_2	IR	1,2

DC(O)OO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C=O stretch	1759.5	O_2	IR	2

References

[1]T-L. Tso, M. Diem, and E. K. C. Lee, Chem. Phys. Lett. **91**, 339 (1982).
[2]T-L. Tso and E. K. C. Lee, J. Phys. Chem. **88**, 5475 (1984).

HNO_3^+

$\tilde{F}$ C_s
T_0 = 56800(900) gas PE[1,2]

$\tilde{E}$ C_s
T_0 = 51640(160) gas PE[1,2]

$\tilde{D}$ $^2A'$ C_s
T_0 = 33400(160) gas PE[1,2]

$\tilde{C}$ $^2A''$ C_s
T_0 = 11620(900) gas PE[1,2]

$\tilde{B}$ $^2A'$ C_s
T_0 = 9760(160) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1210(30)	gas	PE	1

$\tilde{A}$ $^2A'$ C_s
T^a = 3950(240) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1490(30)	gas	PE	1,2
			1070(30)	gas	PE	1,2

$\tilde{X}$ $^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1370(80)	gas	PE	2
			650(30)	gas	PE	1

[a] First detectable component.

References

[1]D. R. Lloyd, P. J. Roberts, and I. H. Hillier, J. Chem. Soc., Faraday Trans. 2 **71**, 496 (1975).
[2]D. C. Frost, S. T. Lee, C. A. McDowell, and N. P. C. Westwood, J. Electron Spectrosc. Relat. Phenom. **7**, 331 (1975).

CF_2=NH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH stretch	3402.3	gas	IR	1
			3388wm	Ar	IR	2
	2	C=N stretch	1785.2	gas	IR	1
			1777s	Ar	IR	2
	3	CF_2 a–stretch	1307	gas	IR	1
			1295vs	Ar	IR	2
	4	CNH deform.	1031.2	gas	IR	1
			1027ms	Ar	IR	2
	5	CF_2 s–stretch	947.2	gas	IR	1
			942m	Ar	IR	2
	6	CF_2 scissors	574vw	Ar	IR	2
	7	CF_2 rock	542.0	gas	IR	1
			542wm	Ar	IR	2
a"	8	Torsion	831.7	gas	IR	1
			828ms	Ar	IR	2
	9	F_2CN OPLA	695.2	gas	IR	1
			694w	Ar	IR	2

CF_2=ND

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ND stretch	2519.3	gas	IR	1
			2508wm	Ar	IR	2
	2	CN stretch	1780.0	gas	IR	1
			1772s	Ar	IR	2
	3	CF_2 a–stretch	1280	gas	IR	1
			1267vs	Ar	IR	2
	4	CF_2 s–stretch	954.0	gas	IR	1
			951wm	Ar	IR	2
	5	CND deform.	836.0	gas	IR	1
			833wm	Ar	IR	2
	6	CF_2 scissors	565vw	Ar	IR	2
	7	CF_2 rock	491.8	gas	IR	1
			491wm	Ar	IR	2
a"	8	F_2CN OPLA	705.1	gas	IR	1
			703wm	Ar	IR	2
	9	Torsion	613.9	gas	IR	1
			612wm	Ar	IR	2

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c–HFC=NF

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C=N stretch	1647wm	Ar	IR	1
		CF stretch	1205s	Ar	IR	1
		NF stretch	951wm	Ar	IR	1

c–DFC=NF

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C=N stretch	1624T	Ar	IR	1
		CF stretch	1217wm	Ar	IR	1
		NF stretch	968wm	Ar	IR	1

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CF_2=PH

$\tilde{X}$ C_s Structure: MW[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	PH stretch	2326.9m	gas	IR	3,4
	2	C=P stretch	1349.5vs	gas	IR	3,4
	3	CF_2 a–stretch	1228.5s	gas	IR	3,4
	4	CPH deform.	884.4m	gas	IR	3,4
	5	CF_2 s–stretch	729.3m	gas	IR	3,4
	6	CF_2 scissors	485.5m	gas	IR	3,4
	7	CF_2 rock	418.3w	gas	IR	4
a″	8	CPH deform.	1088.8w	gas	IR	4
	9	CF_2 wag	568.0w	gas	IR	3,4

A_0 = 0.370; B_0 = 0.159; C_0 = 0.111 MW[1,2]

CF_2=PD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	PD stretch	1690.6m	gas	IR	4
	2	C=P stretch	1350.2vs	gas	IR	4
	3	CF_2 a–stretch	1219.9s	gas	IR	4
	4	CF_2 s–stretch	736.6m	gas	IR	4
	5	CPD deform.	661.5w	gas	IR	4
	6	CF_2 scissors	483.5m	gas	IR	4
	7	CF_2 rock	401.2w	gas	IR	4
a″	9	CF_2 wag	544.7vw	gas	IR	4

A_0 = 0.356; B_0 = 0.156; C_0 = 0.108 MW[1,2]

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$HONO_2$

In the gas phase, continuous absorption begins near 330 nm, with a maximum near 38500 (260 nm), then increasing absorption out to the 190 nm observation limit.[4,5,31] Between 330 and 220 nm, photodissociation to OH + NO_2 predominates.[6,16,33,39] However, at 193 nm photodissociation to HONO + O is the major process.[33] Vacuum ultraviolet spectral observations[7,12] show an absorption maximum near 54900 (182 nm), a more prominent maximum near 73500 (136 nm), and overlapping absorption bands at higher energies. The onset of the photoproduction of OH ($A\ ^2\Sigma$) + NO_2 has been observed[12] at 68000 (147.5 nm).

$\tilde{X}$ C_s Structure: MW[1,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	OH stretch	3550.0m	gas	IR	2
			3522.3	Ar	IR	28
			3519.3			
			3491.8	N_2	IR	8,36
	2	NO_2 a–stretch	1709.57vs	gas	IR,DL	2,9,11,20
					LS	21,23,35
			1699.4	Ar	IR	28
			1696.2			
			1698.3	N_2	IR	8,36
	3	Mixed	1325.74s	gas	IR,DL	2,19,26,27
			1321.4	Ar	IR	28
			1318.7			
			1346.1	N_2	IR	8,36
	4	Mixed	1303.52vs	gas	IR,DL	2,26,27
			1304.4	Ar	IR	28
			1311.9	N_2	IR	8,36
	5	ON stretch	879.11s	gas	IR,DL	2,18,32,34
						37
			896.9	Ar	IR	2
			889.5			
			903.1	N_2	IR	8,36
	6	NO_2 scissors	646.83w	gas	IR	2,25
			656.6	Ar	IR	36
			664.1	N_2	IR	8,36
	7	NO_2 rock	580.30w	gas	IR	2,25
			588.0	Ar	IR	36
			597.5	N_2	IR	8,36
a″	8	ONO_2 OPLA	763.15s	gas	IR	2,25
			763.6	Ar	IR	28
			767.7	N_2	IR	8,36
	9	Torsion	458.23m	gas	IR	2,15,24
			479	N_2	IR	8

A_0 = 0.434; B_0 = 0.404; C_0 = 0.209 MW[1,10,13,14,17,22]IR[11,24,25]

$DONO_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2621.5m	gas	IR	2
			2601.5	Ar	IR	36
			2599.1			
			2576.5	N_2	IR	8,36
	2	NO_2 a-stretch	1687.0vs	gas	IR	2
			1678.6	Ar	IR	36
			1674.9			
			1669.2	N_2	IR	8,36
	3	NO_2 s-stretch	1308.4vs	gas	IR	2
			1310.4	Ar	IR	36
			1311.1	N_2	IR	8,36
	4	DON bend	1013.6m	gas	IR	2
			1013.4	Ar	IR	36
			1012.2			
			1032.4	N_2	IR	8,36
	5	ON stretch	888.0s	gas	IR	2
			894.2	Ar	IR	36
			884.5			
			906.0	N_2	IR	8,36
	6	NO_2 scissors	642.14s	gas	IR	2,38
			660	N_2	IR	8
	7	NO_2 rock	541.58w	gas	IR	2,38
			559.9	N_2	IR	8,36
a"	8	ONO_2 OPLA	762.87s	gas	IR	2,29
			763.7	Ar	IR	36
			767.7	N_2	IR	8,36
	9	Torsion	343.85m	gas	IR	2,15,30
			361	N_2	IR	8

A_0 = 0.433; B_0 = 0.377; C_0 = 0.201 MW^1IR^{38}

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HOONO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OH stretch	3545.5w	Ar	IR	1,2
			3541.7	N_2	IR	1,2
	2	N=O stretch	1703.6s	Ar	IR	1,2
			1701.4	N_2	IR	1,2
	3	HOO bend	1364.4m	Ar	IR	1,2
			1394.9	N_2	IR	1,2
	4	OO stretch	952.0m	Ar	IR	1,2
			960.5	N_2	IR	1,2
	5	ONO bend	772.8m	Ar	IR	1,2
			793.6	N_2	IR	1,2

DOONO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OD stretch	2615.4	Ar	IR	1,2
			2622.3	N_2	IR	2
	2	N=O stretch	1703.7	Ar	IR	1,2
			1701.8	N_2	IR	2
	3	DOO bend	1089.7	Ar	IR	1,2
			1090.7	N_2	IR	2

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	4	OO stretch	950.3	Ar	IR	1,2
			957.3	N_2	IR	2
	5	ONO bend	772.1	Ar	IR	1,2
			790.3	N_2	IR	2

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$HOPO_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3585.4	Ar	IR	1
	2	PO_2 a-stretch	1451.3	Ar	IR	1
	3	PO_2 s-stretch	1192.6	Ar	IR	1
	4	POH deform.	1044.8	Ar	IR	1
	5	P–O stretch	913.4	Ar	IR	1
	6	PO_2 scissors	447.2	Ar	IR	1
	7	PO_2 rock	412.0	Ar	IR	1
a"	8	OH torsion	492.0	Ar	IR	1
	9	OPO_2 OPLA	428.0	Ar	IR	1

$DOPO_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2646.9	Ar	IR	1
	2	PO_2 a-stretch	1450.9	Ar	IR	1
	3	PO_2 s-stretch	1190.7	Ar	IR	1
	6	PO_2 scissors	445.6	Ar	IR	1
	7	PO_2 rock	386.5	Ar	IR	1
a"	8	OPO_2 OPLA	434.4	Ar	IR	1
	9	OD torsion	366.0	Ar	IR	1

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HOOPO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3227	Ar	IR	1
		P=O stretch	1226.3	Ar	IR	1
		O–O stretch	1052.3	Ar	IR	1
		P–O stretch	915.3	Ar	IR	1
		POO bend	742.1	Ar	IR	1
a"		HOOP torsion	492.0	Ar	IR	1

References

[1]R. Withnall and L. Andrews, J. Phys. Chem. **91**, 784 (1987).

$HP(O_2)O$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		PH stretch	2490.1	Ar	IR	1
		P=O stretch	1370.3	Ar	IR	1,2
		PO_2 s-stretch	974.1	Ar	IR	1
		PO stretch	587.3	Ar	IR	1
		OPO_2 deform.	436.7	Ar	IR	1

$DP(O_2)O$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		P=O stretch	1368.3	Ar	IR	1
		PO_2 s-stretch	973.5	Ar	IR	1
		PO stretch	585.6	Ar	IR	1

References

[1]R. Withnall and L. Andrews, J. Phys. Chem. **91**, 784 (1987).
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$HOAsO_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3613	Ar	IR	1
		AsO_2 a-stretch	1061.4	Ar	IR	1
		HOAs deform.	948	Ar	IR	1
		AsO_2 s-stretch	932.2	Ar	IR	1
		As–O stretch	725	Ar	IR	1
		Torsion	424	Ar	IR	1
			414			

$DOAsO_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OD stretch	2664	Ar	IR	1
		AsO_2 s–stretch	951.3	Ar	IR	1
		As–O stretch	778	Ar	IR	1

References

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$HSbO_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SbH stretch	2027	Ar	IR	1
		SbH a–deform.	872.7	Ar	IR	1
		O_3 a–stretch	767.4	Ar	IR	1
		Sb–O_3 stretch	727	Ar	IR	1
		SbH s–deform.	472.4	Ar	IR	1
		O_3 s–bend	425.6	Ar	IR	1

$DSbO_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SbD stretch	1457	Ar	IR	1
		O_3 a–stretch	796.7	Ar	IR	1
		Sb–O_3 stretch	731.8	Ar	IR	1
		SbD a–deform.	617.6	Ar	IR	1
		O_3 s–bend	437.9	Ar	IR	1
		SbD s–deform.	387	Ar	IR	1

References

[1]L. Andrews, B. W. Moores, and K. K. Fonda, Inorg. Chem. **28**, 290 (1989).

$HOSbO_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3604	Ar	IR	1
		SbO stretch	635	Ar	IR	1
		Torsion	370	Ar	IR	1

$DOSbO_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OD stretch	2658	Ar	IR	1
		SbO_2 s–stretch	778.5	Ar	IR	1
		Torsion	276	Ar	IR	1

References

[1]L. Andrews, B. W. Moores, and K. K. Fonda, Inorg. Chem. **28**, 290 (1989).

HCF_3^+

$\tilde{F}\ ^2A_1$ C_{3v}
T^a = 85360(400) gas PE[1,3,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	2660(80)	gas	PE	4
	3	CF_3 stretch	1050(80)	gas	PE	4

$\tilde{D},\tilde{E}\ ^2E,^2A_1$ C_{3v}
$T^a \cong$ 54400 gas PE[1–4]
Broad emission bands between about 230 and 580 nm which appear on excitation of HCF_3 by synchrotron radiation in the 48–62 nm spectral region have been attributed[5,6] to the $\tilde{D}$–$\tilde{X},\tilde{A},\tilde{B},\tilde{C}$ transitions of HCF_3^+.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			480(80)	gas	PE	1

τ = 80(4) ns gas EM[6]

$\tilde{C}\ ^2E$ C_{3v}
T_0 = 26220(400) gas PE[1–4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF_3 stretch	1050(80)	gas	PE	1–4
	3	CF_3 umbrella	550(80)	gas	PE	1,3,4

$\tilde{B}\ ^2E$ C_{3v}
T^a = 18800(1000) gas PE[1–4]

$\tilde{A}\ ^2A_2$ C_{3v}
T^a = 13200(1000) gas PE[1–4]

$\tilde{X}\ ^2A_1$ C_{3v}

DCF_3^+

$\tilde{C}\ ^2E$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF_3 stretch	1050(80)	gas	PE	3
	3	CF_3 umbrella	500(80)	gas	PE	3

[a] From vertical ionization potential.

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[1]A. W. Potts, H. J. Lempka, D. G. Streets, and W. C. Price, Phil. Trans. Roy. Soc. (London) **A268**, 59 (1970).
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HCF_2Cl^+

$\tilde{G},\tilde{H}\ ^2A',^2A''$ C_s
T^a = 59870(800) gas PE[1,2]

$\tilde{F}\ ^2A'$ C_s
T^a = 50910(800) gas PE[1,2]

$\tilde{C},\tilde{D},\tilde{E}\ ^2A'',^2A'',^2A'$ C_s
T^a = 27270(800) gas PE[1,2]

$\tilde{B}\ ^2A'$ C_s
T^a = 10890(800) gas PE[1,2]

$\tilde{X},\tilde{A}\ ^2A'',^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		FCCl deform.	410(80)	gas	PE	2

[a] From vertical ionization potentials.

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$HCFCl_2^+$

$\tilde{F},\tilde{G}\ ^2A',^2A''$ C_s
T^a = 47360(800) gas PE[1,2]

$\tilde{E}\ ^2A'$ C_s
T^a = 22830(800) gas PE[1,2]

$\tilde{D}\ ^2A''$ C_s
T^a = 20570(800) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CCl_2 stretch	610(80)	gas	PE	2
		FCCl deform.	400(80)	gas	PE	2

$\tilde{C}\ ^2A'$ C_s
T^a = 8470(800) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CCl_2 scissors	280(80)	gas	PE	2

$\tilde{B}\ ^2A''$ C_s
T^a = 3630(800) gas PE[1,2]

$\tilde{A}\ ^2A'$ C_s
T^a = 1600(800) gas PE[1,2]

$\tilde{X}\ ^2A''$ C_s

[a] From vertical ionization potentials.

References

[1]J. Doucet, P. Sauvageau, and C. Sandorfy, J. Chem. Phys. **58**, 3708 (1973).
[2]I. Novak, T. Cvitas, L. Klasinc, and H. Güsten, J. Chem. Soc., Faraday Trans. 2 **77**, 2049 (1981).

$HCCl_3^+$

$\tilde{F}\ ^2A_1$ C_{3v}
T^a = 68000(1000) gas PE[1]

$\tilde{E}\ ^2A_1$ C_{3v}
T^a = 45100(320) gas PE[1]

$\tilde{D}\ ^2E$ C_{3v}
T^a = 37280(320) gas PE[1]
A strong, broad absorption with maximum at 388 nm (25800) which appears on argon-resonance photolysis of $HCCl_3$ isolated in solid argon and which has a photodecomposition threshold at a wavelength longer than 470 nm has been assigned[5] to the $\tilde{D}$–$\tilde{X}$ transition of $HCCl_3^+$. The energy difference is attributed to structural relaxation in the condensed phase.

$\tilde{C}\ ^2E$ [b] C_{3v}
T^a = 11940(320) gas PE[1]

$\tilde{B}\ ^2A_1$ [b] C_{3v}
T^a = 5160(320) gas PE[1]

$\tilde{A}\ ^2E$ [b] C_{3v}
T^a = 4360(320) gas PE[1]

$\tilde{X}\ ^2A_2$ [b] C_{3v}

[a] From vertical ionization potential. The first ionization potential of $HCCl_3$ is taken as 11.37(2) eV, as in the photoelectron–photoion coincidence study of Ref. 4.
[b] The assignment of Ref. 2 has been used. An alternate assignment has been proposed by Ref. 3.

References

[1]A. W. Potts, H. J. Lempka, D. G. Streets, and W. C. Price, Phil. Trans. Roy Soc. (London) **A268**, 59 (1970).
[2]R. N. Dixon, J. N. Murrell, and B. Narayan, Mol. Phys. **20**, 611 (1971).
[3]S. Katsumata and K. Kimura, Bull. Chem. Soc. Japan **46**, 1342 (1973).
[4]A. S. Werner, B. P. Tsai, and T. Baer, J. Chem. Phys. **60**, 3650 (1974).
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$HCBr_3^+$

$\tilde{F}\ ^2A_1$ C_{3v}
T^a = 75200(1000) gas PE[1]

$\tilde{E}\ ^2A_1$ C_{3v}
T^a = 43000(320) gas PE[1]

$\tilde{D}\ ^2E$ C_{3v}
T^a = 34130(320) gas PE[1]

$\tilde{C}\ ^2E$ C_{3v}
T^a = 10000(320) gas PE[1]
A = 1290(320) gas PE[1]

$\tilde{B}\ ^2A_1$ C_{3v}
T^a = 6450(320) gas PE[1]

$\tilde{A}\ ^2E$ C_{3v}
T^a = 2660(320) gas PE[1]
A = 1130(320) gas PE[1]

$\tilde{X}\ ^2A_2$ C_{3v}

[a] From vertical ionization potential. The first ionization potential of $HCBr_3$ is taken as 10.48(2) eV, as in the photoelectron–photoion coincidence study of Ref. 2.

References

[1]A. W. Potts, H. J. Lempka, D. G. Streets, and W. C. Price, Phil. Trans. Roy. Soc. (London) **A268**, 59 (1970).
[2]B. P. Tsai, T. Baer, A. S. Werner, and S. F. Lin, J. Phys. Chem. **79**, 570 (1975).

$HSiF_3^+$

$\tilde{F}\ ^2A_1$ C_{3v}
T^a = 52120(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	SiF_3 stretch	725(40)	gas	PE	1
	3	Deformation	330(40)	gas	PE	1

$\tilde{E}\ ^2E$ C_{3v}
T^a = 33320(320) gas PE[1]

$\tilde{D}\ ^2A_1$ C_{3v}
T^a = 30010(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	SiF_3 stretch	790(40)	gas	PE	1

$\tilde{C}\ ^2E$ C_{3v}
T^a = 22270(320) gas PE[1]

$\tilde{B}\ ^2E$ C_{3v}
T^a = 15330(320) gas PE[1]

$\tilde{A}\ ^2A_2$ C_{3v}
T^a = 11780(320) gas PE[1]

$\tilde{X}\ ^2A_1$ C_{3v}

[a] From vertical ionization potentials.

References

[1]S. Cradock, E. A. V. Ebsworth, and R. A. Whiteford, J. Chem. Soc., Dalton Trans. **22**, 2401 (1973).

$HSiCl_3^+$

$\tilde{F}\ ^2A_1$ C_{3v}
T^a = 50020(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiH stretch	2000T	gas	PE	1

$\tilde{E}\ ^2A_1$ C_{3v}
T^a = 24530(320) gas PE[1]

$\tilde{D}\ ^2E$ C_{3v}
T^a = 22670(320) gas PE[1]

$\tilde{C}\ ^2E$ C_{3v}
T^a = 9120(320) gas PE[1]

$\tilde{A},\tilde{B}\ ^2A_1,^2E$ C_{3v}
T^a = 3790(320) gas PE[1]

$\tilde{X}\ ^2A_2$ C_{3v}

[a] From vertical ionization potentials.

References

[1]D. C. Frost, F. G. Herring, A. Katrib, R. A. N. McLean, J. E. Drake, and N. P. C. Westwood, Can. J. Chem. **49**, 4033 (1971).

$HOSO_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3539.8m	Ar	IR	1–3
		SO_2 a–stretch	1309.2s	Ar	IR	1–3
		HOS bend	1296.2wm	Ar	IR	3
		SO_2 s–stretch	1097.2s	Ar	IR	1–3
		S–OH stretch	759.3s	Ar	IR	1–3

$DOSO_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OD stretch	2612.9wm	Ar	IR	3
		SO_2 a–stretch	1302.8m	Ar	IR	3
		SO_2 s–stretch	1097.9wm	Ar	IR	3
		DOS bend	916T	Ar	IR	3
		S–OD stretch	757.2m	Ar	IR	3

References

[1]S. Hashimoto, G. Inoue, and H. Akimoto, Chem. Phys. Lett. **107**, 198 (1984).
[2]S. Nagase, S. Hashimoto, and H. Akimoto, J. Phys. Chem. **92**, 641 (1988).
[3]Y.–P. Kuo, B.–M. Cheng, and Y.–P. Lee, Chem. Phys. Lett. **177**, 195 (1991).

6.11. Five-Atomic Nonhydrides

Na_5

A broad absorption maximum at about 16500 (605 nm) has been observed in depletion photoionization experiments[1,2] on gas–phase Na_5.

References

[1]K. Selby, V. Kresin, J. Masui, M. Vollmer, W. A. de Heer, A. Scheidemann, and W. D. Knight, Phys. Rev. B **43**, 4565 (1991).
[2]C. R. C. Wang, S. Pollack, T. A. Dahlseid, G. M. Koretsky, and M. M. Kappes, J. Chem. Phys. **96**, 7931 (1992).

cyc–C_5^+

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2052T	Ar	IR	1

References

[1]M. Vala, T. M. Chandrasekhar, J. Szczepanski, and R. Pellow, J. Mol. Struct. **222**, 209 (1990).

C_5

$\tilde{A}$?
T_0 = 44228 Ar AB[8] $\tilde{A}$–$\tilde{X}$ 211–226 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1813	Ar	AB	8
			654	Ar	AB	8

$\tilde{X}\ ^1\Sigma_g^-$ $D_{\infty h}$ Structure: ESR[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	2	Sym. stretch	779(10)	gas	TPE	9,10
Σ_u^+	3	Asym. stretch	2169.441	gas	IR,DL	4–7
			2168(3)	Ne	IR	2
			2164	Ar	IR	1–3
	4	Asym. stretch	1446.6	Ar	IR	11
Π_g	5	Bend	218(13)T	gas	DL,TPE	7,9,10
Π_u	6	Bend	535(10)	gas	TPE	9,10
Π_u	7	Bend	118(3)T	gas	DL,TPE	7,9,10

B_0 = 0.0853 IR[4]DL[5–7]

References

[1]K. R. Thompson, R. L. DeKock, and W. Weltner, Jr., J. Am. Chem. Soc. **93**, 4688 (1971).
[2]W. R. M. Graham, K. I. Dismuke, and W. Weltner, Jr., Astrophys. J. **204**, 301 (1976).
[3]M. Vala, T. M. Chandrasekhar, J. Szczepanski, R. Van Zee, and W. Weltner, Jr., J. Chem. Phys. **90**, 595 (1989).
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[8]J. Szczepanski and M. Vala, J. Phys. Chem. **95**, 2792 (1991).
[9]T. N. Kitsopoulos, C. J. Chick, Y. Zhao, and D. M. Neumark, J. Chem. Phys. **95**, 5479 (1991).
[10]D. W. Arnold, S. E. Bradforth, T. N. Kitsopoulos, and D. M. Neumark, J. Chem. Phys. **95**, 8753 (1991).
[11]R. H. Kranze and W. R. M. Graham, J. Chem. Phys. **96**, 2517 (1992).

C_4Si

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CC stretch	2080.1	Ar	IR	2

B_0 = 0.051 MW[1]

References

[1]M. Ohishi, N. Kaifu, K. Kawaguchi, A. Murakami, S. Saito, S. Yamamoto, S. Ishikawa, Y. Fujita, Y. Shiratori, and W. M. Irvine, Astrophys. J. **345**, L83 (1989).
[2]P. A. Withey and W. R. M. Graham, J. Chem. Phys. **96**, 4068 (1992).

SiCCCSi

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	C_3 stretch	1955.2vs	Ar	IR	1
	4	SiC stretch	898.9w	Ar	IR	1

References

[1]J. D. Presilla-Márquez, C. M. L. Rittby, and W. R. M. Graham, Paper TG11, 48th International Symposium on Molecular Spectroscopy, Columbus, Ohio, 1993.

C_5^-

Threshold for electron detachment from ground-state C_5^- = 23020(10) gas TPE[1]PE[2]

$\tilde{X}\ ^2\Pi_u$ $D_{\infty h}$?

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	7	Bend	200T	gas	TPE	1

A = 22T gas TPE[1]

References

[1]T. N. Kitsopoulos, C. J. Chick, Y. Zhao, and D. M. Neumark, J. Chem. Phys. **95**, 5479 (1991).
[2]D. W. Arnold, S. E. Bradforth, T. N. Kitsopoulos, and D. M. Neumark, J. Chem. Phys. **95**, 8753 (1991).

C_4O

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2221.7vs	Ar	IR	1
			1922.7s	Ar	IR	1
			1431.5wm	Ar	IR	1
			774.8w	Ar	IR	1
			484.0wm	Ar	IR	1

References

[1]G. Maier, H. P. Reisenauer, U. Schäfer, and H. Balli, Angew. Chem. **100**, 590 (1988); Angew. Chem. Int. Ed. Engl. **27**, 566 (1988).

C_4S

$\tilde{B}$
$T_0 \cong 41700$ Ar AB[1]

$\tilde{A}$
T_0 = 22220 Ar AB[1] $\tilde{A}$–$\tilde{X}$ 380–450 nm

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1757	Ar	IR	1

References

[1]G. Maier, J. Schrot, and H. P. Reisenauer, Chem. Ber. **124**, 2613 (1991).

$C(CN)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CN a-stretch	1756m	Ar	IR	1
		C_3 a-stretch	1158w	Ar	IR	1
		CCN deform.	392w	Ar	IR	1

References

[1]W. H. Smith and G. E. Leroi, Spectrochim. Acta **25A**, 1917 (1969).

N_3CN^+

$\tilde{F}\ ^2A''$ C_s
T^a = 57280(900) gas PE[1]

$\tilde{E}\ ^2A'$ C_s
T^a = 45500(240) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	NN stretch	1520(40)	gas	PE	1

$\tilde{D}\ ^2A''$ C_s
T^a = 28720(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	C≡N stretch	1960(40)	gas	PE	1
	5	NNN bend	620(40)	gas	PE	1
	6	CNN bend	430(40)	gas	PE	1

$\tilde{C}\ ^2A'$ C_s
T_0 = 24930(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	NN stretch	1380(40)	gas	PE	1
	4	NC stretch	1090(40)	gas	PE	1
	5	NNN bend	620(40)	gas	PE	1

$\tilde{B}\ ^2A'$ C_s
T^a = 19120(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	C≡N stretch	2190(40)	gas	PE	1
	3	NN stretch	1130(40)	gas	PE	1
	5	NNN bend	810(40)	gas	PE	1

$\tilde{A}\ ^2A'$ C_s
T_0 = 8550(240) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	6	CNN bend	640(40)	gas	PE	1

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	NN stretch	1900(40)	gas	PE	1
			1120(40)	gas	PE	1
			800(40)	gas	PE	1

[a] From vertical ionization potential.

References

[1]D. C. Frost, H. W. Kroto, C. A. McDowell, and N. P. C. Westwood, J. Electron Spectrosc. Relat. Phenom. **11**, 147 (1977).

$C_3O_2^+$

$\tilde{D}\ ^2\Pi_u$ $D_{\infty h}$
T_0 = 53680(50) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g	1	CO stretch	2195(40)	gas	PE	1
	2	C_3 s-stretch	629(40)	gas	PE	1

$\tilde{C}\ ^2\Sigma_g$ [a]
T_0 = 51420(50) gas PE[1]

$\tilde{B}\ ^2\Pi_u$ [a]
T_0 = 41520(50) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Bend	662(40)	gas	PE	1

$\tilde{A}\ ^2\Pi_g$ [a]
T_0 = 31440(50) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO a-stretch	2364(40)	gas	PE	1
		Bend	718(30)	gas	PE	1

$\tilde{X}\ ^2\Pi_u$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g	1	CO stretch	2105(40)	gas	PE	1
Π_u	7	Bend	435(40)[b]	gas	PE	1

[a] Symmetry of the orbital which is depopulated on ionization is given. Photoelectron spectrum indicates that the product ion is bent.
[b] Observed as sequence bands. This vibration is highly anharmonic.

References

[1]J. W. Rabalais, L. O. Werme, T. Bergmark, L. Karlsson, M. Hussain, and K. Siegbahn, *Electron Spectroscopy*, D. A. Shirley, Ed., (North-Holland Publishing Co., Amsterdam, 1972), p. 425.

$NCNCO^+$

$\tilde{E}\ ^2A'$ C_s
T^a = 45990(320) gas PE[1]

$\tilde{D}\ ^2A''$ C_s
$T^a \cong$ 26220 gas PE[1]

$\tilde{C}\ ^2A'$ C_s
T_0 = 24450(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			730(60)	gas	PE	1

$\tilde{B}\ ^2A'$ C_s
T^a = 15900(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			2340(60)	gas	PE	1
			1410(60)	gas	PE	1
			600(60)	gas	PE	1

$\tilde{A}\ ^2A'$ C_s
T^a = 4120(320) gas PE[1]

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			2130(60)	gas	PE	1
			540(60)	gas	PE	1

[a] From vertical ionization potential.

References

[1]D. C. Frost, H. W. Kroto, C. A. McDowell, and N. P. C. Westwood, J. Electron Spectrosc. Relat. Phenom. **11**, 147 (1977).

$S(CN)_2^+$

$\tilde{H}\ ^2B_2$ C_{2v}
T^a = 67600(1000) gas PE[1]

$\tilde{G}\ ^2A_1$ C_{2v}
T^a = 41800(1000) gas PE[1]

$\tilde{F}\ ^2B_1$ C_{2v}
T^a = 29850(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CS stretch	560(40)	gas	PE	1

$\tilde{E}\ ^2A_1$ C_{2v}
T^a = 23400(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CS stretch	840(40)	gas	PE	1

$\tilde{D}\ ^2B_2$ C_{2v}
T^a = 21780(320) gas PE[1]

$\tilde{C}\ ^2A_2$ C_{2v}
T^a = 18320(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CN stretch	1980(40)	gas	PE	1

$\tilde{B}\ ^2B_2$ C_{2v}
T^a = 15730(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CN stretch	1840(40)	gas	PE	1

$\tilde{A}\ ^2A_1$ C_{2v}
T^a = 15200(1000) gas PE[1]

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CN stretch	2040(40)	gas	PE	1
	2	SC_2 stretch	640(40)	gas	PE	1

[a] From vertical ionization potentials.

References

[1]P. Rosmus, H. Stafast, and H. Bock, Chem. Phys. Lett. **34**, 275 (1975).

$NCNCS^+$

$\tilde{G}\ ^2A'$ C_s
T^a = 43730(560) gas PE[1]

$\tilde{E},\tilde{F}\ ^2A'',^2A'$ C_s
T^a = 39450(560) gas PE[1]

$\tilde{D}\ ^2A'$ C_s
T^a = 21540(560) gas PE[1]

$\tilde{C}\ ^2A''$ C_s
T^a = 18800(320) gas PE[1]

$\tilde{B}\ ^2A'$ C_s
T^a = 16860(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		NCS a-stretch	1940(60)	gas	PE	1
		NCS bend	645(60)	gas	PE	1

$\tilde{A}\ ^2A'$ C_s
T^a = 2180(560) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			400(60)	gas	PE	1

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		NCS a-stretch	1690(60)	gas	PE	1

[a] From vertical ionization potentials.

References

[1]M. A. King and H. W. Kroto, J. Am. Chem. Soc. **106**, 7347 (1984).

$Se(CN)_2^+$

$\tilde{H}\ ^2B_2$ C_{2v}
T^a = 62450(320) gas PE[1]

$\tilde{G}\ ^2S_1$ C_{2v}
T^a = 42360(320) gas PE[1]

$\tilde{F}\ ^2B_1$ C_{2v}
T^a = 27670(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	SeC stretch	460(50)	gas	PE	1

$\tilde{E}\ ^2B_2$ C_{2v}
T^a = 24120(560) gas PE[1]

$\tilde{D}\ ^2A_1$ C_{2v}
T^a = 23080(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CN stretch	2150(50)	gas	PE	1

$\tilde{C}\ ^2A_2$ C_{2v}
T^a = 19360(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CN stretch	1900(50)	gas	PE	1

$\tilde{B}\ ^2A_1$ C_{2v}
$T^a \cong$ 18480 gas PE[1]

$\tilde{A}\ ^2B_2$ C_{2v}
T^a = 17510(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CN stretch	1900(50)	gas	PE	1

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CN stretch	1900(50)	gas	PE	1
	2	SeC stretch	530(50)	gas	PE	1

[a] From vertical ionization potentials.

References

[1]G. Jonkers, R. Mooyman, and C. A. de Lange, Mol. Phys. **43**, 655 (1981).

$FC{\equiv}CCN^+$

$\tilde{D}\ ^2\Sigma^+$ $C_{\infty v}$
T_0 = 79100(500) gas PE[1]

$\tilde{C}\ ^2\Pi$ $C_{\infty v}$
T_0 = 58900(500) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1300(80)	gas	PE	1
			730(80)	gas	PE	1

$\tilde{B}\ ^2\Pi_{3/2}$ $C_{\infty v}$
T_0 = 20170(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1300(80)	gas	PE	1
			730(80)	gas	PE	1

$\tilde{A}\ ^2\Sigma^+$ $C_{\infty v}$
T_0 = 16060(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2200(80)	gas	PE	1
			680(80)	gas	PE	1

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2360(80)	gas	PE	1
			600(80)	gas	PE	1

References

[1]G. Bieri, E. Heilbronner, V. Hornung, E. Kloster- Jensen, J. P. Maier, F. Thommen, and W. Von Niessen, Chem. Phys. **36**, 1 (1979).

$ClC{\equiv}CCN^+$

$\tilde{D}\ ^2\Sigma^+$ $C_{\infty v}$
T_0 = 56500(500) gas PE[1]

$\tilde{C}\ ^2\Pi$ $C_{\infty v}$
T_0 = 31900(500) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			480(80)	gas	PE	1

$\tilde{B}\ ^2\Pi_{3/2}$ $C_{\infty v}$
T_0 = 20352(3) gas LF[3]
20392(16) Ne AB[3] $\tilde{B}-\tilde{X}$ 446–490 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	C≡C stretch	1990(20)	Ne	AB	3
	3	C–C stretch	970(80)	gas	PE	1
	4	CCl stretch	538(20)	Ne	AB	3

τ = 190(10) ns gas PEFCO[2]

$\tilde{A}\ ^2\Sigma^+$ $C_{\infty v}$
T_0 = 18870(160) gas PE[1]
19662(16) Ne AB[3] $\tilde{A}-\tilde{X}$ 461–509 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	C≡C stretch	2007(20)T	Ne	AB	3
	4	CCl stretch	471(20)	Ne	AB	3

τ = 394(20) ns gas PEFCO[2]

$\tilde{X}\ ^2\Pi_{3/2}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2140(80)	gas	PE	1
		CCl stretch	500(80)	gas	PE	1

References

[1]G. Bieri, E. Heilbronner, V. Hornung, E. Kloster- Jensen, J. P. Maier, F. Thommen, and W. Von Niessen, Chem. Phys. **36**, 1 (1979).
[2]R. Kuhn, J. P. Maier, and F. Thommen, J. Electron Spectrosc. Relat. Phenom. **34**, 253 (1984).
[3]S. Leutwyler, J. P. Maier, and U. Spittel, J. Chem. Soc., Faraday Trans. 2 **81**, 1565 (1985).

BrC≡CCN$^+$

$\tilde{D}\ ^2\Sigma^+$ $C_{\infty v}$
T_0 = 50750(500) gas PE[1]

$\tilde{C}\ ^2\Pi$ $C_{\infty v}$
T_0 = 27400(500) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CBr stretch	400(80)	gas	PE	1

$\tilde{B}\ ^2\Sigma^+$ $C_{\infty v}$
T_0 = 20570(160) gas PE[1]
PEFCO[2] and neon–matrix [3] observations suggest that the $\tilde{A}$ and $\tilde{B}$ states are strongly mixed.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C–C stretch	1020(80)	gas	PE	1

τ = 11(2) ns gas PEFCO[2]

$\tilde{A}\ ^2\Pi_{3/2}$ $C_{\infty v}$
T_0 = 18621(1) gas EF[3,4]LF[3,4] $\tilde{A}-\tilde{X}$ 460–540 nm
18347(3) Ne AB[3] $\tilde{A}-\tilde{X}$ 427–545 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡N stretch	2219(4)	Ne	AB	3
	2	C≡C stretch	2020(2)	gas	LF	4
			1976(4)	Ne	AB	3
	3	C–C stretch	1140(2)	gas	LF	4
			1149(4)	Ne	AB	3
	4	CBr stretch	359(2)	gas	LF	4
			354(4)	Ne	AB	3
Π	6	CCC deform.	259(2)H	gas	LF	4
	7	CCBr deform.	108(2)H	gas	LF	4

τ = 17(2) ns gas PEFCO[2]
A = −1130(160) gas PE[1]

$\tilde{X}\ ^2\Pi_{3/2}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡N stretch	2120(2)	gas	EF	4
	2	C≡C stretch	1983(2)	gas	EF	4
	3	C–C stretch	1095(2)	gas	EF	4
	4	CBr stretch	438(2)	gas	EF	4
Π	6	CCC deform.	302(2)H	gas	EF	4
	7	CCBr deform.	111(2)H	gas	EF	4

A = −890(160) gas PE[1]

References

[1]G. Bieri, E. Heilbronner, V. Hornung, E. Kloster- Jensen, J. P. Maier, F. Thommen, and W. Von Niessen, Chem. Phys. **36**, 1 (1979).
[2]R. Kuhn, J. P. Maier, and F. Thommen, J. Electron Spectrosc. Relat. Phenom. **34**, 253 (1984).
[3]S. Leutwyler, J. P. Maier, and U. Spittel, J. Chem. Soc., Faraday Trans. 2 **81**, 1565 (1985).
[4]R. Kuhn, J. P. Maier, L. Misev, and T. Wyttenbach, J. Electron Spectrosc. Relat. Phenom. **41**, 265 (1986).

IC≡CCN$^+$

$\tilde{D}\ ^2\Sigma^+$ $C_{\infty v}$
T_0 = 43700(500) gas PE[1]

$\tilde{C}\ ^2\Pi_{3/2}$ $C_{\infty v}$
T_0 = 28400(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C–C stretch	1050(80)	gas	PE	1

$\tilde{B}\ ^2\Sigma^+$ $C_{\infty v}$
T_0 = 23870(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2100(80)	gas	PE	1
		CI stretch	400(80)	gas	PE	1

$\tilde{A}\ ^2\Pi_{3/2}$ $C_{\infty v}$

T_0 = 15560(160) gas PE[1]
15371(2) Ne AB[3] $\tilde{A}$–$\tilde{X}$ 530–650 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡N stretch	2214(4)	Ne	AB	3
	2	C≡C stretch	2060(80)	gas	PE	1
	3	C–C stretch	1007(4)	Ne	AB	3
	4	Cl stretch	308(4)	Ne	AB	3

τ < 6 ns gas PEFCO[2]
A = −2340(160) gas PE[1]

$\tilde{X}\ ^2\Pi_{3/2}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2060(80)	gas	PE	1
		Cl stretch	400(80)	gas	PE	1

A = −2820(160) gas PE[1]

References

[1]G. Bieri, E. Heilbronner, V. Hornung, E. Kloster-Jensen, J. P. Maier, F. Thommen, and W. Von Niessen, Chem. Phys. **36**, 1 (1979).
[2]R. Kuhn, J. P. Maier, and F. Thommen, J. Electron Spectrosc. Relat. Phenom. **34**, 253 (1984).
[3]S. Leutwyler, J. P. Maier, and U. Spittel, J. Chem. Soc., Faraday Trans. 2 **81**, 1565 (1985).

Al_2O_3

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1211.2	Ar	IR	1

References

[1]L. Andrews, T. R. Burkholder, and J. T. Yustein, J. Phys. Chem. **96**, 10182 (1992).

Ga_2O_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		GaO a-stretch	979.4	Ar	IR	1

References

[1]T. R. Burkholder, J. T. Yustein, and L. Andrews, J. Phys. Chem. **96**, 10189 (1992).

In_2O_3

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			826	Ar	IR	1

References

[1]T. R. Burkholder, J. T. Yustein, and L. Andrews, J. Phys. Chem. **96**, 10189 (1992).

$Si(CO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1928	Ar	IR	1

References

[1]R. R. Lembke, R. F. Ferrante, and W. Weltner, Jr., J. Am. Chem. Soc. **99**, 416 (1977).

N≡C–CNO

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CNO a-stretch	2356vs	Ar	IR	1
			2192w	Ar	IR	1
		CNO s-stretch	1445wm	Ar	IR	1
			717vw	Ar	IR	1
			407vw	Ar	IR	1

References

[1]G. Maier and J. H. Teles, Angew. Chem. **99**, 152 (1987); Angew. Chem. Int. Ed. Engl. **26**, 155 (1987).

NC–NCO

$\tilde{X}$ C_s Structure: MW[3,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2280vsT	gas	IR	1,5
			2233.1ms	gas	IR	1,5
			1429.4wm	gas	IR	1,5
			1165w	gas	IR	1
			1073.5wm	gas	IR	1,5
			727.3	gas	IR	5
			610.2s	gas	IR	1,5
			455s	gas	IR	1
			365s	gas	IR	1

A_0 = 2.480; B_0 = 0.090; C_0 = 0.087 MW[2,3]

References

[1]E. Mayer, Monatsh. Chem. **101**, 834 (1970).
[2]W. H. Hocking and M. C. L. Gerry, J. Chem. Soc., Chem. Commun. 47 (1973).
[3]W. H. Hocking and M. C. L. Gerry, J. Mol. Spectrosc. **59**, 338 (1976).
[4]B. Bak, H. Svanholt, and A. Holm, Acta Chem. Scand. **A33**, 597 (1979).
[5]T. C. DeVore, J. Mol. Struct. **162**, 287 (1987).

NC–NCS

$\tilde{X}$ C_s ($C_{\infty v}$)[a] Structure: MW[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CN stretch	2260.9	gas	IR	3
	2	CN stretch	2016.4	gas	IR	3
		Skel. bend	97(11)	gas	MW	2

B_0 = 0.051 MW[1,2]

[a] Barrier to linearity 308(34). MW[2]

References

[1]M. A. King and H. W. Kroto, J. Chem. Soc., Chem. Commun. 606 (1980).
[2]M. A. King, H. W. Kroto, and B. M. Landsberg, J. Mol. Spectrosc. **113**, 1 (1985).
[3]T. C. DeVore, J. Mol. Struct. **162**, 287 (1987).

$S(CS)_2$

A weak, broad absorption between 450 and 530 nm has tentatively been attributed[1] to $S(CS)_2$ isolated in solid argon.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CS stretch	1051.1	Ar	IR	1
		CS stretch	686.8	Ar	IR	1

References

[1]R. B. Bohn, Y. Hannachi, and L. Andrews, J. Am. Chem. Soc. **114**, 6452 (1992).

P_4O

$\tilde{X}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	P=O stretch	1241s	Ar	IR	1
	2	P_4 s-stretch	603	Ar	IR	1
	3		441	Ar	IR	1
e	4		501	Ar	IR	1
	5		393	Ar	IR	1
	6	P–P=O deform.	243w	Ar	IR	1

References

[1]L. Andrews and R. Withnall, J. Am. Chem. Soc. **110**, 5605 (1988).

br–P_4O

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			856s	Ar	IR	1
			553w	Ar	IR	1

References

[1]L. Andrews and R. Withnall, J. Am. Chem. Soc. **110**, 5605 (1988).

cyc–P_4S

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			518.1T	Ar	IR	1

References

[1]Z. Mielke, G. D. Brabson, and L. Andrews, J. Phys. Chem. **95**, 75 (1991).

As_4O

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			981.5T	Ar	IR	1

References

[1]L. Andrews and Z. Mielke, Inorg. Chem. **28**, 4001 (1989).

br–As_4O

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		AsOAs a-stretch	590.3s 565.4s	Ar	IR	1
		AsOAs s-stretch	301.5w	Ar	IR	1
		As–As stretch	240.5	Ar	IR	1

References

[1]L. Andrews and Z. Mielke, Inorg. Chem. **28**, 4001 (1989).

Cl_2CCO^+

$\tilde{I}\ ^2A_1$ C_{2v}
T^a = 73100(560) gas PE[1]

$\tilde{H}\ ^2B_2$ C_{2v}
T^a = 65430(560) gas PE[1]

$\tilde{G}\ ^2A_1$ C_{2v}
T^a = 61960(560) gas PE[1]

$\tilde{F}\ ^2B_1$ C_{2v}
T^a = 52850(560) gas PE[1]

$\tilde{E}\ ^2B_2$ C_{2v}
T^a = 47040(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			930(60)	gas	PE	1

$\tilde{D}\ ^2B_1$ C_{2v}
T^a = 38970(320) gas PE[1]

$\tilde{C}\ ^2A_1$ C_{2v}
T^a = 30420(320) gas PE[1]

$\tilde{B}\ ^2A_2$ C_{2v}
T^a = 27840(320) gas PE[1]

$\tilde{A}\ ^2B_2$ C_{2v}
T^a = 25090(320) gas PE[1]

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CCO a-stretch	2200(40)	gas	PE	1
	2	CCO s-stretch	1100(40)	gas	PE	1
	4	CCl_2 scissors	330(40)	gas	PE	1

[a] From vertical ionization potentials.

References

[1]D. Colbourne, D. C. Frost, C. A. McDowell, and N. P. C. Westwood, J. Chem. Soc., Chem. Commun. 250 (1980).

$CF_2N_2^+$

$\tilde{F}\ ^2B_2$ C_{2v}
T_0 = 62930(1600) gas PE[1]

$\tilde{E}\ ^2A_2$ C_{2v}
T^a = 53250(1600) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			600(80)	gas	PE	1

$\tilde{C},\tilde{D}\ ^2B_1,^2A_1$ C_{2v}
T^a = 44780(1000) gas PE[1]

$\tilde{A},\tilde{B}\ ^2B_1,^2A_1$ C_{2v}
T_0 = 30660(1000) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1330(80)	gas	PE	1

$\tilde{X}\ ^2B_2$ C_{2v}

[a] From vertical ionization potential.

References

[1]M. B. Robin, C. R. Brundle, N. A. Kuebler, G. B. Ellison, and K. B. Wiberg, J. Chem. Phys. **57**, 1758 (1972).

PF_2CN^+

$\tilde{E}$ C_s
T^a = 58900(1600) gas PE[1]

$\tilde{D}$ C_s
T^a = 50800(1600) gas PE[1]

$\tilde{C}$ C_s
T^a = 37900(1600) gas PE[1]

$\tilde{B}$ C_s
T^a = 16900(1600) gas PE[1]

$\tilde{A}$ C_s
T^a = 12900(1600) gas PE[1]

[a] From vertical ionization potentials.

References

[1]S. Cradock and D. W. H. Rankin, J. Chem. Soc., Faraday Trans. 2 **68**, 940 (1972).

Cl_2CCO

$\tilde{X}$ C_{2v} Structure: ED[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C=O stretch	2160.3s	gas	IR	2
			2158vs	Ar	IR	1,3
		C=C stretch	1291w	gas	IR	2
			1291w	Ar	IR	1,3
		CCl_2 a-stretch	936s	gas	IR	2
			935m	Ar	IR	1
			605	Ar	IR	3
			441	Ar	IR	3

References

[1]M. Torres, J. Ribo, A. Clement, and O. P. Strausz, Nouv. J. Chim. **5**, 351 (1981).
[2]M. C. L. Gerry, W. Lewis-Bevan, and N. P. C. Westwood, Can. J. Chem. **63**, 676 (1985).
[3]V. N. Khabashesku, A. K. Mal'tsev, I. Bertoti, T. Sekei, and O. M. Nefedov, Dokl. Akad. Nauk SSSR **293**, 924 (1987); Dokl. Phys. Chem. **293**, 347 (1987).
[4]B. Rozsondai, J. Tremmel, I. Hargittai, V. N. Khabashesku, N. D. Kagramanov, and O. M. Nefedov, J. Am. Chem. Soc. **111**, 2845 (1989).

O_2N–NO

In nitrogen– and neon–matrix studies,[4,7] excitation in the region of a weak absorption between 700 and 900 nm, with maximum near 720 nm, leads to isomerization forming O=N–O–N=O.

$\bar{X}$ C_s Structure: MW[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	N=O stretch	1832	gas	IR	1,5
			1830.2s	Ne	IR	7
			1840m	N_2	IR	4
			1867vs	O_2	IR	2
			1861	NO	IR,Ra	6
	2	NO_2 a–stretch	1652	gas	IR	5
			1643.3s	Ne	IR	7
			1630vs	N_2	IR	4
			1596s	O_2	IR	2
			1593	NO	IR,Ra	6
	3	NO_2 s–stretch	1305	gas	IR	1,5
			1302.5vs	Ne	IR	7
			1302s	N_2	IR	4
			1303	O_2	IR	2
			1298	NO	IR,Ra	6
	4	NO_2 deform.	773	gas	IR	1,5
			773.1wm	Ne	IR	7
			776wm	N_2	IR	4
			788	O_2	IR	2
			787	NO	IR,Ra	6
	5	NO_2 rock	414	gas	IR	5
			420w	N_2	IR	4
			405	NO	Ra	6
	6	N–N stretch	241	gas	IR	5
			266	NO	Ra	6
	7	NO_2 wag	205	NO	Ra	6
a''	8	NNO_2 OPLA	627	NO	Ra	6
	9	Torsion	63	gas	IR	5
			70	NO	Ra	6

A_0 = 0.415; B_0 = 0.141; C_0 = 0.105 MW[3]

References

[1]L. D'Or and P. Tarte, Bull. Soc. Roy. Sci. Liège **22**, 276 (1953).
[2]W. G. Fateley, H. A. Bent, and B. Crawford, Jr., J. Chem. Phys. **31**, 204 (1959).
[3]A. H. Brittain, A. P. Cox, and R. L. Kuczkowski, Trans. Faraday Soc. **65**, 1963 (1969).
[4]E. L. Varetti and G. C. Pimentel, J. Chem. Phys. **55**, 3813 (1971).
[5]C. H. Bibart and G. E. Ewing, J. Chem. Phys. **61**, 1293 (1974).
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[7]M. E. Jacox and W. E. Thompson, J. Chem. Phys. **93**, 7609 (1990).

O=N-O-N=O

In nitrogen–matrix studies,[1] absorption maxima were observed at 398, 381, and 363 nm. Excitation in the 370–480 nm spectral region resulted in photoisomerization into O_2N–NO.[1,3]

$\bar{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	N=O s–stretch	1740	NO	Ra	2
	2	N–O s–stretch	973.6m	Ne	IR	3
			969w	N_2	IR	1
			973m	NO	IR,Ra	2
	3	NON bend	387m	N_2	IR	1
			395	NO	Ra	2
	4	O=NO s-bend	366s	N_2	IR	1
a_2	5	Torsion	140	NO	Ra	2
b_1	6	Torsion	105H	NO	Ra	2
b_2	7	N=O a–stretch	1697.2vs	Ne	IR	3
			1690s	N_2	IR	1
			1687vs	NO	IR	2
			1661w	N_2	IR	1
	8	N–O a–stretch	877vw	N_2	IR	1
			865vw	NO	IR	2
	9	O=NO a-bend	704vw	N_2	IR	1
			705vw	NO	IR	2

References

[1]E. L. Varetti and G. C. Pimentel, J. Chem. Phys. **55**, 3813 (1971).
[2]E. M. Nour, L.-H. Chen, and J. Laane, J. Phys. Chem. **87**, 1113 (1983).
[3]M. E. Jacox and W. E. Thompson, J. Chem. Phys. **93**, 7609 (1990).

ON–NSO

$\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO stretch	1827m	Ar	IR	1
			1823m			
		NO stretch	1499wm	Ar	IR	1
			1495wm			
		NS stretch	826w	Ar	IR	1
			822w			

References

[1]M. Hawkins and A. J. Downs, J. Phys. Chem. **88**, 2042 (1984).

ONSNO [a]

$\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO stretch	1669m	Ar	IR	1
		NO stretch	1567m	Ar	IR	1
		Deformation	323w	Ar	IR	1

[a] Alternative assignment of absorptions to SNONO cannot be definitively excluded.

References

[1]M. Hawkins and A. J. Downs, J. Phys. Chem. **88**, 3042 (1984).

$SN–NS_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NS_2 a–stretch	1499.7	Ar	IR	1

References

[1]P. Hassanzadeh and L. Andrews, J. Am. Chem. Soc. **114**, 83 (1992).

CO_4^-

The gas–phase photodestruction cross section of CO_4^- ($O_2C{\cdot}{\cdot}O_2^-$) is small over the 840–350 nm range.[1–4] In a neon matrix,[5] the onset of photodestruction occurs near 260 nm, with evidence for the detachment of O or O^-.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CO_2 a–stretch	1895.2vs	Ne	IR	5
			1892 K	Ar	IR	5
	2	CO_2 s–stretch	1256.5s	Ne	IR	5
			1259 K	Ar	IR	5
	4	CO_2 scissors	697.1m	Ne	IR	5
			692 K	Ar	IR	5

References

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$FC(O)O_2$

A gas–phase absorption between 200 and 285 nm, with maximum at 43100 (232 nm), has been assigned[1] to $FC(O)O_2$.

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C_2F_3

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	C=C stretch	1780.4wm	Ar	IR	2
	2	CF stretch	1290(5)	gas	IR,DL	1
			1282.4s	Ar	IR	2
	3	CF stretch	1225(5)	gas	IR,DL	1
			1216.9vs	Ar	IR	2
	4	C_2F_3 s–stretch	900.0w	Ar	IR	2

References

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cyc–F_2SiO_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SiF_2 s–stretch	1155.2s	O_2	IR	1
		SiF_2 a–stretch	1013.7s	O_2	IR	1
		SiO_2 s–stretch	862.6w	O_2	IR	1

References

[1]A. Patyk, W. Sander, J. Gauss, and D. Cremer, Chem. Ber. **123**, 89 (1990).

cyc–Cl_2SiO_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SiO_2 s–stretch	1054.4s	O_2	IR	1
		$SiCl_2$ stretch	649.9ms	O_2	IR	1
		O–O stretch	576.1wm	O_2	IR	1

References

[1]A. Patyk, W. Sander, J. Gauss, and D. Cremer, Chem. Ber. **123**, 89 (1990).

F_2CSO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C=S stretch	1373vs	Ar	IR	1
		CF_2 a-stretch	1296s	Ar	IR	1
		S=O stretch	1117.5s	Ar	IR	1
			724.5w	Ar	IR	1

References

[1]W. Sander, R. Henn, and W. Sundermeyer, Spectrochim. Acta **42A**, 1281 (1986).

ClFCSO [a]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C=S stretch	1297	Ar	IR	1
		CF stretch	1131	Ar	IR	1
		S=O stretch	1050	Ar	IR	1
			640	Ar	IR	1

[a] More stable isomer.

References

[1]W. Sander, R. Henn, and W. Sundermeyer, Spectrochim. Acta **42A**, 1281 (1986).

ClFCSO [a]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C=S stretch	1246	Ar	IR	1
		CF stretch	1145	Ar	IR	1
		S=O stretch	1082	Ar	IR	1

[a] Less stable isomer.

References

[1]W. Sander, R. Henn, and W. Sundermeyer, Spectrochim. Acta **42A**, 1281 (1986).

$ClONO_2$

The onset of continuous absorption by gas-phase $ClONO_2$ occurs near 25000 (400 nm).[2] Except for two possible shallow maxima, the absorption continues to rise out to the 185 nm cutoff of the observations.

$\tilde{X}$ C_s Structure: MW[4,9]IR[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO_2 a-stretch	1735.4vs	gas	IR	1,3,11
			1727.6s	Ar	IR	8,10,14
			1734.0s	N_2	IR	10,14
			1730.0vs	O_2	IR	6,14
	2	NO_2 s-stretch	1291.9vs	gas	IR	1,3,11
			1285.8vs	Ar	IR	8,10,14
			1291.4vs	N_2	IR	10,14
			1289.7s	O_2	IR	6,14
	3	ClO stretch	809.3s	gas	IR	1,3,11
			801.6m	Ar	IR	8,10,14
			809.7wm	N_2	IR	10,14
			808.1m	O_2	IR	6,14
	4	Mixed	780.22ms	gas	IR,DL	1,3,11,12 13
			775.6m	Ar	IR	8,10,14
			778.6m	N_2	IR	10,14
			776.3m	O_2	IR	6,14
	5	Mixed	560.0s	gas	IR	1
			560.9ms	Ar	IR	8,10,14
			563.2wm	N_2	IR	10,14
			559.0m	O_2	IR	6,14
	6	NO_2 rock	434.1m	gas	IR	1
			426	Ar	IR	8,10
			436.5w	N_2	IR	10
			435.0	O_2	IR	6
	7	ClO rock	270vvw	gas	IR	1
a''	8	NO_2 wag	710.8w	gas	IR	1
			710.8w	Ar	IR	8,10,14
			708.4w	N_2	IR	10,14
			704.6wm	O_2	IR	6,14
	9	Torsion	120.16	gas	IR	1,5,7

A_0 = 0.404; B_0 = 0.093; C_0 = 0.075 MW[4,9]
Torsional barrier = 1900(100) gas IR[5,7]

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$BrONO_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO_2 a–stretch	1714vs	gas	IR	1
			1709vs	Ne	IR	1
			1702vs	N_2	IR	1
	2	NO_2 s–stretch	1288vs	gas	IR	1
			1285vs	Ne	IR	1
			1285vs	N_2	IR	1
	3	NO_2 scissors	806vs	gas	IR	1
			802vs	Ne	IR	1
			805vs	N_2	IR	1
	4	OBr stretch	750w	Ne	IR	1
			750w	N_2	IR	1
	5	NO_2 rock	564s	gas	IR	1
			563s	Ne	IR	1
			574s	N_2	IR	1
			569s			
a''	8	ONO_2 OPLA	728wm	gas	IR	1
			723vw	Ne	IR	1
			725wm	N_2	IR	1

References

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$IONO_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO_2 a–stretch	1673	gas	IR	1
		NO_2 s–stretch	1276	gas	IR	1
			815	gas	IR	1
			580T	gas	IR	1

References

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SO_4

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		S=O stretch	1434s	Ar	IR	1
		S=O stretch	1267s	Ar	IR	1
		O–O stretch	925wm	Ar	IR	1
			777wm	Ar	IR	1
			611m	Ar	IR	1
			498sh	Ar	IR	1
			490sh	Ar	IR	1

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FSO_3^+

$\tilde{D}$ C_{3v}
T^b = 53700(1200) gas PE[1]

$\tilde{C}$ $^3A_2$ [a] C_{3v}
T^b = 40700(1200) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SO_3 s–stretch	920(40)	gas	PE	1
	3	SO_3 umbrella	550(40)	gas	PE	1

$\tilde{B}$ C_{3v}
T^b = 17300(1200) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			850(40)	gas	PE	1

$\tilde{A}$ C_{3v}
T^b = 10100(1200) gas PE[1]

$\tilde{X}$ $^1A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SO_3 s–stretch	1220(40)	gas	PE	1

[a] Tentative assignment.
[b] From vertical ionization potentials.

References

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CF_3O

$\tilde{A}$ $^2A_1$ C_{3v}
T_0 = 28478 gas LF[3] $\tilde{A}$–$\tilde{X}$ 330–400 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CO stretch	709T	gas	LF	3
e	6	FCO deform.	463T	gas	LF	3

τ_0 = 30.1 ns gas LF[3]

$\tilde{X}$ ^2E C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO stretch	1225T	gas	LF	3
	2	CF_3 s–stretch	907T	gas	LF	3
e	4	CF_3 a–stretch	1221.6	Ar	IR	1,2
	6	FCO deform.	483T	gas	LF	3

References

[1]L. Andrews, M. Hawkins, and R. Withnall, Inorg. Chem. **24**, 4234 (1985).
[2]K. C. Clemitshaw and J. R. Sodeau, J. Phys. Chem. **93**, 3552 (1989).
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CF_4^+

$\tilde{D}\ ^2A_1$ T_d Structure: PE,EF[7]
T_0[a] = 78830(160) gas PE[2,3,5]
gas EF[6] $\tilde{D}-\tilde{C}$ 350–420 nm
Broad, unstructured emission maxima at 189 and 160 nm (52900 and 62500) which appear on He^+ or electron impact on CF_4 have been interpreted as arising from the $\tilde{D}-\tilde{B}$ and $\tilde{D}-\tilde{A}$ transitions of CF_4^+, respectively.[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF stretch	800(1)	gas	PE,EF	3,5,6

τ = 2.1(2) ns gas EF[1]
B_0 = 0.180(3)[b] EF[7]

$\tilde{C}\ ^2T_2$ T_d Structure: PE,EF[7]
T_0[a] = 51230(160) gas PE[2,3,5]
gas EF[6] $\tilde{D}-\tilde{C}$ 350–420 nm
Broad, unstructured emission maxima at 290 and 230 nm (34500 and 43500) which result from He^+ or electron impact[6] on CF_4 and from exposure of CF_4 to synchrotron radiation[10] of wavelength shorter than 57.4 nm have been interpreted as arising from the $\tilde{C}-\tilde{A}$ and $\tilde{C}-\tilde{X}$ transitions of CF_4^+, respectively.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF stretch	729	gas	PE,EF	2,3,5,6

A = +16(1) EF[6–8]
τ = 9.0(9) ns gas EF[1]EM[9]
$B_0 \cong$ 0.168[c] PE,EF[7]

$\tilde{B}\ ^2E$
T_0[a] = 23800(1000) gas PE[2–5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF stretch	810(80)	gas	PE	3–5
e		Deformation	500(100)	gas	PE	3–5

$\tilde{A}\ ^2T_2$
T_0[a] = 14100(1000) gas PE[2–5]

$\tilde{X}\ ^2T_1$

[a] Measured with respect to onset of first photoelectron band, estimated by Ref. 3 at 15.35 eV.
[b] From computer simulation of emission bands.
[c] From Franck–Condon analysis of photoelectron spectrum.

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CF_3Cl^+

$\tilde{F}\ ^2E$ C_{3v}
T_0[a] ≤ 66130(400) gas PE[2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF_3 umbrella	589(80)	gas	PE	4
	3	CCl stretch	420(80)	gas	PE	4

$\tilde{E}\ ^2A_1$ C_{3v}
T_0[a] = 60420(400) gas PE[2,4]
Broad emission bands in the 200–600 nm spectral region[8,9] which appear on excitation of CF_3Cl by synchrotron radiation with energy greater than 19 eV and which have a lifetime of 25(3) ns[9] have been attributed[9] to transitions arising from the $\tilde{E}$ state of CF_3Cl^+.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF_3 umbrella	637(80)	gas	PE	4

$\tilde{D}\ ^2E$ C_{3v}
T_0[a] = 39720(400) gas PE[1,2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF_3 umbrella	726(80)	gas	PE	4
	3	CCl stretch	387(80)	gas	PE	4
e	4	CF_3 stretch	1130(80)	gas	PE	4

$\tilde{C}\ ^2E$ C_{3v}
T^{ab} = 34610(400) gas PE[1,2,4]
A broad, unstructured absorption with onset near 400 nm (25000) and maximum at 295 nm (33900) which appears on argon–resonance photolysis of CF_3Cl isolated in solid argon and which has a photodecomposition threshold at a wavelength longer than 340 nm has been assigned[7] to the $\tilde{C}-\tilde{X}$ transition of CF_3Cl^+.

$\tilde{B}\ ^2A_2$ C_{3v}
T^{ab} = 26950(400) gas PE[1,2,4]

$\tilde{A}\ ^2A_1$ C_{3v}
T^{ab} = 22110(400) gas PE[1,2,4]

$\tilde{X}\ ^2E$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1299vs	Ar	IR	5,6
		CCl stretch	734wm	Ar	IR	5,6
		Deformation	460ms 451m	Ar	IR	5,6
		Deformation	416m	Ar	IR	5,6

[a] The first ionization potential of CF_3Cl is taken as 12.42(4) eV, the mean of the values reported in the photoionization studies of Refs. 2 and 3.
[b] From vertical ionization potential.

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CF_3Br^+

$\tilde{G}\ ^2A_1$ C_{3v}
T^a = 93800(1200) gas PE[2]

$\tilde{F}\ ^2E$ C_{3v}
T^a = 71200(1200) gas PE[2]

$\tilde{E}\ ^2A_1$ C_{3v}
T^a = 62300(1200) gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF_3 umbrella	620(80)	gas	PE	2
	3	CBr stretch	360(80)	gas	PE	2

$\tilde{D}\ ^2E$ C_{3v}
T^a = 44300(800) gas PE[1,2]
Emission bands between about 200 and 700 nm which result from the excitation of CF_3Br by synchrotron radiation of wavelength shorter than about 75 nm have been attributed[6] to the $\tilde{D}$–$\tilde{X}, \tilde{A}, \tilde{B}$ transitions of CF_3Br^+.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF_3 stretch	1080(80)	gas	PE	2
	2	CF_3 umbrella	690(80)	gas	PE	2

$\tilde{C}\ ^2E$ C_{3v}
T^a = 36100(800) gas PE[1,2]
A broad, unstructured absorption with maximum near 295 nm (33600) which appears on argon–resonance photolysis of CF_3Br isolated in solid argon and which has a photodecomposition threshold near 340 nm[5] may be contributed by the $\tilde{C}$–$\tilde{X}$ transition of CF_3Br^+.

$\tilde{B}\ ^2A_2$ C_{3v}
T^a = 30500(800) gas PE[1,2]

$\tilde{A}\ ^2A_1$ C_{3v}
T^a = 17750(800) gas PE[1,2]

$\tilde{X}\ ^2E$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1293s	Ar	IR	3,4
		CF stretch	1255vs	Ar	IR	3,4
			469s	Ar	IR	3,4

[a] From vertical ionization potentials.

References

[1]J. Doucet, P. Sauvageau, and C. Sandorfy, J. Chem. Phys. **58**, 3708 (1973).
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CF_3I^+

$\tilde{G}\ ^2A_1$ C_{3v}
T^a = 107700(1200) gas PE[1]

$\tilde{F}\ ^2E$ C_{3v}
T^a = 81900(1200) gas PE[1]

$\tilde{E}\ ^2A_1$ C_{3v}
T^a = 70200(800) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF_3 stretch	1090(80)	gas	PE	1
	2	CF_3 umbrella	600(80)	gas	PE	1
	3	CI stretch	190(80)	gas	PE	1

$\tilde{D}\ ^2E$ C_{3v}
T^a = 55100(800) gas PE[1]

$\tilde{C}\ ^2E$ C_{3v}
T^a = 47360(800) gas PE[1]

$\tilde{B}\ ^2A_2$ C_{3v}
T^a = 41230(800) gas PE[1]

$\tilde{A}\ ^2A_1$ C_{3v}
T^a = 22600(800) gas PE[1]

$\tilde{X}\ ^2E_{3/2}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1229vs	Ar	IR	2
		CF_3 s–stretch	1090(80)	gas	PE	1
			677m	Ar	IR	2
			497s	Ar	IR	2
		CI stretch	240(80)	gas	PE	1

A = 5890(80).[1]

[a] From vertical ionization potentials.

References

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$CF_2Cl_2^+$

$\tilde{H}$ C_{2v}
T^{ab} = 68200(1000) gas PE[2,4,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCl_2 stretch	565T	gas	PE	5

$\tilde{G}$ C_{2v}
T_0^a = 56160(160) gas PE[1,2,4,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCl_2 stretch	550(80)	gas	PE	5

$\tilde{E}, \tilde{F}\ ^2A_2, ^2A_1$ C_{2v}
T^{ab} = 36500(160) gas PE[1,2,4,5]
A broad absorption with maximum near 310 nm (32300) which appears on argon–resonance photolysis of CF_2Cl_2 isolated in solid argon and which has a photodecomposition threshold between 420 and 340 nm has been assigned[7] to the $\tilde{E}, \tilde{F}$–$\tilde{X}$ transitions of $CF_2Cl_2^+$.

$\tilde{D}\ ^2B_2$ C_{2v}
T_0^a = 19150(110) gas PE[1,2,4,5]
It has been proposed[8] that an unstructured emission in the 200–400 nm region, with its principal contribution at wavelengths longer than 300 nm, which appears on electron bombardment of CF_2Cl_2 at electron energies greater than that for the onset of the $\tilde{D}$ state of $CF_2Cl_2^+$ may be contributed by the $\tilde{D}$–$\tilde{X}$ transition of $CF_2Cl_2^+$.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CF_2 scissors	370(40)	gas	PE	1,4,5

$\tilde{C}\ ^2A_1$ C_{2v}
T^{ab} = 13880(160) gas PE[1,2,4,5]

$\tilde{B}\ ^2A_2$ C_{2v}
T_0^a = 11050(120) gas PE[1,2,4,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF_2 stretch	1097(80)	gas	PE	4,5
	2	CCl_2 stretch	565(80)	gas	PE	5
	4	CCl_2 scissors	210(80)	gas	PE	5

$\tilde{A}\ ^2B_1$ C_{2v}
T^{ab} = 6370(160) gas PE[1,2,4,5]

$\tilde{X}\ ^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF_2 a–stretch	1234vs	Ar	IR	6
		CCl_2 a–stretch	1067m	Ar	IR	6
		CF_2 bend	609wm	Ar	IR	6
		FCCl deform.	424m	Ar	IR	6
		FCCl deform.	406m	Ar	IR	6

[a] The first ionization potential of CF_2Cl_2 is taken as 11.75 eV, as determined in the photoionization studies of Refs. 2 and 3.
[b] From vertical ionization potential.

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$CF_2Br_2^+$

$\tilde{G}$ C_{2v}
T^a = 60700(1000) gas PE[1]

$\tilde{F}$ C_{2v}
T^a = 42900(1000) gas PE[1]

$\tilde{E}$ C_{2v}
T^a = 34530(400) gas PE[1]
A very strong, broad absorption with maximum at 357 nm (28000) which appears on argon–resonance photolysis of CF_2Br_2 isolated in solid argon and which has a photodecomposition threshold at a wavelength longer than 420 nm has been assigned[3] to the $\tilde{E}$–$\tilde{X}$ transition of $CF_2Br_2^+$.

$\tilde{D}$ C_{2v}
T^a = 16700(400) gas PE[1]

$\tilde{C}$ C_{2v}
T^a = 9760(400) gas PE[1]

$\tilde{B}$ C_{2v}
T^a = 6780(400) gas PE[1]

$\tilde{A}$ C_{2v}
T^a = 3310(400) gas PE[1]

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF_2 stretch	1244s	Ar	IR	2
			873m	Ar	IR	2
			868m	Ar	IR	2
			428wm	Ar	IR	2
			406wm	Ar	IR	2

[a] From vertical ionization potentials.

References

[1]J. Doucet, R. Gilbert, P. Sauvageau, and C. Sandorfy, J. Chem. Phys. **62**, 366 (1975).
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$CFCl_3^+$

$\tilde{E}, \tilde{F}$ $^2A_1, ^2E$ C_{3v}
T^a = 53650(160) gas PE[1-4]

$\tilde{D}$ ^2E C_{3v}
T_0 = 25390(120) gas PE[1-4]
A prominent, broad absorption with maximum near 405 nm (24700) which appears on argon-resonance photo lysis of $CFCl_3$ isolated in solid argon and which has a photodecomposition threshold at a wavelength longer than 500 nm has been assigned[6] to the $\tilde{D}$–$\tilde{X}$ transition of $CFCl_3^+$.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCl_3 stretch	460T	gas	PE	4
	3	CCl_3 umbrella	275(40)	gas	PE	1,4

$\tilde{C}$ $^2A_1$ C_{3v}
T_0 = 13430(100) gas PE[1-4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF stretch	1010(80)	gas	PE	2
	2	CCl_3 stretch	640(80)	gas	PE	2
	3	CCl_3 umbrella	340(40)	gas	PE	4

$\tilde{B}$ ^2E C_{3v}
T^a = 9680(160) gas PE[1-4]
Band shows a splitting of 1130(240).[4]

$\tilde{A}$ ^2E C_{3v}
T^a = 2980(160) gas PE[1-4]
Band shows a splitting of 1530(160).[4]

$\tilde{X}$ $^2A_2$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1214vs	Ar	IR	5
		CCl a-stretch	1041s	Ar	IR	5
		CCl s-stretch	585m	Ar	IR	5
		Deformation	432m	Ar	IR	5
		Deformation	324mT	Ar	IR	5

[a] From vertical ionization potentials.

References

[1]J. Doucet, P. Sauvageau, and C. Sandorfy, J. Chem. Phys. **58**, 3708 (1973).
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$CFBr_3^+$

$\tilde{E}$ $^2A_1$ C_{3v}
T^a = 55830(160) gas PE[1]

$\tilde{D}$ ^2E C_{3v}
T^a = 26540(160) gas PE[1]
A prominent, broad absorption with maximum near 435 nm (23000) which appears on argon-resonance photolysis of $CFBr_3$ isolated in solid argon and which has a photodecomposition threshold at a wavelength longer than 500 nm has been assigned[3] to the $\tilde{D}$–$\tilde{X}$ transition of $CFBr_3^+$.

$\tilde{C}$ $^2A_1$ C_{3v}
T_0 = 12750(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CBr_3 umbrella	210(80)	gas	PE	1

$\tilde{B}$ ^2E C_{3v}
T^a = 9200(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF stretch	874(80)	gas	PE	1

Splitting of 1690(160) observed.[1]

$\tilde{A}\ ^2E$ C_{3v}
T^a = 3790(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CBr_3 umbrella	213(80)	gas	PE	1

Splitting of 4030(160) observed.[1]

$\tilde{X}\ ^2A_2$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1167vs	Ar	IR	2
			1160vs			
			853vs	Ar	IR	2
			423s	Ar	IR	2
			399s	Ar	IR	2
			316m	Ar	IR	2

[a] From vertical ionization potential.

References

[1]F. T. Chau and C. A. McDowell, J. Electron Spectrosc. Relat. Phenom. **6**, 357 (1975).
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CCl_4^+

$\tilde{D}\ ^2A_1$ T_d
T^{ab} = 68800(900) gas PE[2]

$\tilde{C}\ ^2T_2$ T_d
T_0^a = 39290(900) gas PE[2-4]

$\tilde{B}\ ^2E$
T^{ab} = 15330(240) gas PE[2-4]

$\tilde{A}\ ^2T_2$ T_d
T_0^a = 6450(320) gas PE[2-4]

[a] The first ionization potential is taken as 11.47(1) eV, as in the photoionization study of Ref. 1.
[b] From vertical ionization potential.

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[4]P. J. Bassett and D. R. Lloyd, J. Chem. Soc. A 641 (1971).

CBr_4^+

$\tilde{D}\ ^2A_1$ T_d
T^{ab} = 75000(1000) gas PE[1,2]

$\tilde{C}\ ^2T_2$ T_d
T^{ab} = 38600(600) gas PE[1,2]

$\tilde{B}\ ^2E$
T^{ab} = 14320(400) gas PE[1,2]

$\tilde{A}\ ^2T_2$
T^{ab} = 6050(320) gas PE[1,2]

[a] The first ionization potential of CBr_4 is taken as 10.31(2) eV, as in the photoionization study of Ref. 3.
[b] From vertical ionization potential.

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SiF_4^+

$\tilde{D}\ ^2A_1$ T_d Structure: PE,EF[9]
T^{ab} = 50800(200) gas PE[2]
EF[7]EM[8,10] $\tilde{D}-\tilde{C}$ 530–590 nm

$\tilde{D}-\tilde{C}$ band origin measured at 18146.8 in emission studies on a cooled beam.[7]

Continuous emission between 570 and 730 nm, with a maximum near 610 nm (16400), has been assigned to the $\tilde{D}-\tilde{C}$ transition.[8,10,12]

Broad, unstructured emission maxima at 370 and 304 nm (27000 and 32900) which appear on ion, electron, or photon impact on SiF_4 have been interpreted as arising from the $\tilde{D}-\tilde{B}$ and $\tilde{D}-\tilde{A}$ transitions of SiF_4^+, respectively.[6,8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiF stretch	743.4(5)	gas	EF	7

τ = 9.30(4) ns gas EF[1]EM[12]
B_0 = 0.136(1)[c] EF[9]

$\tilde{C}\ ^2T_2$ T_d[d] Structure: PE,EF[9]
T_0^a = 33130(100) gas PE[2,3,5]
EF[7]EM[8,10] $\tilde{D}-\tilde{C}$ 530–590 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiF stretch	706.6(5)	gas	PE,EF	3,5,7
e	2	Deformation	159.0(5)	gas	EF	7
t_2	4	Deformation	431.0(5)	gas	PE,EF	3,5,7

A = +6.9(2) EF[7,9,11]
B_0 = 0.132[c] PE,EF[9]

$\tilde{B}\ ^2E$
T_0^a = 22580(100) gas PE[2,3,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiF stretch	685(50)	gas	PE	5

$\tilde{A}\ ^2T_2$ T_d
T_0^a = 17000(1000) gas PE[2,3,5]

$\tilde{X}\ ^2T_1$

[a] Measured with respect to a first ionization potential of 15.19 eV, estimated[4] by extrapolation of the photoionization efficiency curve for SiF_4.
[b] From vertical ionization potential.
[c] From Franck–Condon analysis of the photoelectron spectrum and computer simulation of the $\tilde{D}$–$\tilde{C}$ emission.
[d] Dynamic Jahn–Teller distortion, probably to C_{3v}.[7,9]

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SiF_3Cl^+

$\tilde{G}\ ^2A_1$ C_{3v}
T^a = 59870(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiF_3 stretch	890(40)	gas	PE	1
	3	Deformation	200(40)	gas	PE	1

$\tilde{F}\ ^2E$ C_{3v}
T^a = 44210(320) gas PE[1]

$\tilde{E}\ ^2A_1$ C_{3v}
T^a = 38890(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiF_3 stretch	965(40)	gas	PE	1
	2	SiCl stretch	605(40)	gas	PE	1

$\tilde{D}\ ^2E$ C_{3v}
T^a = 32680(320) gas PE[1]

$\tilde{C}\ ^2E$ C_{3v}
T^a = 26300(320) gas PE[1]

$\tilde{B}\ ^2A_2$ C_{3v}
T^a = 23480(320) gas PE[1]

$\tilde{A}\ ^2A_1$ C_{3v}
T^a = 15250(320) gas PE[1]

$\tilde{X}\ ^2E$ C_{3v}

[a] From vertical ionization potentials.

References

[1]S. Cradock, E. A. V. Ebsworth, and R. A. Whiteford, J. Chem. Soc., Dalton Trans. 2401 (1973).

SiF_3Br^+

$\tilde{G}\ ^2A_1$ C_{3v}
T^a = 67290(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiF_3 stretch	755(40)	gas	PE	1
	3	Deformation	240(40)	gas	PE	1

$\tilde{F}\ ^2E$ C_{3v}
T^a = 51150(320) gas PE[1]

$\tilde{E}\ ^2A_1$ C_{3v}
T^a = 45500(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiF_3 stretch	850(40)	gas	PE	1

$\tilde{D}\ ^2E$ C_{3v}
T^a = 39530(320) gas PE[1]

$\tilde{C}\ ^2E$ C_{3v}
T^a = 33640(320) gas PE[1]

$\tilde{B}\ ^2A_2$ C_{3v}
T^a = 29370(320) gas PE[1]

$\tilde{A}\ ^2A_1$ C_{3v}
T^a = 16860(320) gas PE[1]

$\tilde{X}\ ^2E$ C_{3v}

[a] From vertical ionization potentials.

References

[1]S. Cradock, E. A. V. Ebsworth, and R. A. Whiteford, J. Chem. Soc., Dalton Trans. 2401 (1973).

$SiF_2Cl_2^+$

$\tilde{J}\ ^2B_2$ C_{2v}
T^a = 46300(1000) gas PE[1]

$\tilde{H},\tilde{I}\ ^2B_1,^2A_1$ C_{2v}
T^a = 40580(320) gas PE[1]

$\tilde{G}\ ^2A_1$ C_{2v}
T^a = 34200(1000) gas PE[1]

$\tilde{F}\ ^2B_2$ C_{2v}
T^a = 31000(1000) gas PE[1]

$\tilde{E}\ ^2A_2$ C_{2v}
T^a = 26710(320) gas PE[1]

$\tilde{D}\ ^2B_1$ C_{2v}
T^a = 15330(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		$SiCl_2$ s–stretch	450(20)	gas	PE	1

$\tilde{C}\ ^2A_1$ C_{2v}
T^a = 8070(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		$SiCl_2$ s–stretch	490(20)	gas	PE	1

$\tilde{B}\ ^2B_2$ C_{2v}
T^a = 6210(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		$SiCl_2$ s–stretch	440(20)	gas	PE	1

$\tilde{A}\ ^2A_2$ C_{2v}
T^a = 1450(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]O. Grabandt, C. A. de Lange, R. Mooyman, and P. Vernooijs, Chem. Phys. Lett. **184**, 221 (1991).

$SiFCl_3^+$

$\tilde{E}\ ^2A_1$ C_{3v}
T_0 = 39530(320) gas PE[1]

$\tilde{D}\ ^2E$ C_{3v}
T_0 = 22750(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	$SiCl_3$ umbrella	250(50)	gas	PE	1

$\tilde{C}\ ^2A_1$ C_{3v}
T^a = 15890(320) gas PE[1]

$\tilde{B}\ ^2E$ C_{3v}
T^a = 13150(320) gas PE[1]

$\tilde{A}\ ^2E$ C_{3v}
T^a = 6940(320) gas PE[1]

[a] From vertical ionization potential.

References

[1]O. Grabandt, C. A. de Lange, R. Mooyman, and P. Vernooijs, Chem. Phys. Lett. **184**, 221 (1991).

$SiCl_4^+$

$\tilde{D}\ ^2A_1$ T_d
T_0 = 48900(400) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiCl stretch	290T	gas	PE	3

$\tilde{C}\ ^2T_2$
T_0 = 26620(160) gas PE[1,2]
A broad, unstructured emission with maxima at 410 and 570 nm (24400 and 17500) has been assigned[5,6] to the $\tilde{C}$–$\tilde{X}$ and $\tilde{C}$–$\tilde{A}$ transitions, respectively, of gas-phase $SiCl_4^+$. Using pulsed synchrotron excitation of $SiCl_4$, a radiative lifetime of 38.4(1) ns has been determined[6] for the $\tilde{C}$ state of $SiCl_4^+$.

A broad absorption with maximum at 475 nm (21000) which appears on argon–resonance photolysis of $SiCl_4$ isolated in an argon matrix has been assigned[4] to the $\tilde{C}$–$\tilde{X}$ transition of $SiCl_4^+$. The energy difference is attributed to structural relaxation in the argon matrix. The absorption can be destroyed by exposure of the sample to 290–1000 nm radiation.

$\tilde{B}\ ^2E$
T^a = 13880(400) gas PE[1,2]

$\tilde{A}\ ^2T_2$
T_0 = 7750(160) gas PE[1,2]

$\tilde{X}\ ^2T_1$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		$SiCl_2$ a–stretch	717T	Ar	IR	4

[a] From vertical ionization potential.

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$SiBr_4^+$

$\tilde{D}\ ^2A_1$ T_d
T^a = 50600(320) gas PE[1]

$\tilde{C}\ ^2T_2$ T_d
T^a = 24300(400) gas PE[1]
A broad, unstructured emission with maxima at 435 and 550 nm (23000 and 18200) has been assigned[2] to the $\tilde{C}$–$\tilde{X}$ and $\tilde{C}$–$\tilde{A}$ transitions, respectively, of gas-phase $SiBr_4^+$, excited by electron impact. Using pulsed synchrotron excitation of $SiBr_4$, a radiative lifetime of 47.6(3) ns has been determined[2] for the $\tilde{C}$ state of $SiBr_4^+$.

$\tilde{B}\ ^2E$ T_d
T^a = 10400(320) gas PE[1]

$\tilde{A}\ ^2T_2$ T_d
T^a = 6000(400) gas PE[1]

$\tilde{X}\ ^2T_1$ T_d

[a] From vertical ionization potentials.

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GeF_4^+

$\tilde{D}\ ^2A_1$ T_d
T^{ab} = 45300(1000) gas PE[2,4]
EF[6] $\tilde{D}$–$\tilde{C}$ 390–420 nm
Broad, unstructured emission maxima at 290 and 255 nm (34500 and 39200) which appear on ion impact on GeF_4 have been interpreted as arising from the $\tilde{D}$–$\tilde{B}$ and $\tilde{D}$–$\tilde{A}$ transitions of GeF_4^+, respectively.[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	GeF stretch	644.3	gas	EF	6

Biexponential. τ_1 = 3.1(3) ns, τ_2 = 6.3(4) ns EM[7]

$\tilde{C}\ ^2T_2$ [c]
T_0^a = 20330(240) gas PE[1–4]
EF[6] $\tilde{D}$–$\tilde{C}$ 390–420 nm
$\tilde{D}$–$\tilde{C}$ band origin measured at 25064.0 in emission studies on a cooled beam.[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	GeF stretch	620.8	gas	EF	6
e	2	Deformation	82.8	gas	EF	6
t_2	4	Deformation	288.3	gas	EF	6

A = −18.6[d] EF[6]

$\tilde{B}\ ^2E$
T^{ab} = 11210(320) gas PE[1–4]

$\tilde{A}\ ^2T_2$
T^{ab} = 7020(320) gas PE[1–4]

$\tilde{X}\ ^2T_1$

[a] First ionization potential taken to be 15.69(2) eV, as in Ref. 1.
[b] From vertical ionization potential.
[c] Distorted by Jahn–Teller interaction.
[d] Tentative value.

References

[1]P. J. Bassett and D. R. Lloyd, J. Chem. Soc. A 641 (1971).
[2]S. Cradock, Chem. Phys. Lett. **10**, 291 (1971).
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[6]S. M. Mason and R. P. Tuckett, Mol. Phys. **62**, 979 (1987).
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$GeCl_4^+$

$\tilde{D}\ ^2A_1$ T_d
T_0 = 51070(400) gas PE[1,2]

$\tilde{C}\ ^2T_2$ T_d
T_0 = 21620(240) gas PE[1,2]
A broad, unstructured emission with maxima at 495 and 615 nm (20200 and 16300) has been assigned[3,4] to the $\tilde{C}$–$\tilde{X}$ and $\tilde{C}$–$\tilde{A}$ transitions, respectively, of gas-phase $GeCl_4^+$. Using pulsed synchrotron excitation of $GeCl_4$, a radiative lifetime of 65.4(4) ns has been determined[4] for the $\tilde{C}$ state of $GeCl_4^+$.

$\tilde{B}\ ^2E$
T^a = 9440(240) gas PE[1,2]

$\tilde{A}\ ^2T_2$
T^a = 6130(320) gas PE[1,2]

$\tilde{X}\ ^2T_1$

[a] From vertical ionization potential.

References

[1]J. C. Green, M. L. H. Green, P. J. Joachim, A. F. Orchard, and D. W. Turner, Phil. Trans. Roy. Soc. (London) **A268**, 111 (1970).
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$GeBr_4^+$

$\tilde{D}\ ^2A_1$ T_d
T^a = 53400(1000) gas PE[1]

$\tilde{C}\ ^2T_2$ T_d
T^a = 21660(160) gas PE[1]
A broad, unstructured emission maximum at 475 nm (21000) has been assigned[2] to the $\tilde{C}$–$\tilde{X}$ transition of gas-phase $GeBr_4^+$, excited by Penning ionization in collisions of $GeBr_4$ with He^*. Using pulsed synchrotron excitation of $GeBr_4$, a radiative lifetime of 67(4) ns has been determined[2] for the $\tilde{C}$ state of $GeBr_4^+$.

$\tilde{B}\ ^2E$ T_d
T^a = 7340(160) gas PE[1]

$\tilde{A}\ ^2T_2$ T_d
T^a = 4680(400) gas PE[1]

$\tilde{X}\ ^2T_1$ T_d

[a] From vertical ionization potentials.

References

[1]J. C. Green, M. L. H. Green, P. J. Joachim, A. F. Orchard, and D. W. Turner, Phil. Trans. Roy. Soc. (London) **A268**, 111 (1970).
[2]J. C. Creasey, I. R. Lambert, R. P. Tuckett, and A. Hopkirk, J. Chem. Soc., Faraday Trans. **86**, 2021 (1990).

F_3NO^+

$\tilde{F}\ ^2A_1$ C_{3v}
T^{ab} = 62450(900) gas PE[2]

$\tilde{E}\ ^2E$ C_{3v}
T_0^b = 52770(240) gas PE[2]

$\tilde{C},\tilde{D}\ ^2A_1,^2E$ C_{3v}
T_0^b = 24040(320) gas PE[2]

$\tilde{A},\tilde{B}\ ^2A_2,^2E$ C_{3v}
T_0^b = 11860(560) gas PE[2]

$\tilde{X}\ ^2E$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NO stretch	1025(25)	gas	PE	2

[a] From vertical ionization potential.
[b] The first ionization potential is taken as 13.36(1) eV, the value obtained in the PES study of Ref. 2. The difference between that value and the alternate value of 13.26(1) eV, obtained in the photoionization study of Ref. 1, does not correspond with the excitation of a whole number of vibrational quanta.

References

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[2]P. J. Bassett and D. R. Lloyd, J. Chem. Soc., Dalton Trans. 248 (1972).

F_3NS^+

$\tilde{C}\ ^2A_2$? C_{3v}
T^a = 47200(320) gas PE[1]

$\tilde{B}\ ^2E$ C_{3v}
T^a = 33480(320) gas PE[1]

$\tilde{A}\ ^2A_1$ C_{3v}
T^a = 13310(320) gas PE[1]

$\tilde{X}\ ^2E$ C_{3v}

[a] From vertical ionization potentials.

References

[1]D. O. Cowan, R. Gleiter, O. Glemser, and E. Heilbronner, Helv. Chim. Acta **55**, 2418 (1972).

F_3PO^+

$\tilde{G}\ ^2A_1$ C_{3v}
T^a = 85800(1100) gas PE[1]

$\tilde{F}\ ^2E$ C_{3v}
T_0 = 61240(480) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			654(80)	gas	PE	1

$\tilde{E}\ ^2A_1$ C_{3v}
T^a = 55190(400) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			718(50)	gas	PE	1

$\tilde{D}\ ^2E$ C_{3v}
T_0 = 45830(480) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			718(25)	gas	PE	1

$\tilde{C}\ ^2E$ C_{3v}
$T^a \cong$ 39620 gas PE[1]

$\tilde{B}\ ^2A_2$ C_{3v}
T_0 = 31630(720) gas PE[1]

$\tilde{A}\ ^2A_1$ C_{3v}
T_0 = 19280(640) gas PE[1]

$\tilde{X}\ ^2E$ C_{3v}

[a] From vertical ionization potential.

References

[1]P. J. Bassett and D. R. Lloyd, J. Chem. Soc., Dalton Trans. 248 (1972).

Cl_3PO^+

$\tilde{G}\ ^2A_1$ C_{3v}
T^a = 66080(320) gas PE[1,2]

$\tilde{F}\ ^2E$ C_{3v}
T_0 = 38490(320) gas PE[1-3]

$\tilde{E}\ ^2A_1$ C_{3v}
T_0 = 30180(320) gas PE[1-3]

$\tilde{D}\ ^2E$ C_{3v}
T^a = 20090(320) gas PE[1-3]

$\tilde{C}\ ^2A_1$ C_{3v}
T^a = 17020(320) gas PE[1-3]

$\tilde{B}\ ^2E$ C_{3v}
T^a = 12910(600) gas PE[1-3]
A = 650(240) gas PE[2,3]

$\tilde{A}\ ^2A_2$ C_{3v}
T^a = 8230(320) gas PE[1-3]

$\tilde{X}\ ^2E$ C_{3v}

[a] From vertical ionization potential.

References

[1]P. A. Cox, S. Evans, A. F. Orchard, N. V. Richardson, and P. J. Roberts, Faraday Discuss. Chem. Soc. **54**, 26 (1972).
[2]J. C. Bünzli, D. C. Frost, and C. A. McDowell, J. Electron Spectrosc. Relat. Phenom. **1**, 481 (1972/73).
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Br_3PO^+

$\tilde{F}\ ^2E$ C_{3v}
T^a = 37280(320) gas PE[1-3]

$\tilde{E}\ ^2A_1$ C_{3v}
T_0 = 29210(320) gas PE[1-3]

$\tilde{D}\ ^2E$ C_{3v}
T^a = 15000(500) gas PE[1-3]

$\tilde{C}\ ^2A_1$ C_{3v}
T^a = 13390(320) gas PE[1-3]

$\tilde{B}\ ^2E$ C_{3v}
T^a = 8960(320) gas PE[1-3]
A = 1940(320) gas PE[1-3]

$\tilde{A}\ ^2A_2$ C_{3v}
T^a = 5083(320) gas PE[1-3]

$\tilde{X}\ ^2E$ C_{3v}
A = 890(240) gas PE[1-3]

[a] From vertical ionization potential. The first ionization potential is taken as 10.75(2) eV, the onset of ionization to form Br_3PO^+ ($\tilde{X}\ ^2E_{3/2}$) determined by Ref. 2, and the positions of higher levels are calculated with respect to that energy level.

References

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[2]J. C. Bünzli, D. C. Frost, and C. A. McDowell, J. Electron Spectrosc. Relat. Phenom. **1**, 481 (1972/73).
[3]J. L. Berkosky, F. O. Ellison, T. H. Lee, and J. W. Rabalais, J. Chem. Phys. **59**, 5342 (1973).

F_3PS^+

$\tilde{G}\ ^2E$ C_{3v}
T^a = 72450(320) gas PE[1]

$\tilde{F}\ ^2A_1$ C_{3v}
$T^a \cong$ 70300 gas PE[1]

$\tilde{E}\ ^2A_1$ C_{3v}
T^a = 60110(500) gas PE[1]

$\tilde{D}\ ^2E$ C_{3v}
T^a = 56160(320) gas PE[1]

$\tilde{C}\ ^2E$ C_{3v}
T^a = 46960(500) gas PE[1]

$\tilde{B}\ ^2A_2$ C_{3v}
T^a = 42840(320) gas PE[1]

$\tilde{A}\ ^2A_1$ C_{3v}
T^a = 27350(320) gas PE[1]

$\tilde{X}\ ^2E$ C_{3v}

[a] From vertical ionization potentials.

References

[1]S. Elbel and H. tom Dieck, J. Chem. Soc., Dalton Trans. 1757 (1976).

Cl_3PS^+

$\tilde{G}\ ^2A_1$ C_{3v}
T_0 = 70270(320) gas PE[1-3]

$\tilde{F}\ ^2E$ C_{3v}
T_0 = 46230(320) gas PE[1-4]

$\tilde{E}\ ^2A_1$ C_{3v}
T_0 = 39620(320) gas PE[1-4]

$\tilde{D}\ ^2E$ C_{3v}
T^a = 30340(320) gas PE[1-4]

$\tilde{C}\ ^2E$ C_{3v}
$T^a \cong$ 24400 gas PE[1-4]

$\tilde{B}\ ^2A_1$ C_{3v}
$T^a \cong$ 22400 gas PE[1-4]

$\tilde{A}\ ^2A_2$ C_{3v}
T_0 = 8390(320) gas PE[1-4]

$\tilde{X}\ ^2E$ C_{3v}

[a] From vertical ionization potential.

References

[1]P. A. Cox, S. Evans, A. F. Orchard, N. V. Richardson, and P. J. Roberts, Faraday Discuss. Chem. Soc. **54**, 26 (1972).
[2]J. C. Bünzli, D. C. Frost, and C. A. McDowell, J. Electron Spectrosc. Relat. Phenom. **1**, 481 (1972/73).
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Br_3PS^+

$\tilde{F}\ ^2E$ C_{3v}
T^a = 42520(320) gas PE[1-3]

$\tilde{E}\ ^2A_1$ C_{3v}
T_0 = 34450(320) gas PE[1-3]

$\tilde{D}\ ^2E$ C_{3v}
T^a = 22510(320) gas PE[1-3]

$\tilde{C}\ ^2A_1$ C_{3v}
T^a = 19530(320) gas PE[1-3]

$\tilde{B}\ ^2E$ C_{3v}
T^a = 15170(320) gas PE[1-3]
A = 1780(320) gas PE[1-3]

$\tilde{A}\ ^2A_2$ C_{3v}
T^a = 12180(320) gas PE[1-3]

$\tilde{X}\ ^2E$ C_{3v}

[a] From vertical ionization potential.

References

[1]P. A. Cox, S. Evans, A. F. Orchard, N. V. Richardson, and P. J. Roberts, Faraday Discuss. Chem. Soc. **54**, 26 (1972).
[2]J. C. Bünzli, D. C. Frost, and C. A. McDowell, J. Electron Spectrosc. Relat. Phenom. **1**, 481 (1972/73).
[3]J. L. Berkosky, F. O. Ellison, T. H. Lee, and J. W. Rabalais, J. Chem. Phys. **59**, 5342 (1973).

FSO_3

$\tilde{C}\ ^2E$ C_{3v} Structure: AB[3]
T_0 = 19383.1 gas AB[1-3] $\tilde{C}$–$\tilde{X}$ 360–550 nm
19077(5) Ar AB[4] $\tilde{C}$–$\tilde{X}$ 420–525 nm
18986(5) N_2 AB[4] $\tilde{C}$–$\tilde{X}$ 420–525 nm
Overlapped by continuum beyond 460 nm.[1,6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SO stretch	952.9	gas	AB	2
			947(10)	Ar	AB	4
			966(10)	N_2	AB	4
	2	SF stretch	800.5	gas	AB	2
			796(10)	Ar	AB	4
			820(10)	N_2	AB	4
	3	SO deform.	515.0	gas	AB	2
			512(10)	Ar	AB	4
			511(10)	N_2	AB	4
e	4	SO stretch	1114.5	gas	AB	2
	5	SO deform.	505.7	gas	AB	2
	6	SF wag	346.9	gas	AB	2

A = 66 gas AB[2]
A_0 = 0.172; B_0 = 0.158 AB[3] [a]

$\tilde{B}\ ^2E$ C_{3v}
gas AB[1-3] $\tilde{B}$–$\tilde{X}$ 570–1000 nm

$\tilde{A}\ ^2A_1$ C_{3v}
gas AB[1-3] $\tilde{A}$–$\tilde{X}$ 1000–2000 nm

$\tilde{X}\ ^2A_2$ C_{3v} Structure: AB[1,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SO stretch	1055.5	gas	AB,LF	2,5
			1053vs	Ar	IR	4
	2	SF stretch	839.3	gas	AB,LF	2,5
			833vs	Ar	IR	4
	3	SO deform.	533.5	gas	AB,LF	2,5
			531m	Ar	IR	4
e	4	SO stretch	1177.5	gas	AB,LF	2,5
			1177m	Ar	IR	4
	5	SO deform.	604.1	gas	AB,LF	2,5
			601vw	Ar	IR	4
	6	SF wag	369.4	gas	AB,LF	2,5
			366vw	Ar	IR	4

A_0 = 0.183; B_0 = 0.158 AB[3]

[a] For upper Jahn–Teller potential surface.

References

[1]G. W. King, D. P. Santry, and C. H. Warren, J. Mol. Spectrosc. **32**, 108 (1969).
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[5]C. H. Warren, J. Mol. Spectrosc. **83**, 451 (1980).
[6]A. E. Croce, J. Photochem. Photobiol., A:Chem. **51**, 293 (1990).

$FClO_3^+$

$\tilde{F}\ ^2A_1$ C_{3v}
T^a = 67400(900) gas PE[1]

$\tilde{E}\ ^2E$ C_{3v}
T_0 = 54500(120) gas PE[1]

$\tilde{D}\ ^2E$ C_{3v}
T^a = 33770(200) gas PE[1]

$\tilde{C}\ ^2E$ C_{3v}
T_0 = 19690(100) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ClO_3 stretch	790(40)	gas	PE	1

$\tilde{B}\ ^2A_1$ C_{3v}
T^a = 10850(200) gas PE[1]

$\tilde{A}\ ^2E$ C_{3v}
T_0 = 5930(200) gas PE[1]

$\tilde{X}\ ^2A_2$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ClO_3 stretch	900(40)	gas	PE	1
	3	ClO_3 umbrella	520(40)	gas	PE	1

[a] From vertical ionization potential.

References

[1]R. L. DeKock, D. R. Lloyd, I. H. Hillier, and V. R. Saunders, Proc. Roy. Soc. (London) **A328**, 401 (1972).

$F_2SO_2^+$

$\tilde{G}\ ^2A_1$ C_{2v}
T_0 = 53730(140) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	SF_2 stretch	855(30)	gas	PE	1,3
	3	SO_2 scissors	500(20)	gas	PE	1,3

$\tilde{F}\ ^2B_2$ C_{2v}
T_0 = 49500(140) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	SF_2 stretch	850(30)	gas	PE	1
	3	SO_2 scissors	485(40)	gas	PE	1

$\tilde{E}\ ^2B_1$ C_{2v}
T_0 = 40580(320) gas PE[1-3]

$\tilde{D}\ ^2B_2$ C_{2v}
T_0 = 29340(120) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SO_2 stretch	1135(16)	gas	PE	1–3
	2	SF_2 stretch	805(30)	gas	PE	1–3
	3	SO_2 scissors	510(20)	gas	PE	1–3

$\tilde{C}\ ^2A_1$ C_{2v}
T_0 = 17270(130) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SO_2 stretch	1025(30)	gas	PE	1–3

$\tilde{B}\ ^2B_1$ C_{2v}
T_0 = 14600(160) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4	SF_2 scissors	340(16)	gas	PE	1–3

$\tilde{A}\ ^2A_2$ C_{2v}
T_0 = 4280(240) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	SO_2 scissors	475(60)	gas	PE	1–3

$\tilde{X}\ ^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			370(40)	gas	PE	1

References

[1]R. L. DeKock, D. R. Lloyd, I. H. Hillier, and V. R. Saunders, Proc. Roy. Soc. (London) **A328**, 401 (1972).
[2]G. W. Mines, R. K. Thomas, and H. Thompson, Proc. Roy. Soc. (London) **A329**, 275 (1972).
[3]D. Chadwick, D. C. Frost, F. G. Herring, A. Katrib, C. A. McDowell, and R. A. N. McLean, Can. J. Chem. **51**, 1893 (1973).

$FClSO_2^+$

T^a = 49900(1000) gas PE[1]

T^a = 33800(1000) gas PE[1]

T^a = 32030(320) gas PE[1]

T^a = 19610(320) gas PE[1]

T^a = 16300(320) gas PE[1]

T^a = 12340(320) gas PE[1]

T^a = 6050(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]G. W. Mines, R. K. Thomas, and H. Thompson, Proc. Roy. Soc. (London) **A329**, 275 (1972).

$Cl_2SO_2^+$

T^a = 48970(320) gas PE[1,2]

T^a = 44860(320) gas PE[1,2]

T_0 = 39370(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SO_2 stretch	1170(40)	gas	PE	2
	2	SO_2 scissors	580(40)	gas	PE	2
	3	SCl_2 stretch	380(40)	gas	PE	2
	4	SCl_2 scissors	200(40)	gas	PE	2

T^a = 16540(1000) gas PE[1,2]

T^a = 13640(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			640(40)	gas	PE	2

T_0 = 7660(1000) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			500(40)	gas	PE	2

[a] From vertical ionization potential.

References

[1]G. W. Mines, R. K. Thomas, and H. Thompson, Proc. Roy. Soc. (London) **A329**, 275 (1972).
[2]D. Chadwick, D. C. Frost, F. G. Herring, A. Katrib, C. A. McDowell, and R. A. N. McLean, Can. J. Chem. **51**, 1893 (1973).

BF_4^-

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BF stretch	1197vs Cs	Ar	IR	1
		BF stretch	1014 Cs	Ar	IR	1
		Deformation	524 Cs	Ar	IR	1

References

[1]R. L. Hunt and B. S. Ault, Spectrochim. Acta **37A**, 63 (1981).

BF_3Cl^-

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BF stretch	1210 Cs	Ar	IR	1
		BCl stretch	840 Cs	Ar	IR	1

References

[1]R. L. Hunt and B. S. Ault, Spectrochim. Acta **37A**, 63 (1981).

BCl_4^-

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BCl stretch	766 Cs	Ar	IR	1
		BCl stretch	642 Cs	Ar	IR	1

References

[1]R. L. Hunt and B. S. Ault, Spectrochim. Acta **37A**, 63 (1981).

CF_3O^-

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1514 Cs	Ar	IR	1
		CF stretch	1039 Cs	Ar	IR	1
		CF stretch	919 Cs	Ar	IR	1
		CF stretch	808 Cs	Ar	IR	1
		OCF deform.	555 Cs	Ar	IR	1

References

[1]B. S. Ault, J. Phys. Chem. **84**, 3448 (1980).

$Cl_2CCl–Cl$

A strong, broad absorption with maximum near 415 nm (24000) which appears on argon–resonance photolysis of CCl_4 isolated in an argon matrix was originally assigned[2,3] to the $\tilde{C}–\tilde{X}$ transition of CCl_4^+. Subsequent argon–matrix studies[4] showed that this absorption can also be produced by 220 or 193 nm irradiation of the sample. *Ab initio* calculations are consistent with the alternate assignment of this band and of the associated infrared absorption pattern to $Cl_2CCl–Cl$. The product absorptions are destroyed, and the absorptions of ordinary CCl_4 are intensified, by exposure of the sample to radiation of wavelength longer than 360 nm.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CCl stretch	1019.7m	Ar	IR	1,4
	2	CCl stretch	501.9m	Ar	IR	1,4
	3	Deformation	373.9wm	Ar	IR	1,4
	4	Deformation	291.2wm	Ar	IR	1,4
	5	Cl–Cl stretch	246.4wm	Ar	IR	4
a''	7	CCl stretch	929.1vs	Ar	IR	1,4

References

[1]F. T. Prochaska and L. Andrews, J. Chem. Phys. **67**, 1091 (1977).
[2]L. Andrews and F. T. Prochaska, J. Phys. Chem. **83**, 368 (1979).
[3]L. Andrews, B. J. Kelsall, J. H. Miller, and B. W. Keelan, J. Chem. Soc., Faraday Trans. 2 **79**, 1417 (1983).
[4]G. Maier, H. P. Reisenauer, J. Hu, B. A. Hess, Jr., and L. J. Schaad, Tetrahed. Lett. **30**, 4105 (1989).

Cl_2O_3

An unstructured gas–phase absorption between 220 and 320 nm, with maximum at 37450 (267 nm), has been assigned[2,4,5] to Cl_2O_3.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1225vs	gas	IR	1,4
			1226.1	Ar	IR	3
			1057s	gas	IR	4
			1058.4	Ar	IR	3
			740w	gas	IR	4
			560wm	gas	IR	4

References

[1]A. J. Schell-Sorokin, D. S. Bethune, J. R. Lankard, M. M. T. Loy, and P. P. Sorokin, J. Phys. Chem. **86**, 4653 (1982).
[2]G. D. Hayman and R. A. Cox, Chem. Phys. Lett. **155**, 1 (1989).
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[4]J. B. Burkholder, J. J. Orlando, and C. J. Howard, J. Phys. Chem. **94**, 687 (1990).
[5]J. B. Burkholder, R. L. Mauldin III, R. J. Yokelson, S. Solomon, and A. R. Ravishankara, J. Phys. Chem. **97**, 7597 (1993).

CF_3Cl^-

$\tilde{X}$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		938s	Ar	IR	1,2
		933s	Ar	IR	1,2
		666m	Ar	IR	1,2

References

[1]F. T. Prochaska and L. Andrews, J. Am. Chem. Soc. **100**, 2102 (1978).
[2]F. T. Prochaska and L. Andrews, J. Chem. Phys. **68**, 5577 (1978).

CF_3Br^-

$\tilde{X}$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CF stretch	918s	Ar	IR	1,2
		914s	Ar	IR	1,2
	CF_3 deform.	662m	Ar	IR	1,2

References

[1]F. T. Prochaska and L. Andrews, J. Am. Chem. Soc. **100**, 2102 (1978).
[2]F. T. Prochaska and L. Andrews, J. Phys. Chem. **82**, 1731 (1978).

CF_3I^-

$\tilde{X}$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CF stretch	893m	Ar	IR	1
	CF_3 deform.	660wm	Ar	IR	1

References

[1]F. T. Prochaska and L. Andrews, J. Am. Chem. Soc. **100**, 2102 (1978).

$CF_2Cl_2^-$

$\tilde{X}$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CF_2 a-stretch	1029m	Ar	IR	1
		626m	Ar	IR	1
		564vs	Ar	IR	1

References

[1]F. T. Prochaska and L. Andrews, J. Chem. Phys. **68**, 5577 (1978).

CF_2ClBr^-

$\tilde{X}$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CF_2 a-stretch	1013	Ar	IR	1
		622	Ar	IR	1
		564	Ar	IR	1

References

[1]F. T. Prochaska and L. Andrews, J. Chem. Phys. **68**, 5577 (1978).

$CF_2Br_2^-$

$\tilde{X}$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		1001sT	Ar	IR	1
		554vsT	Ar	IR	1

References

[1]F. T. Prochaska and L. Andrews, J. Phys. Chem. **82**, 1731 (1978).

$CFCl_3^-$

$\tilde{X}$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CF stretch	1056ms	Ar	IR	1
	CCl stretch	776m	Ar	IR	1
		486s	Ar	IR	1
		440ms	Ar	IR	1

References

[1]F. T. Prochaska and L. Andrews, J. Chem. Phys. **68**, 5568 (1978).

$CFBr_3^-$

$\tilde{X}$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CF stretch	1029m	Ar	IR	1
		1019m	Ar	IR	1
	CBr stretch	626m	Ar	IR	1
	Deformation	465s	Ar	IR	1

References

[1]F. T. Prochaska and L. Andrews, J. Phys. Chem. **82**, 1731 (1978).

PF_4^-

$\tilde{X}$ C_{2v} ?

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PF eq. stretch	789 Cs	Ar	IR	1
	2	PF ax. stretch	621 Cs	Ar	IR	1
b_1	6	PF stretch	710 Cs	Ar	IR	1
b_2	8	PF eq. stretch	780 Cs	Ar	IR	1

References

[1]P. Wermer and B. S. Ault, Inorg. Chem. **20**, 970 (1981).

$PClF_3^-$

$\tilde{X}$ C_{2v} ?

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PF eq. stretch	780 Cs	Ar	IR	1
	2	PF ax. stretch	621 Cs	Ar	IR	1
b_2	8	PF eq. stretch	767 Cs	Ar	IR	1

References

[1]P. Wermer and B. S. Ault, Inorg. Chem. **20**, 970 (1981).

SOF_3^-

$\tilde{X}$ C_s ?

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SO stretch	1264m Cs	Ar	IR	1
		SF stretch	695 Cs	Ar	IR	1
		SF stretch	667 Cs	Ar	IR	1
		SF stretch	623 Cs	Ar	IR	1

References

[1]K. Garber and B. S. Ault, Inorg. Chem. **22**, 2509 (1983).

$SClF_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SF eq. stretch	841wm	Ar	IR	1
		SF ax. a–str.	668s	Ar	IR	1
		SF ax. s–str.	606m	Ar	IR	1
		SCl stretch	506m	Ar	IR	1

References

[1]R. Minkwitz, U. Nass, and J. Sawatzki, J. Fluorine Chem. **31**, 175 (1986).

SCl_2F_2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SF ax. stretch	592	Ar	IR,Ra	1
	2	SCl eq. stretch	527	Ar	IR	1
	4	Deformation	162	Ar	Ra	1
b_1	6	SF ax. stretch	770	Ar	IR	1
	7	Deformation	296	Ar	IR,Ra	1
b_2	8	SCl eq. stretch	533	Ar	IR	1
	9	Deformation	274	Ar	IR,Ra	1

References

[1]R. Minkwitz, U. Nass, and J. Sawatzki, J. Fluorine Chem. **31**, 175 (1986).

SCl_3F

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SF stretch	656m	Ar	IR	1
		SCl eq. a–str.	458m	Ar	IR	1
		SCl eq. s–str.	420m	Ar	IR	1
		SCl ax. stretch	332m	Ar	IR	1

References

[1]R. Minkwitz, U. Nass, and J. Sawatzki, J. Fluorine Chem. **31**, 175 (1986).

XeO_2F_2

$\tilde{X}$ C_{2v} Structure: ND[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	XeO stretch	849wm	Ar	IR	1,3
	2	XeF stretch	537w	Ar	IR	3
	3	XeO_2 scissors	331sh	Ar	IR	3
	4	XeF_2 scissors	202w	Ar	IR	3
a_2	5	XeO_2 twist	329sh	Ar	IR	3
b_1	6	XeO stretch	906s	Ar	IR	1,3
b_2	8	XeF stretch	585vs	Ar	IR	1
	9	XeO_2 rock	324m	Ar	IR	1,3

References

[1]H. H. Claassen, E. L. Gasner, H. Kim, and J. L. Huston, J. Chem. Phys. **49**, 253 (1968).
[2]S. W. Peterson, R. D. Willett, and J. L. Huston, J. Chem. Phys. **59**, 453 (1973).
[3]K. O. Christe and W. W. Wilson, Inorg. Chem. **27**, 3763 (1988).

XeF_4^+

$\tilde{I}\ ^2A_{2u}$ D_{4h}
$T^{ab} \cong 57200$ gas PE[1]ESCA[4]

$\tilde{H}\ ^2E_u$ D_{4h}
$T^{ab} \cong 43800$ gas ESCA[4]

$\tilde{G}\ ^2B_{2g}$ D_{4h}
$T^{ab} = 29400(1000)$ gas PE[1]

$\tilde{F}\ ^2E_g$ D_{4h}
$T^{ab} \cong 27000$ gas PE[1]

$\tilde{E}\ ^2B_{2g}$ D_{4h}
$T^{ab} = 25300(1000)$ gas PE[1]

$\tilde{D}\ ^2E_u$ D_{4h}
$T^{ab} \cong 22200$ gas PE[1]

$\tilde{C}\ ^2A_{2g}$ D_{4h}
$T^{ab} = 20100(1000)$ gas PE[1]

$\tilde{B}\ ^2B_{1g}$ D_{4h}
$T^{ab} = 14600(1000)$ gas PE[1]

$\tilde{A}\ ^2A_{1g}$ D_{4h}
$T_0^a = 5890(1000)$ gas PE[1]UV[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1	Sym. stretch	490(80)	gas	PE	1

$\tilde{X}\ ^2A_{2u}$ D_{4h}

[a] The first ionization potential is taken as 12.65(10) eV, as in the photoionization study of Ref. 2.
[b] From vertical ionization potential.

References

[1]C. R. Brundle, G. R. Jones, and H. Basch, J. Chem. Phys. **55**, 1098 (1971).
[2]J. Berkowitz, W. A. Chupka, P. M. Guyon, J. H. Holloway, and R. Spohr, J. Phys. Chem. **75**, 1461 (1971).
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[4]G. M. Bancroft, P.-Å. Malmquist, S. Svensson, E. Basilier, U. Gelius, and K. Siegbahn, Inorg. Chem. **17**, 1595 (1978).

6.12. Six-Atomic Molecules

$LiBH_4$

$\tilde{X}$ C_{3v} Structure: MW[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			700(150)	gas	MW	1
e			400(150)	gas	MW	1

$B_0 = 0.769$ MW[1]

References

[1]Y. Kawashima and E. Hirota, J. Chem. Phys. **96**, 2460 (1992).

$NaBH_4$

$\tilde{X}$ C_{3v} Structure: MW[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			435T	gas	MW	1

$B_0 = 0.322$ MW[1]

References

[1]Y. Kawashima, C. Yamada, and E. Hirota, J. Chem. Phys. **94**, 7707 (1991).

$HCaH_2CaH$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1124.3	Kr	IR	1
			1024.3	Kr	IR	1
			869.7	Kr	IR	1
			596.6	Kr	IR	1

$DCaD_2CaD$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			813.1	Kr	IR	1
			738.6	Kr	IR	1
			628.2	Kr	IR	1

References

[1]Z. L. Xiao, R. H. Hauge, and J. L. Margrave, High Temp. Sci. **31**, 59 (1991).

$CaBH_4$

$\tilde{B}\ ^2E$ C_{3v}
$T_0 = 15426(10)$ gas LF[1] $\tilde{B}$–$\tilde{X}$ 627–669 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		Ca···BH_4 stretch	472(10)	gas	LF	1

$A = 59(10)$ gas LF[1]

$\tilde{A}\ ^2A_1$ C_{3v}
T_0 = 14804(10) gas LF[1] $\tilde{A}$–$\tilde{X}$ 635–720 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		Ca···BH_4 stretch	469(10)	gas	LF	1

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		Ca···BH_4 stretch	455(10)	gas	LF	1

References

[1]F. S. Pianalto, A. M. R. P. Bopegedera, W. T. M. L. Fernando, R. Hailey, L. C. O'Brien, C. R. Brazier, P. C. Keller, and P. F. Bernath, J. Am. Chem. Soc. **112**, 7900 (1991).

$SrBH_4$

$\tilde{B}\ ^2E$ C_{3v}
T_0 = 14430(10) gas LF[1] $\tilde{B}$–$\tilde{X}$ 651–718 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		Sr···BH_4 stretch	408(10)	gas	LF	1

A = 200(10) gas LF[1]

$\tilde{A}\ ^2A_1$ C_{3v}
T_0 = 13723(10) gas LF[1] $\tilde{A}$–$\tilde{X}$ 707–772 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		Sr···BH_4 stretch	404(10)	gas	LF	1

$\tilde{X}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		Sr···BH_4 stretch	388(10)	gas	LF	1

References

[1]F. S. Pianalto, A. M. R. P. Bopegedera, W. T. M. L. Fernando, R. Hailey, L. C. O'Brien, C. R. Brazier, P. C. Keller, and P. F. Bernath, J. Am. Chem. Soc. **112**, 7900 (1990).

$B_2H_4^+$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1300(100)	gas	PI	1

References

[1]B. Ruscic, M. Schwarz, and J. Berkowitz, J. Chem. Phys. **91**, 4576 (1989).

$HFeCH_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		FeH stretch	1684.2	Ar	IR	1
		FeCH rock	540.2	Ar	IR	1
		CFe stretch	524.3	Ar	IR	1

$DFeCD_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		FeD stretch	1210.8	Ar	IR	1
		CFe stretch	480.2	Ar	IR	1

References

[1]J. W. Kauffman, R. H. Hauge, and J. L. Margrave, High Temp. Sci. **17**, 237 (1984).

$HNiCH_3$

Threshold for dissociation into Ni + CH_4 near 400 nm.[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	2950.5	Ar	IR	1
		CH stretch	2861.0	Ar	IR	1
		NiH stretch	1945.1	Ar	IR	1
		CH_3 deform.	1139.0	Ar	IR	1
		CH_3 deform.	1120.3	Ar	IR	1
		CH_3 rock	642.7	Ar	IR	1
		NiC stretch	554.9	Ar	IR	1

$DNiCD_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD stretch	2197.5	Ar	IR	1
		NiD stretch	1406.8	Ar	IR	1
		CD_3 deform.	895.8	Ar	IR	1
		CD_3 deform.	891.9	Ar	IR	1

References

[1]S.-C. Chang, R. H. Hauge, W. E. Billups, J. L. Margrave, and Z. H. Kafafi, Inorg. Chem. **27**, 205 (1988).

SiH_3AlH

In an argon matrix, an absorption maximum at 34200 (292 nm) and a weak, broad absorption with maximum near 19200 (520 nm) have been assigned[1] to SiH_3AlH. Irradiation of the sample at approximately 520 nm leads to the formation of SiH_4 + Al.

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SiH stretch	2116wm	Ar	IR	1
		AlH stretch	1784m	Ar	IR	1
		SiH_3 deform.	842ms	Ar	IR	1

SiD_3AlD

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SiD stretch	1522w	Ar	IR	1
		AlD stretch	1300wm	Ar	IR	1
		SiD_3 deform.	628m	Ar	IR	1

References

[1]M. A. Lefcourt and G. A. Ozin, J. Phys. Chem. **95**, 2623 (1991).

CH_3GaH

In an argon matrix, an absorption with maximum at 45900 (218 nm) behaves appropriately for assignment to CH_3GaH.[1]

In an argon matrix, a weak, broad (100 nm FWHM) absorption at 16700 (600 nm) has also been attributed[1] to CH_3GaH. Irradiation of the sample in the region of this absorption leads to photodestruction of CH_3GaH.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	2970	Ar	IR	1
		CH stretch	2914	Ar	IR	1
		GaH stretch	1719	Ar	IR	1
		CH_3 deform.	1432	Ar	IR	1
		CH_3 deform.	1161	Ar	IR	1
		CH_3 rock	754	Ar	IR	1
		CH_3 rock	642	Ar	IR	1
		GaC stretch	528	Ar	IR	1

CD_3GaD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD stretch	2222	Ar	IR	1
		CD stretch	2137	Ar	IR	1
		GaD stretch	1244	Ar	IR	1
		CD_3 deform.	1026	Ar	IR	1
		CD_3 deform.	899	Ar	IR	1
		CD_3 rock	579	Ar	IR	1
		GaC stretch	484	Ar	IR	1

References

[1]R. D. Lafleur and J. M. Parnis, J. Phys. Chem. **96**, 2429 (1992).

$H_2BNH_2^+$

$\tilde{D}\ ^2A_1$ C_{2v}
T^a = 59100(1200) gas PE[1]

$\tilde{C}\ ^2B_2$ C_{2v}
T^a = 51500(1200) gas PE[1]

$\tilde{B}\ ^2A_1$ C_{2v}
T^a = 26800(1200) gas PE[1]

$\tilde{A}\ ^2B_2$ C_{2v}
T^a = 10300(1200) gas PE[1]

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		BN stretch	1100(80)	gas	PE	1

[a] From vertical ionization potential.

References

[1]N. P. C. Westwood and N. H. Werstiuk, J. Am. Chem. Soc. **108**, 891 (1986).

$C_2H_4^+$

$\tilde{D}\ ^2B_1$ D_2
$T_0 \cong$ 67230 gas PE[1-3]

$\tilde{C}\ ^2B_2$ D_2
T_0 = 42140(350)[a] gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	2	CC stretch	1245(20)	gas	PE	1-3,6

$\tilde{B}\ ^2A$ D_2
T_0 = 31570(200)[a] gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	CH stretch	1900(100)	gas	PE	3

$\tilde{A}\ ^2B_3$ D_2
T_0 = 15600(200)[a] gas PE[2,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	CH stretch	2900(50)	gas	PE	1,3
	2		1150(100)	gas	PE	3
	3		800(100)	gas	PE	1,3

$\tilde{X}\ ^2B_3$ D_2 Structure: PE[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	2	CC stretch	1494(1)[b]	gas	PE	5,6
	3	CH_2 scissors	1261(3)[b]	gas	PE	5,6
	4	Torsion	220HT	gas	PE	5,6

Barrier to inversion = 270(150).[6]

$C_2D_4^+$

$\tilde{D}\ ^2B_1$ D_2
$T_0 \cong$ 66740 gas PE[2,3]

$\tilde{C}\ ^2B_2$ D_2
T_0 = 42050(100)[a] gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	2	CC stretch	1100(80)	gas	PE	2
	3	CD_2 scissors	930(40)	gas	PE	2,3

$\tilde{B}\ ^2A$ D_2
T_0 = 31480(100)[a] gas PE[2,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a			1000(100)	gas	PE	3

$\tilde{A}\ ^2B_3$ D_2
T_0 = 15670(100)[a] gas PE[2,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	CD stretch	2640(100)	gas	PE	3
	2	CC stretch	900(100)	gas	PE	3

$\tilde{X}\ ^2B_3$ D_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	2	CC stretch	1332(8)	gas	PE	4,8
	3	CD_2 scissors	961(8)	gas	PE	4,8
	4	Torsion	23(10)[c]	gas	PE	8

[a] First ionization potential of C_2H_4 taken as 10.517(2) and of C_2D_4 as 10.528(2), from threshold PE study of Ref. 4.
[b] For reassignment see Refs. 7 and 8.
[c] $2\nu_4$ = 269(7).[4,8]

References

[1]A. D. Baker, C. Baker, C. R. Brundle, and D. W. Turner, Int. J. Mass Spectrom. Ion Phys. **1**, 285 (1968).
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$CH_2{=}SiH_2^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_2 deform.	1010(40)	gas	PE	1
		Si=C stretch + SiH_2 deform.	840(40)	gas	PE	1
		Si=C stretch + SiH_2 deform.	620(40)	gas	PE	1
		Torsion	200T	gas	PE	1

$CH_2{=}SiD_2^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Si=C stretch + SiD_2 deform.	770(40)	gas	PE	1
		Si=C stretch + SiD_2 deform.	550(40)	gas	PE	1
		Torsion	120T	gas	PE	1

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[1]P. Rosmus, H. Bock, B. Solouki, G. Maier, and G. Mihm, Angew. Chem. **93**, 616 (1981); Angew. Chem. Int. Ed. Engl. **20**, 598 (1981).

H_2BNH_2

$\tilde{X}$ C_{2v} Structure: MW[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NH stretch	3451	gas	IR	2
			3437	Ar	IR	4
			3439	N_2	IR	4
	2	BH stretch	2495	gas	IR	2
			2499	Ar	IR	4
			2506	N_2	IR	4
	3	NH_2 scissors	1625	gas	IR	2
			1620	Ar	IR	4
			1617	N_2	IR	4
	4	BN stretch	1337.47	gas	IR	2
			1334	Ar	IR	4
			1346	N_2	IR	4
	5	BH_2 scissors	1225	gas	IR	2
a_2	6	Torsion	820T[a]	gas	IR	3
b_1	7	NH_2 wag	1005[b]	gas	IR	2
			1002	Ar	IR	4
			1001	N_2	IR	4
	8	BH_2 wag	612s[b]	gas	IR	3
			608s	Ar	IR	4
			647s	N_2	IR	4
b_2	9	NH stretch	3534	gas	IR	2
			3519	Ar	IR	4
			3523	N_2	IR	4
	10	BH stretch	2564	gas	IR	2
			2568	Ar	IR	4
			2568	N_2	IR	4
	11	NH_2 rock	1131[b]	gas	IR	2
			1120	Ar	IR	4
			1122	N_2	IR	4
	12	BH_2 rock	742vwT[b]	gas	IR	3

A_0 = 4.611; B_0 = 0.917; C_0 = 0.763 MW[1,5]

[a] Value estimated from appearance of perturbation.
[b] Ref. 4 proposes a reassignment of the absorptions below 1250 cm^{-1}.

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$CH_2{=}SiH_2$

In an Ar or N_2 matrix, absorption maximum at 258 nm.[1-4] On irradiation at 254 nm, photoisomerizes to CH_3SiH.[2,4]

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		SiH s-stretch	2219m	Ar	IR	1-3
			2214m	N_2	IR	2,4
		CH_2 scissors	1350w	Ar	IR	2,3
			1350w	N_2	IR	2,4
		Si=C stretch	985w	Ar	IR	1-3
			985w	N_2	IR	1,2,4
		SiH_2 scissors	927w	Ar	IR	1-3
			927w	N_2	IR	2,4
b_1		CH_2 wag	741s	Ar	IR	1-3
			747s	N_2	IR	2,4
b_2		SiH a-stretch	2239m	Ar	IR	1-3
			2235m	N_2	IR	2,4
		CH_2 rock	817s	Ar	IR	1-3
			817s	N_2	IR	2,4

$CH_2{=}SiD_2$

In an Ar matrix, absorption maximum at 259 nm.[1,4]

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		SiD s-stretch	1600m	Ar	IR	1,3
			1600	N_2	IR	4
		CH_2 scissors	1335	Ar	IR	3
			1352	N_2	IR	4
		Si=C stretch	952w	Ar	IR	1,3
			952	N_2	IR	4
b_1		CH_2 wag	719s	Ar	IR	1,3
			725	N_2	IR	4
b_2		SiD a-stretch	1635m	Ar	IR	1,3
			1635	N_2	IR	4
		CH_2 rock	759s	Ar	IR	1,3
			760	N_2	IR	4
		SiD_2 rock	396w	Ar	IR	1,3
			396	N_2	IR	4

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[2]H. P. Reisenauer, G. Mihm, and G. Maier, Angew. Chem. **94**, 864 (1982); Angew. Chem. Int. Ed. Engl. **21**, 854 (1982).
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CH_3SiH

In an Ar matrix, absorption maximum at 480 nm. On irradiation in this spectral region, photoisomerizes to $CH_2{=}SiH_2$. An absorption band with similar behavior appears at 330 nm in N_2-matrix studies.[1,2]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2004m	Ar	IR	1,2
			1986w	N_2	IR	1,2
			1978w	N_2	IR	1,2
			1971m	N_2	IR	1,2
			1935w	Ar	IR	1,2

References

[1]H. P. Reisenauer, G. Mihm, and G. Maier, Angew. Chem. **94**, 864 (1982); Angew. Chem. Int. Ed. Engl. **21**, 854 (1982).
[2]G. Maier, G. Mihm, H. P. Reisenauer, and D. Littmann, Chem. Ber. **117**, 2369 (1984).

$CH_2NH_2^+$

$\tilde{X}\ ^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CN stretch	1810(50)	gas	PE	1
b_1		CH_2 OPLA	1190(50)	gas	PE	1

References

[1]J. M. Dyke, E. P. F. Lee, and M. H. Zamanpour Niavaran, Int. J. Mass Spectrom. Ion Proc. **94**, 221 (1989).

CH_3OH^+

$\tilde{D}\ ^2A'$ C_s
T_0 = 49600(120) gas PE[1-3]

$\tilde{C}\ ^2A''$ C_s
T_0 = 38300(120) gas PE[1-3]

$\tilde{B}\ ^2A'$ C_s
T_0 = 29420(120) gas PE[1-3]

$\tilde{A}\ ^2A'$ C_s
T_0 = 10060(120) gas PE[1-3]

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CH_3 umbrella	1372(80)	gas	PE	2,3
		CO stretch ?	895(80)	gas	PE	1-3

CD_3OD^+

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1030(30)	gas	PE	2
			763(30)	gas	PE	2

References

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[2]K. A. G. MacNeil and R. N. Dixon, J. Electron Spectrosc. Relat. Phenom. **11**, 315 (1977).
[3]L. Karlsson, R. Jadrny, L. Mattsson, F. T. Chau, and K. Siegbahn, Phys. Scripta **16**, 224 (1977).

CH_3SH^+

$\tilde{C}\ ^2A''$ C_s
T^a = 49930(160) gas PE[1-3]

$\tilde{B}\ ^2A'$ C_s
T^a = 34110(160) gas PE[1-3]

$\tilde{A}\ ^2A'$ C_s
T^a = 21280(160) gas PE[1-3]

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CH_3 umbrella	1250(80)	gas	PE	2
		CS stretch	680(40)	gas	PE,PI	1,2,4

[a] From vertical ionization potential. The first ionization potential of CH_3SH is taken as 9.442 eV, as in the photoionization study of Ref. 4.

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SiH_3SH^+

$\tilde{C}\ ^2A'$ C_s
T^a = 35820(320) gas PE[1]

$\tilde{B}\ ^2A''$ C_s
T^a = 20400(1000) gas PE[1]

$\tilde{A}\ ^2A'$ C_s
T^a = 14360(320) gas PE[1]

$\tilde{X}\ ^2A''$ C_s

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, J. Chem. Soc., Faraday Trans. 2 **68**, 281 (1972).

GeH_3SH^+

$\tilde{C}\ ^2A'$ C_s
T^a = 35420(320) gas PE[1]

$\tilde{B}\ ^2A''$ C_s
T^a = 22700(1000) gas PE[1]

$\tilde{A}\ ^2A'$ C_s
T^a = 13720(320) gas PE[1]

$\tilde{X}\ ^2A''$ C_s

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, J. Chem. Soc., Faraday Trans. 2 **68**, 281 (1972).

$N_2H_4^+$

$\tilde{D}\ ^2A$ C_2
T^a = 59600(1000) gas PE[2]

$\tilde{C}\ ^2B$ C_2
T^a = 54460(320) gas PE[1,2]

$\tilde{B}\ ^2A$ C_2
T^a = 45990(320) gas PE[1,2]

$\tilde{A}\ ^2B$ [b] C_2
T^a = 5890(320) gas PE[1,2]

$\tilde{X}\ ^2A$ [b] C_2

[a] From vertical ionization potentials.
[b] Ref. 2 reverses these two assignments.

References

[1]K. Osafune, S. Katsumata, and K. Kimura, Chem. Phys. Lett. **19**, 369 (1973).
[2]V. I. Vovna, F. I. Vilesov, and S. N. Lopatin, Opt. Spectrosk. **38**, 259 (1975); Opt. Spectrosc. **38**, 143 (1975).

$P_2H_4^+$

$\tilde{D},\tilde{E}\ ^2A,^2B$ C_2
T^a = 33730(320) gas PE[1]

$\tilde{C}\ ^2A$ C_2
T^a = 20090(320) gas PE[1]

$\tilde{B}$ C_2
$T^a \cong$ 14600 gas PE[1]

$\tilde{A}\ ^2B$ C_2
T^a = 5570(320) gas PE[1]

$\tilde{X}\ ^2A$ C_2

[a] From vertical ionization potentials.

References

[1]S. Elbel, H. tom Dieck, G. Becker, and W. Ensslin, Inorg. Chem. **15**, 1235 (1976).

SiH_3OH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Si–O stretch	859T	Ar	IR	1

SiD_3OD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Si–O stretch	874T	Ar	IR	1

References

[1]R. Withnall and L. Andrews, J. Phys. Chem. **89**, 3261 (1985).

GeH_3OH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		GeOH bend	924	Ar	IR	1
		GeH_3 deform.	877.2	Ar	IR	1
		GeH_3 deform.	867.6	Ar	IR	1
		Ge–O stretch	688.6	Ar	IR	1
a''		GeH_3 deform.	871.7	Ar	IR	1

GeD_3OD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		Ge–O stretch	710.6	Ar	IR	1
		GeD_3 deform.	623.4	Ar	IR	1
a''		GeD_3 deform.	635	Ar	IR	1

References

[1]R. Withnall and L. Andrews, J. Phys. Chem. **94**, 2351 (1990).

HFe_2NH_2 [a]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		FeH stretch	1687	Ar	IR	1
		FeN stretch	581	Ar	IR	1

[a] ^{15}N.

References

[1]J. W. Kauffman, R. H. Hauge, and J. L. Margrave, High Temp. Sci. **17**, 237 (1984).

CH_2CCH^+

$\tilde{A}$ C_{2v}
$T_0 \cong 13900$ gas PE[1]

CD_2CCH^+

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C≡C stretch ?	2020(150)	gas	PE	1

References

[1]D. W. Minsek and P. Chen, J. Phys. Chem. **94**, 8399 (1990).

BH_3CO^+

$\tilde{C}\ ^2A_1$ C_{3v}
$T_0 = 59220(320)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1660(30)	gas	PE	1

$\tilde{B}\ ^2E$ C_{3v}
$T_0 = 39940(320)$ gas PE[1]

$\tilde{A}\ ^2A_1$ C_{3v}
$T_0 = 20900(240)$ gas PE[1]

$\tilde{X}\ ^2E_{3/2}$ C_{3v}
$A = 4760(320)$ gas PE[1]

References

[1]D. R. Lloyd and N. Lynaugh, J. Chem. Soc., Faraday Trans. 2 **68**, 947 (1972).

CH_2CCH

$T_0 = 30109$[a] gas AB[1] 290–345 nm
Ar AB[2] 288–359 nm
All bands in the gas-phase spectrum are diffuse.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C–C stretch	961(10)	gas	AB	1
			965(10)	Ar	AB	2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3322.29	gas	CC	5
			3308.8m	Ar	IR	2,4
		CCH bend	686.5m[b]	Ar	IR	2
		CCH OPLA bend	510(10)	gas	PE	3
		C_3 deformation	483.5m	Ar	IR	2,4

$B_0 = 0.318$; $C_0 = 0.307$ CC[5]

CD_2CCD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD stretch	2546.8m	Ar	IR	2,4
		CCD bend	552.9m[b]	Ar	IR	2
			479.8	Ar	IR	4

[a] Assignment of gas-phase band origin is tentative. The extension of the progression to 27886 in the argon-matrix study suggests that as many as two quanta of the C–C stretching vibration may be excited in the gas phase band at 30109.
[b] Ref. 4 presents arguments for the reassignment of this absorption to *cyc*-C_3H_3.

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[2]M. E. Jacox and D. E. Milligan, Chem. Phys. **4**, 45 (1974).
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CH_3CN^+

$\tilde{C}\ ^2A_1$ C_{3v}
$T_0 = 38600(1000)$ gas PE[1,4]

$\tilde{B}\ ^2E$ C_{3v}
$T_0 = 26630(320)$ gas PE[1,2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CH_3 umbrella	1440(80)	gas	PE	4
	4	C–C stretch	860(80)	gas	PE	4

Jahn–Teller splitting ≅ 4000 gas PE[4]

$\tilde{A}\ ^2A_1$ C_{3v}
$T_0 = 7580(320)$ gas PE[1,2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CH_3 umbrella	1290(80)	gas	PE	2–4

$\tilde{X}\ ^2E$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C≡N stretch	2010(80)	gas	PE	1–4
	3	CH_3 umbrella	1430(80)	gas	PE	3,4
	4	C–C stretch	810(80)	gas	PE	2–4

CD_3CN^+

$\tilde{B}\ ^2E$ C_{3v}
T_0 = 23720(320) gas PE[2]

$\tilde{A}\ ^2A_1$ C_{3v}
T_0 = 7340(320) gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CD_3 umbrella	970(80)	gas	PE	2,3

$\tilde{X}\ ^2E$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C≡N stretch	1990(80)	gas	PE	2,3
	3	CD_3 umbrella	1070(80)	gas	PE	3
	4	C–C stretch	810(80)	gas	PE	3

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[1]D. C. Frost, F. G. Herring, C. A. McDowell, and I. A. Stenhouse, Chem. Phys. Lett. **4**, 533 (1970).
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$CH_2{=}C{=}NH^+$

$\tilde{B}\ ^2A'$ C_s
T^a = 30340(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	7	CH_2 wag	600(40)	gas	PE	1

$\tilde{A}\ ^2A''$ C_s
T^a = 21220(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CCN a–stretch	1900(40)	gas	PE	1
	5	CCN s–stretch	860(40)	gas	PE	1

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CCN s–stretch	1040(40)	gas	PE	1
		CNH bend	550(40)	gas	PE	1

[a] From vertical ionization potentials.

References

[1]H. W. Kroto, G. Y. Matti, R. J. Suffolk, J. D. Watts, M. Rittby, and R. J. Bartlett, J. Am. Chem. Soc. **112**, 3779 (1990).

CH_3NC^+

$\tilde{C}\ ^2A_1$ C_{3v}
T^a = 55900(1000) gas PE[3]

$\tilde{B}\ ^2E$ C_{3v}
T_0 = 34860(320) gas PE[2,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			770T	gas	PE	2

$\tilde{A}\ ^2E$ C_{3v}
T_0 = 7830(320) gas PE[2,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	N≡C stretch	1870(100)	gas	PE	1–3
	3	CH_3 umbrella	1130(80)	gas	PE	1,2

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	N≡C stretch	2280(80)	gas	PE	1–3
	3	CH_3 umbrella	1410(80)	gas	PE	1–3

CD_3NC^+

$\tilde{B}\ ^2E$ C_{3v}
T^a = 39700(320) gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			730T	gas	PE	2

$\tilde{A}\ ^2E$ C_{3v}
T_0 = 10090(320) gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	N≡C stretch	1820(80)	gas	PE	2
	3	CD_3 umbrella	880(80)	gas	PE	2

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	N≡C stretch	2240(80)	gas	PE	2
	3	CD_3 umbrella	1030(80)	gas	PE	2

[a] From adiabatic ionization potential.

References

[1]D. W. Turner, Phil. Trans. Roy. Soc. (London) **A268**, 7 (1970).
[2]R. F. Lake and H. W. Thompson, Spectrochim. Acta **27A**, 783 (1971).
[3]L. Åsbrink, W. von Niessen, and G. Bieri, J. Electron Spectrosc. Relat. Phenom. **21**, 93 (1980).

CH_3CP^+

$\tilde{C}\ ^2A_1$ C_{3v}
T_0 = 46070(880) gas PE[1]

$\tilde{B}\ ^2E$ C_{3v}
T_0 = 38800(1700) gas PE[1]

$\tilde{A}\ ^2A_2$ C_{3v}
T_0 = 18656(1) gas PE[1]EF[2] $\tilde{A}$–$\tilde{X}$ 530–590 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1230(50)	gas	PE	1

$\tilde{X}\ ^2E$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CP stretch	1503(2)	gas	EF	2

A = −85(2) gas EF[2]

References

[1]N. P. C. Westwood, H. W. Kroto, J. F. Nixon, and N. P. C. Simmons, J. Chem. Soc., Dalton Trans. 1405 (1979).
[2]J. Lecoultre, M. A. King, R. Kuhn, and J. P. Maier, Chem. Phys. Lett. **120**, 524 (1985).

$CaOCH_3$

$\tilde{B}\ ^2A_1$ C_{3v}
T_0 = 17674(5) gas CL[1]LF[1,2] $\tilde{B}$–$\tilde{X}$ 525–590 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CO stretch	1150(5)	gas	LF	1
	4	CaO stretch	491(5)	gas	LF	1,2
e	8	CaOC bend	168(5)	gas	LF	1,2

$\tilde{A}\ ^2E$ C_{3v}
T_0 = 15930(10) gas CL[1]LF[1,2] $\tilde{A}$–$\tilde{X}$ 605–635 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CO stretch	1140(5)	gas	LF	1,2
	4	CaO stretch	500(10)	gas	LF	1,2
e	8	CaOC bend	145(5)	gas	LF	1

A = 68(5) gas LF[1]

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CO stretch	1156(5)	gas	LF	2
	4	CaO stretch	488(5)	gas	LF	1,2
e	8	CaOC bend	144(5)	gas	LF	1,2

$CaOCD_3$

$\tilde{B}\ ^2A_1$ C_{3v}
T_0 = 17674(5) gas LF[1] $\tilde{B}$–$\tilde{X}$ 528–600 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CO stretch	1156(5)	gas	LF	1
	4	CaO stretch	476(5)	gas	LF	1
e	8	CaOC bend	166(5)	gas	LF	1

$\tilde{A}\ ^2E$ C_{3v}
T_0 = 15935(10) gas LF[1] $\tilde{A}$–$\tilde{X}$ 584–630 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CO stretch	1156(5)	gas	LF	1
	4	CaO stretch	480(5)	gas	LF	1
e	8	CaOC bend	140(5)	gas	LF	1

A = 72(5) gas LF[1]

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4	CaO stretch	467(5)	gas	LF	1
e	8	CaOC bend	142(5)	gas	LF	1

References

[1]R. F. Wormsbecher and R. D. Suenram, J. Mol. Spectrosc. **95**, 391 (1982).
[2]C. R. Brazier, L. C. Ellingboe, S. Kinsey-Nielsen, and P. F. Bernath, J. Am. Chem. Soc. **108**, 2126 (1986).

$CaSCH_3$

$\tilde{B}\ ^2A''$ C_s
T_0 = 15807 gas LF[1]

$\tilde{A}\ ^2A'$ C_s
T_0 = 15509 gas LF[1]

References

[1]W. T. M. L. Fernando, R. S. Ram, L. C. O'Brien, and P. F. Bernath, J. Phys. Chem. **95**, 2665 (1991).

$SrOCH_3$

$\tilde{B}\ ^2A_1$ C_{3v}
T_0 = 16069(5)[a] gas CL[1]LF[1,2] $\tilde{B}$–$\tilde{X}$ 603–622 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4	SrO stretch	420(5)	gas	LF	1
e	8	SrOC bend	154(15)	gas	LF	1

$\tilde{A}\ ^2E$ C_{3v}
T_0 = 14658.872 gas CL[1]LF[1-3] $\tilde{A}$–$\tilde{X}$ 627–689 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CO stretch	1140(5)	gas	LF	1,3
	4	SrO stretch	418(5)	gas	LF	1–3

τ = 30(20) ns gas LF[1]
A = 267.5(3) gas LF[1-3]
A_0 = 5.163; B_0 = 0.085 LF[3]

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 deform.	1450(5)	gas	LF	3
	3	CO stretch	1138(5)	gas	LF	2,3
	4	SrO stretch	405(5)	gas	LF	2,3
e	8	SrOC bend	136(5)H	gas	LF	3

$A_0 \cong 5.185$; B_0 = 0.084 LF[3]

$SrOCD_3$

$\tilde{B}\ ^2A_1$ C_{3v}
T_0 = 16069(5) gas LF[1] $\tilde{B}$–$\tilde{X}$ 604–622 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4	SrO stretch	417(5)	gas	LF	1
e	8	SrOC bend	157(15)	gas	LF	1

$\tilde{A}\ ^2E$ C_{3v}
T_0 = 14650(10) gas LF[1] $\tilde{A}$–$\tilde{X}$ 627–690 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CO stretch	1159(5)	gas	LF	1
	4	SrO stretch	401(5)	gas	LF	1

A = 274(5) gas LF[1]

[a] Ref. 2 gives 16098(5).

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[1]R. F. Wormsbecher and R. D. Suenram, J. Mol. Spectrosc. **95**, 391 (1982).
[2]C. R. Brazier, L. C. Ellingboe, S. Kinsey-Nielsen, and P. F. Bernath, J. Am. Chem. Soc. **108**, 2126 (1986).
[3]L. C. O'Brien, C. R. Brazier, and P. F. Bernath, J. Mol. Spectrosc. **130**, 33 (1988).

$SrSCH_3$

$\tilde{C}\ ^2A'$ C_s
T_0 = 15468 gas LF[1]

$\tilde{B}\ ^2A''$ C_s
T_0 = 14780 gas LF[1]

$\tilde{A}\ ^2A'$ C_s
T_0 = 14407 gas LF[1]

References

[1]W. T. M. L. Fernando, R. S. Ram, L. C. O'Brien, and P. F. Bernath, J. Phys. Chem. **95**, 2665 (1991).

$BaOCH_3$

$\tilde{B}\ ^2A_1$ C_{3v}
T_0 = 12923(5) gas CL[1]LF[2]

$\tilde{A}\ ^2E$ C_{3v}
T_0 = 11448(5) gas CL[1]LF[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4	BaO stretch	342(5)	gas	LF	2

A = 660(10) gas LF[2]

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4	BaO stretch	375(5)	gas	LF	2
e	8	BaOC bend	127H	gas	LF	2

References

[1]R. F. Wormsbecher and R. D. Suenram, J. Mol. Spectrosc. **95**, 391 (1982).
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$CH_2{=}C{=}NH$

$\tilde{X}$ C_s Structure: MO^2MW^5

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CCN a-stretch	2043.58	gas	IR	6
			2040vs	Ar	IR	1,3
	5	CCN s-stretch; NH deform.	1124wm	Ar	IR	1,3
	6	NH deform.	1000s	Ar	IR	1,3
	7	H_2CC OPLA	690m	Ar	IR	1,3
a''	11	Torsion	872m	Ar	IR	1,3

$A_0 = 6.719$; $B_0 = 0.322$; $C_0 = 0.316$ $MW^{4,5}IR^6$

$CD_2{=}C{=}ND$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CCN a-stretch	1998vs	Ar	IR	1,3
	5	CD_2 scissors	921m	Ar	IR	1,3
	6	ND deform.	800s	Ar	IR	1,3
a''	11	Torsion	648m	Ar	IR	1,3

References

[1]M. E. Jacox and D. E. Milligan, J. Am. Chem. Soc. **85**, 278 (1963).
[2]A. C. Hopkinson, M. H. Lien, K. Yates, P. G. Mezey, and I. G. Csizmadia, J. Chem. Phys. **67**, 517 (1977).
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[6]F. Ito, T. Nakanaga, K. Sugawara, H. Takeo, M. Sugie, C. Matsumura, and Y. Hamada, J. Mol. Spectrosc. **140**, 177 (1990).

$HC{\equiv}CNH_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C≡C stretch	2162	Ar	IR	1

References

[1]C. Wentrup, H. Briehl, P. Lorencak, U. J. Vogelbacher, H.-W. Winter, A. Maquestiau, and R. Flammang, J. Am. Chem. Soc. **110**, 1337 (1988).

CH_3CP

$\tilde{X}$ C_{3v} Structure: MW^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C≡P stretch	1558.74	gas	IR	2,3
e	6	CH_3 deform.	1437.47	gas	IR	4

$B_0 = 0.166$ MW^1

CD_3CP

$\tilde{X}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C≡P stretch	1554.96	gas	IR	2

$B_0 = 0.143$ MW^1

References

[1]H. W. Kroto, J. F. Nixon, and N. P. C. Simmons, J. Mol. Spectrosc. **77**, 270 (1979).
[2]K. Ohno, Y. Yamamoto, H. Matsuura, and H. Murata, Chem. Lett. 413 (1984).
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$HCr(OH)_2$ [a]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CrH stretch	1601.8	Ar	IR	1
		OCrO stretch	735.7	Ar	IR	1

$DCr(OD)_2$ [a]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OCrO stretch	721	Ar	IR	1

[a] Alternatively, peaks may be contributed by an $H_xCr(OH)_2$ species with $x > 1$.

References

[1]J. W. Kauffman, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **89**, 3541 (1985).

CH_3CO

A broad, unstructured gas-phase absorption between 200 and 240 nm, with maximum near 215 nm, has been attributed[2,3] to CH_3CO.

$\tilde{A}$

A broad, unstructured gas-phase absorption with onset near 700 nm and maximum near 550 nm has been attributed[4] to CH_3CO. In an argon matrix,[5] the threshold for the photodecomposition of CH_3CO into CH_3 + CO lies near 600 nm.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch[a]	1875m	Ar[b]	IR	5
			1842m	Ar[b]	IR	1,5
		CH_3 deform.	1420wm	Ar[b]	IR	5
		CH_3 deform.	1329wm	Ar[b]	IR	1,5

CD_3CO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1855m	Ar[b]	IR	5

[a] Fermi resonance with overtone or combination band.
[b] In Ref. 1, LiCl trapped in nearby site; in Ref. 5, HF trapped in nearby site.

References

[1]J. S. Shirk, Ph.D. Thesis, Univ. of California, Berkeley (1966); J. S. Shirk and G. C. Pimentel, J. Am. Chem. Soc. **90**, 3349 (1968).
[2]H. Adachi, N. Basco, and D. G. L. James, Chem. Phys. Lett. **59**, 502 (1978).
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[4]H. E. Hunziker, unpublished data.
[5]M. E. Jacox, Chem. Phys. **69**, 407 (1982).

CH_2CHO

$\tilde{B}\ ^2A''$ C_s
T_0 = 28784.09(1) gas AB[1]LF[2,4,6] $\tilde{B}$–$\tilde{X}$ 300–405 nm
The failure to detect fluorescence on excitation above 30000 suggests[2] the onset of predissociation near 330 nm. In the argon matrix experiments,[5] the threshold for the photodecomposition of CH_2CHO to produce CH_3 + CO was observed between 280 and 300 nm.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1122	gas	LF	2,6
			917	gas	LF	2,6
		CCO bend	450	gas	LF	2,6

τ = 0.84(13) μs gas LF[2]AB[3]
A_0 = 2.103(4); B_0 = 0.344(1); C_0 = 0.296(1) LF[6]

$\tilde{A}\ ^2A'$ C_s
T_0 = 8006 gas AB[3] $\tilde{A}$–$\tilde{X}$ 1000–1250 nm

$\tilde{X}$ C_s Structure: MW[8,9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CH_2 scissors	1558m HF	Ar	IR	5
		C=O stretch	1540	gas	LF	2,6
			1542m[a] HF	Ar	IR	5
			1525m			
		OCH deform.	1375m HF	Ar	IR	5
		CC stretch	1143	gas	LF,PD	2,6,7
		CCO bend	496[b]	gas	LF,PD	2,6,7
a''			765ms HF	Ar[c]	IR	5
			723m HF	Ar[c]	IR	5
			692ms HF	Ar[c]	IR	5
		Torsion	100[c]	gas	PD	7

A_0 = 2.224; B_0 = 0.382; C_0 = 0.326 LF[6]MW[8]

CD_2CDO

$\tilde{B}\ ^2A''$ C_s
T_0 = 28840 gas LF[2] $\tilde{B}$–$\tilde{X}$ 335–411 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			980	gas	LF	2
			768	gas	LF	2

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		C=O stretch	1540	gas	LF	2
			1513ms HF	Ar	IR	5
			1223w HF	Ar	IR	5
		CC stretch	1050	gas	LF	2
		CCO bend	445[b]	gas	LF	2

A_0 = 1.442; B_0 = 0.336; C_0 = 0.272 MW[9]

[a] Fermi resonance with overtone of 765-cm^{-1} fundamental.
[b] Ref. 2 attributed a band displaced by approximately 950 cm^{-1} in the fluorescence spectrum of CH_2CHO, with a counterpart near 800 cm^{-1} in the fluorescence spectrum of CD_2CDO, to a H–deformation fundamental of a'' symmetry. However, measurements of Ref. 6 for CH_2CHO support reassignment to the first overtone of the CCO bend, which has a rather large anharmonic constant.
[c] The tentative assignment[7] of the torsional fundamental at 100 cm^{-1} would require that one of these three argon–matrix absorptions not be a fundamental of a'' symmetry. A possible alternate assignment of that peak would be to the CH_2 in–plane rocking vibration.

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CH_3NO^+

$\tilde{D},\tilde{E}\ ^2A',^2A''$ C_s
T^a = 58300(1200) gas PE[1,3–5]

$\tilde{C}\ ^2A'$ C_s
T^a = 49400(1200) gas PE[1,4,5]

$\tilde{B}\ ^2A''$ C_s
T^a = 37300(1200) gas PE[1–5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		NO stretch	1900T	gas	PE	3

$\tilde{A}\ ^2A'$ C_s
T^a = 33200 gas PE[1–5]

$\tilde{X}\ ^2A'$ C_s

[a] From vertical ionization potentials.

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CH_2NOH^+

$\tilde{F}\ ^2A''$ C_s
T^a = 62200(1000) gas PE[2]

$\tilde{E}\ ^2A'$ C_s
T^a = 55800(1000) gas PE[2]

$\tilde{D}\ ^2A'$ C_s
T^a = 44500(1000) gas PE[2]

$\tilde{C}\ ^2A'$ C_s
T^a = 34290(320) gas PE[2,3]

$\tilde{B}\ ^2A''$ C_s
T^a = 29370(320) gas PE[1–3]

$\tilde{A}\ ^2A'$ C_s
T^a = 4280(320) gas PE[1–3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CNO bend	444(80)	gas	PE	3

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		NO stretch	928(80)	gas	PE	3

[a] From vertical ionization potentials.

References

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$HCONH_2^+$

$\tilde{E}\ ^2A'$ C_s
$T^a \cong$ 71600 gas PE[1]

$\tilde{D}\ ^2A'$ C_s
T_0 = 48650(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1100(30)	gas	PE	1

$\tilde{C}\ ^2A''$ C_s
T_0 = 36230(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1050(30)	gas	PE	1

$\tilde{B}\ ^2A'$ C_s
T_0 = 29290(320) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		1090(30)	gas	PE	1

$\tilde{A}\ ^2A''$ C_s
T^a = 3150(320) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		640(30)	gas	PE	1

$\tilde{X}\ ^2A'$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	CO stretch	1600(30)	gas	PE	1

[a] From vertical ionization potential.

References

[1]C. R. Brundle, D. W. Turner, M. B. Robin, and H. Basch, Chem. Phys. Lett. **3**, 292 (1969).

$HCSNH_2^+$

$\tilde{G}\ ^2A'$ C_s
T^a = 82400(1000) gas PE[2]

$\tilde{F}\ ^2A'$ C_s
T^a = 72700(1000) gas PE[2]

$\tilde{E}\ ^2A'$ C_s
T^a = 55110(320) gas PE[2]

$\tilde{D}\ ^2A'$ C_s
T^a = 44100(600) gas PE[2]

$\tilde{C}\ ^2A''$ C_s
T^a = 36390(320) gas PE[1,2]

$\tilde{B}\ ^2A'$ C_s
T^a = 33400(320) gas PE[1,2]

$\tilde{A}\ ^2A''$ C_s
T_0 = 4110(320) gas PE[1,2]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		730(80)	gas	PE	1,2

$\tilde{X}\ ^2A'$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		1460(80)	gas	PE	1,2

[a] From vertical ionization potential.

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$CH_2{=}CHF^+$

$\tilde{F}\ ^2A'$ C_s
T_0 = 76410(320) gas PE[2,3]

$\tilde{E}\ ^2A'$ C_s
T^a = 61320(320) gas PE[1-3]

$\tilde{C},\tilde{D}\ ^2A'',^2A'$ C_s
T^a = 51560(320) gas PE[1-3]

$\tilde{B}\ ^2A'$ C_s
T^a = 33810(320) gas PE[1-3]

$\tilde{A}\ ^2A'$ C_s
T^a = 27670(320) gas PE[1-3]

$\tilde{X}\ ^2A''$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	C=C stretch	1570(80)	gas	PE	1,2
	CF stretch	1300(80)	gas	PE	1,2
	HCF bend	500(80)	gas	PE	1,2

[a] From vertical ionization potential.

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$CH_2{=}CHCl^+$

$\tilde{F}\ ^2A'$ C_s
T^a = 70600(1000) gas PE[1-3]

$\tilde{E}\ ^2A'$ C_s
T^a = 50830(320) gas PE[1-3]

$\tilde{D}\ ^2A'$ C_s
T^a = 43410(320) gas PE[1-3]

$\tilde{C}\ ^2A'$ C_s
T^a = 28640(500) gas PE[1-3]

$\tilde{B}\ ^2A''$ C_s
T^a = 25250(320) gas PE[1-3]

$\tilde{A}\ ^2A'$ C_s
T_0 = 13400(500) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CH_2 scissors	1130(80)	gas	PE	2,3
		HCCl bend	440(80)	gas	PE	2,3

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		C=C stretch	1300(80)	gas	PE	1-3
		CCl stretch	820(80)	gas	PE	1-3
		HCCl bend	350(80)	gas	PE	1-3

[a] From vertical ionization potential.

References

[1]R. F. Lake and H. Thompson, Proc. Roy. Soc. (London) **A315**, 323 (1970).
[2]G. W. Mines and H. W. Thompson, Spectrochim. Acta **A29**, 1377 (1973).
[3]K. Wittel and H. Bock, Chem. Ber. **107**, 317 (1974).

CH_2CHO^-

Dipole-Bound State C_s
T_0 = 14712.747(5) gas PD[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		C-C stretch	1143	gas	PD	2
		CCO bend	499	gas	PD	2
a''		Torsion	102H	gas	PD	2

A_0 = 2.221(2); B_0 = 0.376; C_0 = 0.320 PD[2,3]

$\tilde{X}$ C_s Structure: PD[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CCO bend	525.82	gas	PD	2,3
a''		Torsion	375T	gas	PD	2

A_0 = 2.494; B_0 = 0.362; C_0 = 0.316 PD[2,3]

CD_2CDO^-

Dipole-Bound State C_s
T_0 = 14665.97(5) gas PD[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1382(10)	gas	PD	1
			981(10)	gas	PD	1
		CCO bend	437(10)	gas	PD	1
a''		Torsion	80HT	gas	PD	1

A_0 = 1.419(3); B_0 = 0.330; C_0 = 0.268 PD[2]

$\tilde{X}$ C_s
A_0 = 1.554(1); B_0 = 0.319; C_0 = 0.264 PD[2]

References

[1]R. L. Jackson, P. C. Hiberty, and J. I. Brauman, J. Chem. Phys. **74**, 3705 (1981).
[2]R. D. Mead, K. R. Lykke, W. C. Lineberger, J. Marks, and J. I. Brauman, J. Chem. Phys. **81**, 4883 (1984).
[3]A. S. Mullin, K. K. Murray, C. P. Schulz, D. M. Szaflarski, and W. C. Lineberger, Chem. Phys. **166**, 207 (1992).

CH_3NO

$\tilde{X}$ C_s Structure: MW[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CH_3 a-stretch	2991wm	Ar	IR	2
		CH_3 s-stretch	2901wm	Ar	IR	2
		N=O stretch	1564	gas	IR	1
			1549s	Ar	IR	2
		CH_3 a-deform.	1410s	Ar	IR	2
		CH_3 s-deform.	1348s	Ar	IR	2
		CH_3 rock	967w	Ar	IR	2
		C-N stretch	842	gas	IR	1
			870m	Ar	IR	2
		CNO bend	574wm	Ar	IR	2
a''		CH_3 a-stretch	2955w	Ar	IR	2
		CH_3 a-deform.	1410s	Ar	IR	2
		CH_3 rock	916wm	Ar	IR	2

References

[1]W. Lüttke, Z. Elektrochem. **61**, 302 (1957).
[2]A. J. Barnes, H. E. Hallam, S. Waring, and J. R. Armstrong, J. Chem. Soc., Faraday Trans. 2 **72**, 1 (1976).
[3]P. H. Turner and A. P. Cox, J. Chem. Soc., Faraday Trans. 2 **74**, 533 (1978).

CH_2NOH

$\tilde{X}$ C_s Structure: MW[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3650.29vs	gas	IR	1,4,7
	2	CH_2 stretch	3109.72w	gas	IR	1,4,7
	3	CH_2 stretch	2973.17wm	gas	IR	1,4,7
	4	C=N stretch	1647wm	gas	IR	1,4

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	5	CH_2 scissors	1410ms	gas	IR	1,4
	6	OH bend	1318vs	gas	IR	1,4
	7	CH_2 rock	1166m	gas	IR	1,4
	8	NO stretch	892.6s	gas	IR	1,4,6
	9	CNO deform.	530w	gas	IR	1,4
a"	10	CH_2 OPLA	952.61s	gas	IR	1,4,6
	11	CH_2 torsion	774.1m	gas	IR	1,4,6
	12	OH torsion	400T	gas	IR	1,4

A_0 = 2.258; B_0 = 0.396; C_0 = 0.336 MW[2,3,5,8]

References

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[2]I. N. Levine, J. Mol. Spectrosc. **8**, 276 (1962).
[3]I. N. Levine, J. Chem. Phys. **38**, 2326 (1963).
[4]A. Azman, D. Hadzi, J. Kidric, B. Orel, and C. Trampuz, Spectrochim. Acta **27A**, 2499 (1970).
[5]V. K. Kaushik and K. Takagi, J. Phys. Soc. Japan **45**, 1975 (1978).
[6]G. Duxbury, R. M. Percival, D. Devoy, and M. R. M. Mahmoud, J. Mol. Spectrosc. **132**, 380 (1988).
[7]G. Duxbury, J. Mol. Spectrosc. **132**, 393 (1988).
[8]A. Klesing and D. H. Sutter, Z. Naturforsch. **45A**, 817 (1990).

$CH_2{=}SiHCl$

In an Ar or N_2 matrix, an absorption maximum appears at 255 nm. On 254–nm irradiation, photoisomerization to CH_3SiCl occurs.[1,2]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SiH stretch	2230w	Ar	IR	1,2
			2230w	N_2	IR	1,2
			984m	Ar	IR	1,2
			980m	N_2	IR	1,2
			843s	Ar	IR	1,2
			840s	N_2	IR	1,2
			699w	Ar	IR	1,2
			544m	Ar	IR	1,2
			539w	Ar	IR	1,2

References

[1]H. P. Reisenauer, G. Mihm, and G. Maier, Angew. Chem. **94**, 864 (1982); Angew. Chem. Int. Ed. Engl. **21**, 854 (1982).
[2]G. Maier, G. Mihm, H. P. Reisenauer, and D. Littmann, Chem. Ber. **117**, 2369 (1984).

CH_3SiCl

In an Ar matrix, an absorption maximum appears at 407 nm. A similar band appears at 387 nm in a N_2 matrix. On irradiation of the sample in this absorption region, photoisomerization to $CH_2{=}SiHCl$ occurs.[1,2]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1223m	Ar	IR	1,2
			1220	N_2	IR	2
			485m	Ar	IR	1,2
			480w	Ar	IR	1,2

References

[1]H. P. Reisenauer, G. Mihm, and G. Maier, Angew. Chem. **94**, 864 (1982); Angew. Chem. Int. Ed. Engl. **21**, 854 (1982).
[2]G. Maier, G. Mihm, H. P. Reisenauer, and D. Littmann, Chem. Ber. **117**, 2369 (1984).

CH_3O_2

An unstructured gas–phase absorption between 200 and 300 nm, with a maximum at 235 nm, has been assigned[1,3,4,6,7,9] to CH_3O_2. In the gas phase, CH_3O_2 photolyzes on exposure to 248–nm radiation,[8] and, in an argon matrix, on exposure to 254–nm radiation.[5]

$\tilde{A}\ ^2A'$ C_s
T_0 = 7375(6) gas AB[2] $\tilde{A}$–$\tilde{X}$ 7375–9149 cm^{-1}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		OO stretch	896(9)	gas	AB	2

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CH_3 deform.	1453(2)	Ar	IR	5
	4	CH_3 deform.	1440(2)	Ar	IR	5
	5	CH_3 rock	1183(2)	Ar	IR	5
	6	OO stretch	1112(2)	Ar	IR	5
	7	CO stretch	902(2)	Ar	IR	5
	8	COO bend	492(2)	Ar	IR	5
a"	9	CH_3 stretch	2968(2)	Ar	IR	5
	10	CH_3 deform.	1414(2)	Ar	IR	5
	11	CH_3 rock	1120T	Ar	IR	5

CD_3O_2

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		OO stretch	1146(2)	Ar	IR	5
		CD_3 deform.	1048(2)	Ar	IR	5
		CO stretch	821(2)	Ar	IR	5
		COO bend	445(2)	Ar	IR	5
a"	9	CD_3 stretch	2176(2)	Ar	IR	5
	10	CD_3 deform.	1078(2)	Ar	IR	5
	11	CD_3 rock	860(2)	Ar	IR	5

References

[1]D. A. Parkes, D. M. Paul, C. P. Quinn, and R. C. Robson, Chem. Phys. Lett. **23**, 425 (1973).
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[8]D. Hartmann, J. Karthäuser, and R. Zellner, J. Phys. Chem. **94**, 2963 (1990).
[9]M. M. Maricq and T. J. Wallington, J. Phys. Chem. **96**, 986 (1992).

CH_3S_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		SS stretch	*610(160)*	gas	PE	1

CD_3S_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		SS stretch	610(140)	gas	PE	1

References

[1]S. Moran and G. B. Ellison, J. Phys. Chem. **92**, 1794 (1988).

CH_3OF^+

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OF stretch	950(100)	gas	PI	1

References

[1]B. Ruscic, E. H. Appelman, and J. Berkowitz, J. Chem. Phys. **95**, 7957 (1991).

CH_3OCl^+

$\tilde{F}\ ^2A'$ C_s
T^a = 54140(560) gas PE[1]

$\tilde{D}, \tilde{E}\ ^2A'', ^2A'$ C_s
T^a = 45670(560) gas PE[1]

$\tilde{C}\ ^2A'$ C_s
T^a = 25250(560) gas PE[1]

$\tilde{B}\ ^2A''$ C_s
T^a = 21700(560) gas PE[1]

$\tilde{A}\ ^2A'$ C_s
T^a = 10890(320) gas PE[1]

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		OCl stretch	710(50)	gas	PE	1

[a] From vertical ionization potential.

References

[1]D. Colbourne, D. C. Frost, C. A. McDowell, and N. P. C. Westwood, J. Electron Spectrosc. Relat. Phenom. **23**, 109 (1981).

$CH_3S_2^-$

Threshold for electron detachment from ground-state $CH_3S_2^-$ = 14180(180) gas PE[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		SS stretch	530(220)	gas	PE	1

$CD_3S_2^-$

Threshold for electron detachment from ground-state $CD_3S_2^-$ = 14100(180) gas PE[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		SS stretch	500(230)	gas	PE	1

References

[1]S. Moran and G. B. Ellison, J. Phys. Chem. **92**, 1794 (1988).

CH_3OF

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_3 stretch	2991s	gas	IR	1
		CH_3 stretch	2914m	gas	IR	1
		CH_3 stretch ?	2803w	gas	IR	1
		CH_3 deform.	1479m	gas	IR	1
		CH_3 deform.	1476m	gas	IR	1

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_3 deform.	1418m	gas	IR	1
		CH_3 rock	1188m	gas	IR	1
		Skel. stretch	994m	gas	IR	1
		Skel. stretch	824.5s	gas	IR	1

References

[1]M. Kol, S. Rozen, and E. Appelman, J. Am. Chem. Soc. **113**, 2648 (1991).

$ClCH_2OH$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3591	Ar	IR	1
		CH_2 a–stretch	2981	Ar	IR	1
			2971			
		CH_2 s–stretch	2913	Ar	IR	1
		COH bend	1374	gas	IR	2
			1393	Ar	IR	1
		CH_2 wag	1318	gas	IR	2
			1323	Ar	IR	1
			1319			
			1231	Ar	IR	1
		CH_2 twist	1114	Ar	IR	1
		CO stretch	1083	gas	IR	2
			1096	Ar	IR	1
		CH_2 rock	959	gas	IR	2
			959	Ar	IR	1
		CCl stretch	669	Ar	IR	1
		ClCO deform.	469	Ar	IR	1
			463			
		OH torsion	372	Ar	IR	1
			368			

References

[1]H. Kunttu, M. Dahlqvist, J. Murto, and M. Räsänen, J. Phys. Chem. **92**, 1495 (1988).
[2]G. S. Tyndall, T. J. Wallington, M. D. Hurley, and W. F. Schneider, J. Phys. Chem. **97**, 1576 (1993).

CH_3IO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_3 s–stretch	2945	Ar	IR	1
		CH_3 deform.	1400s	Ar	IR	1
		CH_3 deform.	1223ms	Ar	IR	1
		CH_3 rock	859m	Ar	IR	1
		CH_3 rock	848m	Ar	IR	1
		IO stretch	724vs	Ar	IR	1
		CI stretch	497w	Ar	IR	1

CD_3IO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD_3 s–stretch	2132	Ar	IR	1
		CD_3 deform.	939	Ar	IR	1
		IO stretch	723	Ar	IR	1
		CD_3 rock	646	Ar	IR	1
		CD_3 rock	640	Ar	IR	1
		CI stretch	460	Ar	IR	1

References

[1]M. Hawkins and L. Andrews, Inorg. Chem. **24**, 3285 (1985).

CH_3OI

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1074	Ar	IR	1
		OI stretch	528	Ar	IR	1

CD_3OI

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OI stretch	509	Ar	IR	1

References

[1]M. Hawkins and L. Andrews, Inorg. Chem. **24**, 3285 (1985).

ICH_2OH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3350	Ar	IR	1
		CH stretch	2937	Ar	IR	1
		CH stretch	2815	Ar	IR	1
		CH_2 deform.	1466	Ar	IR	1
		CO stretch	999	Ar	IR	1

ICD_2OD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OD stretch	2478	Ar	IR	1
		CD stretch	2234	Ar	IR	1
		CD stretch	2063	Ar	IR	1
		CO stretch	972	Ar	IR	1
		CD deform.	845	Ar	IR	1

References

[1]M. Hawkins and L. Andrews, Inorg. Chem. **24**, 3285 (1985).

NH_2NHF

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		HNF wag	1311s HF	Ar	IR	1
		HNF rock	1282s HF	Ar	IR	1
		NH_2 wag	1091w HF	Ar	IR	1
		NF stretch	1013w,br HF	Ar	IR	1

References

[1]R. Lascola, R. Withnall, and L. Andrews, Inorg. Chem. **27**, 642 (1988).

CH_3ClF

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ClF stretch	599vs	Ar	IR	1

CD_3ClF

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ClF stretch	595vs	Ar	IR	1

References

[1]M. E. Jacox, J. Chem. Phys. **83**, 3255 (1985).

CH_3BrF

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BrF stretch	538vs 533vs	Ar	IR	1

CD_3BrF

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BrF stretch	536vs	Ar	IR	1

References

[1]M. E. Jacox, J. Chem. Phys. **83**, 3255 (1985).

CH_3IF

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		IF stretch	520s	Ar	IR	1

CD_3IF

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		IF stretch	518s	Ar	IR	1

References

[1]M. E. Jacox, J. Chem. Phys. **83**, 3255 (1985).

PH_3F_2

$\tilde{X}$ D_{3h} Structure: IR[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	3	PH_3 deform.	1266.15w	gas	IR	1,3
	4	PF_2 a–stretch	755.99vs	gas	IR	1,3
			755	Ar	IR	2
e'	5	PH_3 a–stretch	2501.7m[a]	gas	IR	1,3
			2480w,br	Ar	IR	2
	6	PH_3 deform.	965.45s[b]	gas	IR	1,3
			974	Ar	IR	2
	7	PF_2 deform.	341.55	gas	IR	4

A_0 = 2.868(15); B_0 = 0.159 gas IR[3,4]

PD_3F_2

$\tilde{X}$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	4	PF_2 a-stretch	749	Ar	IR	2
e'	6	PD_3 deform.	719	Ar	IR	2

[a] Effective value; deperturbed value = 2488.48.
[b] Deperturbed value.

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[1]F. Seel and K. Velleman, Z. Anorg. Allg. Chem. **385**, 123 (1971).
[2]L. Andrews and R. Withnall, Inorg. Chem. **28**, 494 (1989).
[3]H. Beckers, J. Breidung, H. Bürger, R. Kuna, A. Rahner, W. Schneider, and W. Thiel, J. Chem. Phys. **93**, 4603 (1990).
[4]H. Beckers, H. Bürger, and A. Rahner, J. Mol. Spectrosc. **151**, 197 (1992).

AsH_3F_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			894w	Ar	IR	1
		AsF a-stretch	610s	Ar	IR	1

AsD_3F_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			644	Ar	IR	1
			583	Ar	IR	1

References

[1]L. Andrews and T. C. McInnis, Inorg. Chem. **30**, 2990 (1991).

$C_4H_2^+$

$\tilde{B}$
T_0 = 51960(160) gas PE[2]

$\tilde{A}\ ^2\Pi_u$ $D_{\infty h}$ Structure: LF[9]
T_0 = 19722.610(2) gas $EM^1EF^7LF^{7,9}$ $\tilde{A}$–$\tilde{X}$ 485–650 nm
19708(2) Ne LF^4 $\tilde{A}$–$\tilde{X}$ 443–604 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	CH stretch	2858	gas	EM	1
			2821(2)	Ne	LF	4
	2	C≡C stretch	1860(40)	gas	PE	2
			2002(2)	Ne	LF	4
	3	C–C stretch	820(10)[a]	gas	PE,EF	2,3
			807(2)	Ne	LF	4
Π_g	7	Skel. deform.	430[ab]	Ne	LF	4

τ = 72(3) ns gas $EF^3PEFCO^5LF^6$
A = −31.1(2.0) gas $EM^1LF^{7,9}$
−30(2) Ne LF^4
B_0 = 0.140 $LF^{7,9}$

$\tilde{X}\ ^2\Pi_g$ $D_{\infty h}$ Structure: LF^9

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	CH stretch	3136.9	gas	EM	1
			3143(2)	Ne	LF	4
	2	C≡C stretch	2176.6	gas	EM	1
			2177(2)	Ne	LF	4
	3	C–C stretch	971.5	gas	EM,LF	1,8
			973(3)	Ne	LF	4
Σ_u^+	4	CH stretch	2820(40)[b]	gas	PE	2
Π_g	7	Skel. deform.	432.2[b]	gas	EM,LF	1,8
			430.3[b]			
			432.5[b]	Ne	LF	4

A = −33.5(1.9) gas $EM^1LF^{4,9}EF^7$
B_0 = 0.147 $EM^1EF^7LF^9$

$C_4D_2^+$

$\tilde{B}$
T_0 = 52930(160) gas PE[2]

$\tilde{A}\ ^2\Pi_u$ $D_{\infty h}$
T_0 = 19740.683(2) gas $EM^1LF^{7,9}EF^7$ $\tilde{A}$–$\tilde{X}$ 485–640 nm
19727(2) Ne LF^4 $\tilde{A}$–$\tilde{X}$ 468–600 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	CD stretch	2296	gas	EM	1
	2	C≡C stretch	1770(40)	gas	PE	2
			1892(2)	Ne	LF	4
	3	C–C stretch	800(40)[a]	gas	PE	2
			782(2)	Ne	LF	4
Π_g	7	Skel. deform.	418H[a]	Ne	LF	4

τ = 79(4) ns gas $EF^5PEFCO^5LF^6$
A = −31.1(2.0) gas $LF^{7,9}$
B_0 = 0.122 $LF^{7,9}$

$\tilde{X}\ ^2\Pi_g$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	CD stretch	2531.1	gas	EM	1
			2534(2)	Ne	LF	4
	2	C≡C stretch	2066.3	gas	EM	1
			2067(2)	Ne	LF	4
	3	C–C stretch	939.6	gas	EM	1
			932(3)	Ne	LF	4

$\tilde{X}\ ^2\Pi_g$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	4	CD stretch	2180(40)H	gas	PE	2
Π_g	7	Deformation	412.8H	gas	EM	1
			414(2)H	Ne	LF	4

$A = -33.3(2.0)$ gas EF^7LF^9
$B_0 = 0.127$ EF^7LF^9

[a] Alternate assignment in which values of ν_3 and $2\nu_7$ are interchanged is also possible.

References

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[2]C. Baker and D. W. Turner, Proc. Roy. Soc. (London) **A308**, 19 (1968).
[3]M. Allan, E. Kloster-Jensen, and J. P. Maier, Chem. Phys. **17**, 11 (1976).
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[8]F. G. Celii, J. P. Maier, and M. Ochsner, J. Chem. Phys. **85**, 6230 (1986).
[9]J. Lecoultre, J. P. Maier, and M. Rösslein, J. Chem. Phys. **89**, 6081 (1988).

H_2CCCC

$\tilde{X}$ C_{2v}
$A_0 = 9.489$; $B_0 = 0.150$; $C_0 = 0.148$ MW^1

References

[1]T. C. Killian, J. M. Vrtilek, C. A. Gottlieb, E. W. Gottlieb, and P. Thaddeus, Astrophys. J. **365**, L89 (1990).

$HCCCNH^+$

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NH stretch	3513.96	gas	LD	1
	3	CN stretch	2315.14	gas	DL	2

$B_0 = 0.144$ LD^1

References

[1]S. K. Lee and T. Amano, Astrophys. J. **323**, L145 (1987).
[2]K. Kawaguchi, M. Kajita, K. Tanaka, and E. Hirota, J. Mol. Spectrosc. **144**, 451 (1990).

HCONHCa

$\tilde{C}\ ^2A''$ C_s
$T_0 = 16248(20)$ gas LF^1 $\tilde{C}-\tilde{X}$ 600–630 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Ca stretch	353(10)	gas	LF	1

$\tilde{B}\ ^2A'$ C_s
$T_0 = 15083(20)$ gas LF^1 $\tilde{B}-\tilde{X}$ 645–680 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Ca stretch	357(10)	gas	LF	1

$\tilde{A}\ ^2A'$ C_s
$T_0 = 14154(20)$ gas LF^1 $\tilde{A}-\tilde{X}$ 670–765 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Ca stretch	355(10)	gas	LF	1

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Ca stretch	351(10)	gas	LF	1

References

[1]A. M. R. P. Bopegedera, W. T. M. L. Fernando, and P. F. Bernath, J. Phys. Chem. **94**, 3547 (1990).

HCONHSr

$\tilde{C}\ ^2A''$ C_s
$T_0 = 14580(20)$ gas LF^1 $\tilde{C}-\tilde{X}$ 655–700 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Sr stretch	315(10)	gas	LF	1

$\tilde{B}\ ^2A'$ C_s
$T_0 = 13917(20)$ gas LF^1 $\tilde{B}-\tilde{X}$ 700–750 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Sr stretch	284(10)	gas	LF	1

$\tilde{A}\ ^2A'$ C_s
T_0 = 13077(20) gas LF[1] $\tilde{A}-\tilde{X}$ 730–820 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Sr stretch	278(10)	gas	LF	1

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Sr stretch	288(10)	gas	LF	1

References

[1]A. M. R. P. Bopegedera, W. T. M. L. Fernando, and P. F. Bernath, J. Phys. Chem. **94**, 3547 (1990).

$H_2C=C=C=O^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2000(100)	gas	PE	1

References

[1]D. McNaughton and R. J. Suffolk, J. Chem. Research (S) 32 (1985).

$HN=CHCN^+$

$\tilde{D}$
T^a = 23500(400) gas PE[1]

$\tilde{C}$
T^a = 18000(400) gas PE[1]

$\tilde{B}$
T^a = 12000(400) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CN stretch	1850(50)	gas	PE	1

$\tilde{A}$
T^a = 6000(400) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1450(50)	gas	PE	1

[a] From vertical ionization potentials.

References

[1]R. A. Evans, S. M. Lacombe, M. J. Simon, G. Pfister-Guillouzo, and C. Wentrup, J. Phys. Chem. **96**, 4801 (1992).

$H_2C=NCN^+$

$\tilde{D}\ ^2A'$ C_s
T^a = 30700(800) gas PE[1–3]

$\tilde{C}\ ^2A''$ C_s
T^a = 20000(320) gas PE[2,3]

$\tilde{B}\ ^2A'$ C_s
T^a = 15300(320) gas PE[1–3]

$\tilde{A}\ ^2A''$ C_s
T^a = 4400(320) gas PE[1–3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1900T	gas	PE	1-3
			1300T	gas	PE	3

[a] From vertical ionization potentials.

References

[1]I. B'Shary, C. Guimon, M. Grimaud, G. Pfister-Guillouzo, and D. Liotard, Can. J. Chem. **66**, 2123 (1988).
[2]H. Bock, R. Dammel, P. Lorenčak, and C. Wentrup, Z. Naturforsch. **45B**, 59 (1990).
[3]R. A. Evans, S. M. Lacombe, M. J. Simon, G. Pfister-Guillouzo, and C. Wentrup, J. Phys. Chem. **96**, 4801 (1992).

c-HN=CHCN

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH stretch	3288w	gas	IR	4
	3	C≡N stretch	2246.5w	gas	IR	4
			2240w	Ar	IR	2,4
	4	C=N stretch	1609m	gas	IR	4
			1611s	Ar	IR	2,4
	5	CH,NH a-def.	1386m	gas	IR	4
			1375m	Ar	IR	2,4
	6	NH,CH s-def.	1218s	gas	IR	4
			1219m	Ar	IR	2,4
	7	Mixed	908m	gas	IR	4
			895s	Ar	IR	2,4
a''	10	Torsion	1075vw	Ar	IR	2,4
	11	NH,CH wag	800m	gas	IR	4
			800m	Ar	IR	4

A_0 = 2.091; B_0 = 0.166; C_0 = 0.153 MW[1,3]

References

[1]H. Takeo, M. Sugie, C. Matsumura, Y. Hamada, and M. Tsuboi, Chem. Phys. Lett. **123**, 229 (1986).
[2]P. Lorencak, G. Raabe, J. J. Radziszewski, and C. Wentrup, J. Chem. Soc., Chem. Commun. 916 (1986).

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[4]R. A. Evans, P. Lorencak, T.-K. Ha, and C. Wentrup, J. Am. Chem. Soc. **113**, 7261 (1991).

t-HN=CHCN

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH stretch	3288w	gas	IR	5
	3	C≡N stretch	2239.5w	gas	IR	5
			2227w	Ar	IR	3,5
	4	C=N stretch	1609m	gas	IR	2,5
			1600s	Ar	IR	3,5
	5	CH,NH a–def.	1387m	gas	IR	2,5
			1388m	Ar	IR	3,5
	6	NH,CH s–def.	1217s	gas	IR	2,5
			1221s	Ar	IR	3,5
			1216vs			
	7	Mixed	908m	gas	IR	2,5
			902s	Ar	IR	3,5
a"	10	NH,CH s–wag	1095s	gas	IR	2,5
			1096s	Ar	IR	3,5
			1093vs			
	11	Torsion	815m	gas	IR	5
			816m	Ar	IR	5

A_0 = 1.806; B_0 = 0.169; C_0 = 0.155 MW[1,4]

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[1]H. Takeo, M. Sugie, C. Matsumura, Y. Hamada, and M. Tsuboi, Chem. Phys. Lett. **123**, 229 (1986).
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[3]P. Lorencak, G. Raabe, J. J. Radziszewski, and C. Wentrup, J. Chem. Soc., Chem. Commun. 916 (1986).
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H_2C=NCN

$\tilde{X}$ C_s Structure: MW[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH_2 a–stretch	3137w	Ar	IR	6
	3	C≡N stretch	2208vs	Ar	IR	6
	4	C=N stretch	1621s	Ar	IR	6
	5	CH_2 scissors	1456ms	Ar	IR	6
	6	CH_2 rock	1215m	Ar	IR	6
a"	10	CH_2 wag	1090m	Ar	IR	6

A_0 = 2.114; B_0 = 0.182; C_0 = 0.167 MW[1,3–5]

D_2C=NCN

$\tilde{X}$

A_0 = 1.689; B_0 = 0.167; C_0 = 0.151 MW[2,3]

References

[1]B. Bak, O. J. Nielsen, and H. Svanholt, Chem. Phys. Lett. **59**, 330 (1978).
[2]B. Bak and H. Svanholt, Chem. Phys. Lett. **66**, 387 (1979).
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HC≡CC-OH

In an argon matrix, the threshold for rearrangement to propynal (HC≡CCHO) lies between 380 and 360 nm.[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		C≡C stretch	1992.8s	Ar	IR	1
		COH bend	1459.6	Ar	IR	1
		C–O stretch	1252.5	Ar	IR	1
		C–C stretch	1016.1	Ar	IR	1
a"		COH bend	1221.7	Ar	IR	1

References

[1]B. J. Ortman, R. H. Hauge, J. L. Margrave, and Z. H. Kafafi, J. Phys. Chem. **94**, 7973 (1990).

H_2C=C=C=O

$\tilde{X}$ C_s Structure: MW[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3049	Ar	IR	3
			3024			
			3037	N_2	IR	3
			3026			
		CH stretch	2978	Ar	IR	3
			2974			
			2978	N_2	IR	3
			2968			
			2177	Ar	IR	3
			2172	N_2	IR	3

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C=O stretch	2125	Ar	IR	3
			2124	N_2	IR	3
			2079	Ar	IR	3
			2075	N_2	IR	3
			1959	Ar	IR	3
			1973	N_2	IR	3
			1690	Ar	IR	3
			1685	N_2	IR	3
			1444	Ar	IR	3
			1457	N_2	IR	3
			1046	Ar	IR	3
			1047	N_2	IR	3
			980	Ar	IR	3
			988	N_2	IR	3
			903	Ar	IR	3
			910	N_2	IR	3
			668	Ar	IR	3
			674	N_2	IR	3
			473	Ar	IR	3
			479	N_2	IR	3

A_0 = 4.998; B_0 = 0.146; C_0 = 0.142 MW[1,2]

$D_2C=C=C=O$

$\tilde{X}$ C_s

B_0 = 0.133; C_0 = 0.128 MW[1]

References

[1]G. L. Blackman, R. D. Brown, R. F. C. Brown, F. W. Eastwood, and G. L. McMullen, J. Mol. Spectrosc. **68**, 488 (1977).

[2]R. D. Brown, P. D. Godfrey, R. Champion, and D. McNaughton, J. Am. Chem. Soc. **103**, 5711 (1981).

[3]O. L. Chapman, M. D. Miller, and S. M. Pitzenberger, J. Am. Chem. Soc. **109**, 6867 (1987).

$H_2C=C=C=S$

$\tilde{X}$ C_{2v} Structure: MW[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C_3 a–stretch	1999vs	Ar	IR	2
		CH_2 deform.	1487wm	Ar	IR	2
		C_3 s–stretch	1330m	Ar	IR	2
		CH_2 OPLA	927m	Ar	IR	2
		C=S stretch	710w	Ar	IR	2

References

[1]R. D. Brown, K. G. Dyall, P. S. Elmes, P. D. Godfrey, and D. McNaughton, J. Am. Chem. Soc. **110**, 789 (1988).

[2]E. Suzuki and F. Watari, Chem. Phys. Lett. **168**, 1 (1990).

$H_2C=C=C=Se$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1993s			
		C_3 a–stretch	1985vs	Ar	IR	1
			1981s			
		CH_2 scissors	1467m	Ar	IR	1
		C_3 s–stretch	1279s	Ar	IR	1
		CCH_2 OPLA	909s	Ar	IR	1

References

[1]W. W. Sander and O. L. Chapman, J. Org. Chem. **50**, 543 (1985).

$HC\equiv C–CHSe$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3322s	Ar	IR	1
		C≡C stretch	2072m	Ar	IR	1
		C=Se stretch ?	1058m	Ar	IR	1
		CH deform.	615m	Ar	IR	1

References

[1]W. W. Sander and O. L. Chapman, J. Org. Chem. **50**, 543 (1985).

$(HCO)_2^+$

$\tilde{E}$ C_{2h}

T_0^a = 51000(700) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g			1410(80)	gas	PE	1
			990(80)	gas	PE	1

$\tilde{C},\tilde{D}$ C_{2h}

$T^{ab} \cong$ 44200 gas PE[1]

$\tilde{B}$ C_{2h}

T_0^a = 26870(700) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2	CO stretch	1360(80)	gas	PE	1

$\tilde{A}$ C_{2h}
T_0[a] = 13470(700) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2	CO stretch	1610(80)	gas	PE	1
	4	CC stretch	970(80)	gas	PE	1
	5	Skel. deform.	400(80)	gas	PE	1

[a] The first ionization potential of $(HCO)_2$ is taken as 10.52(7) eV, the position of the maximum of the first photoelectron band.[2,3]
[b] From vertical ionization potential.

References

[1]D. W. Turner, C. Baker, A. D. Baker, and C. R. Brundle, *Molecular Photoelectron Spectroscopy*, pp. 252–261. Wiley-Interscience, London, 1970.
[2]D. O. Cowan, R. Gleiter, J. A. Hashmall, E. Heilbronner, and V. Hornung, Angew. Chem. **83**, 405 (1971); Angew Chem. Int. Ed. Engl. **10**, 401 (1971).
[3]J. F. Arnett, G. Newkome, W. L. Mattice, and S. P. McGlynn, J. Am. Chem. Soc. **96**, 4385 (1974).

CH_2FCN^+

$\tilde{D}$ $^2A'$ C_s
T[a] = 18960(320) gas PE[1]

$\tilde{C}$ $^2A''$ C_s
T[a] = 15410(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1450(80)	gas	PE	1
			810(80)	gas	PE	1

$\tilde{B}$ $^2A'$ C_s
T[a] = 6860(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1050(80)	gas	PE	1

$\tilde{A}$ $^2A'$ C_s
T[a] = 4110(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1450(80)	gas	PE	1

$\tilde{X}$ $^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		C≡N stretch	2020(80)	gas	PE	1
			1210(80)	gas	PE	1
		C–C stretch	810(80)	gas	PE	1

[a] From vertical ionization potentials.

References

[1]R. Botter, Y. Gounelle, Y. Henry, J. Jullien, F. Menes, and D. Solgadi, J. Electron Spectrosc. Relat. Phenom. **10**, 393 (1977).

CH_2ClCN^+

$\tilde{G}$ C_s
T[a] = 47840(320) gas PE[1]

$\tilde{F}$ C_s
T[a] = 40020(320) gas PE[1]

$\tilde{E}$ C_s
T[a] = 29930(320) gas PE[1]

$\tilde{D}$ $^2A'$ C_s
T[a] = 13230(320) gas PE[1,2]

$\tilde{C}$ $^2A''$ C_s
T[a] = 10250(320) gas PE[1,2]

$\tilde{B}$ $^2A'$ C_s
T[a] = 7910(320) gas PE[1,2]

$\tilde{A}$ $^2A'$ C_s
T[a] = 1210(320) gas PE[2]

$\tilde{X}$ $^2A''$ C_s

[a] From vertical ionization potentials.

References

[1]R. F. Lake and H. Thompson, Proc. Roy. Soc. (London) **A317**, 187 (1970).
[2]R. Botter, Y. Gounelle, Y. Henry, J. Jullien, F. Menes, and D. Solgadi, J. Electron Spectrosc. Relat. Phenom. **10**, 393 (1977).

CHOCHS

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2885w	Ar	IR	1
			2860m	Ar	IR	1
			2825w	Ar	IR	1
		C=O stretch	1700s	Ar	IR	1
			1698s	Ar	IR	1
			1368w	Ar	IR	1
			1268m	Ar	IR	1
			1095m	Ar	IR	1
		C=S stretch ?	1023s	Ar	IR	1
			788m	Ar	IR	1
			483m	Ar	IR	1

References

[1]M. Torres, A. Clement, and O. P. Strausz, Nouv. J. Chim. **7**, 269 (1983).

HS–CH=C=S

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3040w	Ar	IR	1
		C=S stretch	1750s	Ar	IR	1
			945w	Ar	IR	1
			935w	Ar	IR	1
			735w	Ar	IR	1
			695w	Ar	IR	1

References

[1]M. Torres, A. Clement, O. P. Strausz, A. C. Weedon, and P. de Mayo, Nouv. J. Chim. **6**, 401 (1982).

H_2NNCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NH_2 a–stretch	3362m	Ar	IR	1
		NH_2 s–stretch	3297w	Ar	IR	1
		NCO a–stretch	2262m	Ar	IR	1
			2210vs			
		NH_2 scissors	1612w	Ar	IR	1
			1303vw	Ar	IR	1
			1026wm	Ar	IR	1
		NN stretch	844vw	Ar	IR	1
		NNC deform.	642w	Ar	IR	1
		NCO deform.	563w	Ar	IR	1

D_2NNCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NCO a–stretch	2260vs	Ar	IR	1
			2213vs			
		ND_2 scissors	1181w	Ar	IR	1
			876w	Ar	IR	1
			790w	Ar	IR	1
		NN stretch	843w	Ar	IR	1
		NNC deform.	638w	Ar	IR	1
		NCO deform.	563w	Ar	IR	1

References

[1]J. H. Teles and G. Maier, Chem. Ber. **122**, 745 (1989).

CH_2NO_2

In an Ar matrix, threshold for photodecomposition into H_2CO + NO near 290 nm.[1]

$^2A_2$ C_{2v}

T_0 = 12840(80) gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	NO_2 s–stretch	1444(25)	gas	PE	3
	4	CN stretch ?	936(25)	gas	PE	3
	5	NO_2 scissors	605(25)	gas	PE	3

$\tilde{X}$ $^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s–stretch	3055 HF	Ar	IR	1,2
	2	CH_2 scissors	1419 HF	Ar	IR	1,2
	3	NO_2 s–stretch	1300(25)	gas	PE	3
			1297 HF	Ar	IR	1,2
	4	CN stretch	954(25)	gas	PE	3
			986 HF	Ar	IR	1,2
	5	NO_2 scissors	693 HF	Ar	IR	1,2
a_2	6	Torsion	205H	gas	PE	3
b_1	7	CNO_2 OPLA[a]	719 HF	Ar	IR	1,2
	8	H_2CN OPLA[a]	606 HF	Ar	IR	1,2
b_2	9	CH_2 a–stretch	3200 HF	Ar	IR	1,2
	10	NO_2 a–stretch	1484[b] HF	Ar	IR	1,2
			1461			
	11	CH_2 rock	1095 HF	Ar	IR	1,2
	12	NO_2 rock	484T[c] HF	Ar	IR	1,2

CD_2NO_2

$\tilde{X}$ $^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	NO_2 s–stretch	1292(25)	gas	PE	3
			1296 DF	Ar	IR	1,2
	4	CN stretch + CD_2 scissors	906 DF	Ar	IR	1,2
	5	NO_2 scissors	668 DF	Ar	IR	1,2
a_2	6	Torsion	140H	gas	PE	3
b_1	7	CNO_2 OPLA	694 DF	Ar	IR	1,2
b_2	10	NO_2 a–stretch	1460 DF	Ar	IR	1,2

[a] The two out–of–plane modes are strongly mixed.
[b] In Fermi resonance with (ν_4 + ν_{12}).
[c] Estimated from (ν_4 + ν_{12}).

References

[1]M. E. Jacox, J. Phys. Chem. **87**, 3126 (1983).
[2]M. E. Jacox, J. Phys. Chem. **91**, 5038 (1987).
[3]R. B. Metz, D. R. Cyr, and D. M. Neumark, J. Phys. Chem. **95**, 2900 (1991).

$NH_2BF_2^+$

$\tilde{H}\ ^2A_1$ C_{2v}
T^a = 74200(1600) gas PE[2]

$\tilde{G}\ ^2B_2$ C_{2v}
T^a = 63900(1100) gas PE[2]

$\tilde{F}\ ^2A_1$ C_{2v}
T^a = 58500(1100) gas PE[1,2]

$\tilde{E}\ ^2B_1$ C_{2v}
T^a = 49700(1100) gas PE[2]

$\tilde{D}\ ^2B_2$ C_{2v}
T^a = 48400(1600) gas PE[1,2]

$\tilde{B},\tilde{C}\ ^2B_2,^2A_2$ C_{2v}
T^a = 35700(1100) gas PE[1,2]

$\tilde{A}\ ^2A_1$ C_{2v}
T^a = 32400(1100) gas PE[1,2]

$\tilde{X}\ ^2B_1$ C_{2v}

[a] From vertical ionization potential.

References

[1]H. W. Kroto and D. McNaughton, J. Chem. Soc., Dalton Trans. 1767 (1985).
[2]C. A. Kingsmill, N. H. Werstiuk, and N. P. C. Westwood, J. Am. Chem. Soc. **109**, 2870 (1987).

$NH_2BCl_2^+$

$\tilde{F}\ ^2A_1$ C_{2v}
T^a = 38800(1100) gas PE[1]

$\tilde{E}\ ^2B_2$ C_{2v}
T^a = 26600(1600) gas PE[1]

$\tilde{D}\ ^2B_1$ C_{2v}
T^a = 23100(1100) gas PE[1]

$\tilde{C}\ ^2A_1$ C_{2v}
T^a = 12400(1100) gas PE[1]

$\tilde{B}\ ^2A_2$ C_{2v}
T^a = 9600(1100) gas PE[1]

$\tilde{A}\ ^2B_2$ C_{2v}
T^a = 6500(1100) gas PE[1]

$\tilde{X}\ ^2B_1$ C_{2v}

[a] From vertical ionization potential.

References

[1]C. A. Kingsmill, N. H. Werstiuk, and N. P. C. Westwood, J. Am. Chem. Soc. **109**, 2870 (1987).

$NH_2BBr_2^+$

$\tilde{F}\ ^2A_1$ C_{2v}
T^a = 36600(1100) gas PE[1]

$\tilde{E}\ ^2B_2$ C_{2v}
T^a = 24200(1600) gas PE[1]

$\tilde{D}\ ^2B_1$ C_{2v}
T^a = 21200(1100) gas PE[1]

$\tilde{C}\ ^2A_1$ C_{2v}
T^a = 10200(1100) gas PE[1]

$\tilde{B}\ ^2A_2$ C_{2v}
T^a = 7100(1100) gas PE[1]

$\tilde{A}\ ^2B_2$ C_{2v}
T^a = 5300(1100) gas PE[1]

$\tilde{X}\ ^2B_1$ C_{2v}

[a] From vertical ionization potential.

References

[1]C. A. Kingsmill, N. H. Werstiuk, and N. P. C. Westwood, J. Am. Chem. Soc. **109**, 2870 (1987).

$CH_2{=}CF_2^+$

$\tilde{G}\ ^2B_2$ C_{2v}
T^a = 75920(320) gas PE[1-3]

$\tilde{E},\tilde{F}\ ^2A_1,^2B_1$ C_{2v}
T^a = 63820(320) gas PE[1-3]

$\tilde{C},\tilde{D}\ ^2B_2,^2A_2$ C_{2v}
$T^a \cong$ 47000 gas PE[3]

$\tilde{B}\ ^2A_1$ C_{2v}
T^a = 43890(320) gas PE[1-3]

$\tilde{A}\ ^2B_2$ C_{2v}
T_0 = 30420(320) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1050(80)	gas	PE	2

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C=C stretch	1530(80)	gas	PE	1,2
	4	CF_2 s-stretch	700(80)	gas	PE	1,2

[a] From vertical ionization potential.

References

[1]R. F. Lake and H. Thompson, Proc. Roy. Soc. (London) **A315**, 323 (1970).
[2]J. A. Sell and A. Kupperman, J. Chem. Phys. **71**, 4703 (1979).
[3]G. Bieri, W. von Niessen, L. Åsbrink, and A. Svensson, Chem. Phys. **60**, 61 (1981).

c-CHF=CHF$^+$

$\tilde{F},\tilde{G}\ ^2A_1,^2A_2$ C_{2v}
T^a = 69150(320) gas PE[2,5]

$\tilde{D},\tilde{E}\ ^2B_2,^2B_1$ C_{2v}
T^a = 55110(320) gas PE[2,5]
F-atom detachment has been observed in this transition. PEPICO[3]

$\tilde{C}\ ^2A_2$ C_{2v}
T^a = 47850(320) gas PE[2,5]
F-atom detachment has been observed in this transition. PEPICO[3]

$\tilde{B}\ ^2B_2$ C_{2v}
T_0 = 37680(160) gas PE[1,2,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH s-stretch	2610(80)	gas	PE	2
		CF s-stretch	1100(80)	gas	PE	2

$\tilde{A}\ ^2A_1$ C_{2v}
T_0 = 28880(10) gas PE[1]EF[1] $\tilde{A}$–$\tilde{X}$ 340–380 nm
The threshold for fragmentation into HCCF$^+$ + HF is near the onset of the transition. PEPICO[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CH deform.	1430(80)	gas	PE	1,2
	4	CF s-stretch	1020(80)	gas	PE	1,2
	5	CF deform.	260(10)	gas	EF,PE	1

τ_0 = 320(30) ns gas EF[1]PEFCO[4]

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C=C stretch	1600(10)	gas	EF	1
	3	CH deform.	1330(10)	gas	EF	1
	4	CF stretch	1030(10)	gas	EF	1
	5	CF deform.	250(10)	gas	EF	1

[a] From vertical ionization potential.

References

[1]J. P. Maier, O. Marthaler, and G. Bieri, Chem. Phys. **44**, 131 (1979).
[2]J. A. Sell and A. Kupperman, J. Chem. Phys. **71**, 4703 (1979).
[3]J.-P. Stadelmann and J. Vogt, Int. J. Mass Spectrom. Ion Phys. **35**, 83 (1980).
[4]J. P. Maier and F. Thommen, J. Chem. Soc., Faraday Trans. 2 **77**, 845 (1981).
[5]G. Bieri, W. von Niessen, L. Åsbrink, and A. Svensson, Chem. Phys. **60**, 61 (1981).

t-CHF=CHF$^+$

$\tilde{F},\tilde{G}\ ^2A_g,^2B_u$ C_{2h}
T^a = 69060(320) gas PE[2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g			920(80)	gas	PE	2
			450(80)	gas	PE	2

$\tilde{D},\tilde{E}\ ^2A_g,^2A_u$ C_{2h}
T^a = 54780(320) gas PE[2,4]
F-atom detachment has been observed in this transition. PEPICO[3]

$\tilde{C}\ ^2B_g$ C_{2h}
T^a = 49780(320) gas PE[2,4]
F-atom detachment has been observed in this transition. PEPICO[3]

$\tilde{B}\ ^2B_u$ C_{2h}
T_0 = 39370(160) gas PE[1,2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	CH s-stretch	2820(80)	gas	PE	2
		CF s-stretch	1180(80)	gas	PE	2

$\tilde{A}\ ^2A_g$ C_{2h}
T_0 = 26630(160) gas PE[1,2,4]
The threshold for fragmentation into HCCF$^+$ + HF is near the onset of the transition. PEPICO[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g		CF deform.	500(80)	gas	PE	2

$\tilde{X}\ ^2A_u$ C_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2	C=C stretch	1600(80)	gas	PE	2
	3	CH deform.	1230(80)	gas	PE	2
	4	CF s-stretch	850(80)	gas	PE	2
	5	CF deform.	550(80)	gas	PE	2

[a] From vertical ionization potential.

References

[1]J. P. Maier, O. Marthaler, and G. Bieri, Chem. Phys. **44**, 131 (1979).
[2]J. A. Sell and A. Kupperman, J. Chem. Phys. **71**, 4703 (1979).
[3]J.-P. Stadelmann and J. Vogt, Int. J. Mass Spectrom. Ion Phys. **35**, 83 (1980).
[4]G. Bieri, W. von Niessen, L. Åsbrink, and A. Svensson, Chem. Phys. **60**, 61 (1981).

$CH_2=CFCl^+$

$\tilde{F}\ ^2A''$ C_s
T^a = 61890(240) gas PE[1,2]

$\tilde{E}\ ^2A'$ C_s
T^a = 57690(240) gas PE[1,2]

$\tilde{D}\ ^2A'$ C_s
T^a = 39620(240) gas PE[1,2]

$\tilde{C}\ ^2A'$ C_s
T^a = 34130(240) gas PE[1,2]

$\tilde{B}\ ^2A''$ C_s
T_0 = 24200(160) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CCl stretch	521(20)	gas	PE	2

$\tilde{A}\ ^2A'$ C_s
T_0 = 17910(160) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CCl stretch	524(30)	gas	PE	1,2
		CFCl deform.	291(15)	gas	PE	2

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		C=C stretch	1400(40)	gas	PE	2
		CCl stretch	722(20)	gas	PE	1,2
		CFCl deform.	380(25)	gas	PE	2

[a] From vertical ionization potential.

References

[1]A. W. Potts, J. M. Benson, I. Novak, and W. A. Svensson, Chem. Phys. **115**, 253 (1987).
[2]G. Tornow, R. Locht, R. Kaufel, H. Baumgärtel, and H. W. Jochims, Chem. Phys. **146**, 115 (1990).

c–$CHF=CHCl^+$

$\tilde{F}$ C_s
T^a = 59950(240) gas PE[1]

$\tilde{E}$ C_s
T^a = 54380(240) gas PE[1]

$\tilde{D}$ C_s
T^a = 43000(240) gas PE[1]

$\tilde{C}$ C_s
T_0 = 32030(160) gas PE[1]

$\tilde{B}$ C_s
T_0 = 25740(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CF rock	448(40)	gas	PE	1

$\tilde{A}$ C_s
T_0 = 16140(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CH deform.	1268(40)	gas	PE	1

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		C=C stretch	1464(50)	gas	PE	1
		CF stretch	910(40)	gas	PE	1

[a] From vertical ionization potential.

References

[1]G. Tornow, R. Locht, R. Kaufel, H. Baumgärtel, and H. W. Jochims, Chem. Phys. **146**, 115 (1990).

t-$CHF=CHCl^+$

$\tilde{F}$ C_s
T^a = 66800(240) gas PE[1]

$\tilde{E}$ C_s
T^a = 58740(240) gas PE[1]

$\tilde{D}$ C_s
T^a = 41150(240) gas PE[1]

$\tilde{C}$ C_s
T^a = 35340(240) gas PE[1]

$\tilde{B}$ C_s
T_0 = 26540(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CF rock	374(15)	gas	PE	1

$\tilde{A}$ C_s
T_0 = 17510(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CH deform.	1094(10)	gas	PE	1

$\tilde{X}$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	C=C stretch	1529(30)	gas	PE	1
	CCl stretch	489(20)	gas	PE	1

[a] From vertical ionization potential.

References

[1]G. Tornow, R. Locht, R. Kaufel, H. Baumgärtel, and H. W. Jochims, Chem. Phys. **146**, 115 (1990).

$CH_2{=}CCl_2^+$

$\tilde{H}\ ^2A_1$ C_{2v}
T^a = 69710(320) gas PE[1-5]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		1290(80)	gas	PE	1

$\tilde{F},\tilde{G}\ ^2A_1,^2B_2$ C_{2v}
T^a = 51400(1000) gas PE[1-5]

$\tilde{E}\ ^2B_1$ C_{2v}
T^a = 35580(320) gas PE[1-5]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		1010(80)	gas	PE	1

$\tilde{D}\ ^2B_2$ C_{2v}
T^a = 32030(320) gas PE[1-5]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		930(100)	gas	PE	3,4

$\tilde{C}\ ^2A_1$ C_{2v}
T^a = 21860(320) gas PE[1-5]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	CCl_2 scissors	320(40)	gas	PE	1,4

$\tilde{B}\ ^2A_2$ C_{2v}
T_0 = 17990(320) gas PE[1-5]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	CCl_2 scissors	270(40)	gas	PE	1,4

$\tilde{A}\ ^2B_2$ C_{2v}
T_0 = 13150(320) gas PE[1-5]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	CCl_2 scissors	270(40)	gas	PE	1,4

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	C=C stretch	1290(80)	gas	PE	1–4
	CCl stretch	560(80)	gas	PE	1,3,4

[a] From vertical ionization potential.

References

[1]R. F. Lake and H. Thompson, Proc. Roy. Soc. (London) **A315**, 323 (1970).
[2]N. Jonathan, K. Ross, and V. Tomlinson, Int. J. Mass Spectrom. Ion Phys. **4**, 51 (1970).
[3]K. Wittel and H. Bock, Chem. Ber. **107**, 317 (1974).
[4]J. C. Bünzli, D. C. Frost, F. G. Herring, and C. A. McDowell, J. Electron Spectrosc. Relat. Phenom. **9**, 289 (1976).
[5]W. von Niessen, L. Åsbrink, and G. Bieri, J. Electron Spectrosc. Relat. Phenom. **26**, 173 (1982).

c-$CHCl{=}CHCl^+$

$\tilde{G}\ ^2A_1$ C_{2v}
T^a = 57700(1000) gas PE[1-4]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	CH s-stretch	1940(80)	gas	PE	1

$\tilde{F}\ ^2A_1$ C_{2v}
$T^a \cong$ 49600 gas PE[1-4]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	CCl s-stretch	600(80)	gas	PE	1

$\tilde{E}\ ^2B_2$ C_{2v}
$T^a \cong$ 36700 gas PE[1-4]

$\tilde{D}\ ^2B_1$ C_{2v}
$T^a \cong$ 33500 gas PE[1-4]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	CCl s-stretch	640(80)	gas	PE	1,3

$\tilde{C}\ ^2A_2$ C_{2v}
T^a = 22750(500) gas PE[1-4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CCl s–stretch	640(80)	gas	PE	1–3

$\tilde{B}\ ^2A_1$ C_{2v}
T^a = 18960(320) gas PE[1-4]

$\tilde{A}\ ^2B_2$ C_{2v}
T^a = 16100(1000) gas PE[1-4]

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		C=C stretch	1370(80)	gas	PE	1,3
		CCl s–stretch	800(80)	gas	PE	1–3

[a] From vertical ionization potential.

References

[1]R. F. Lake and H. Thompson, Proc. Roy. Soc. (London) **A315**, 323 (1970).
[2]N. Jonathan, K. Ross, and V. Tomlinson, Int. J. Mass Spectrom. Ion Phys. **4**, 51 (1970).
[3]K. Wittel and H. Bock, Chem. Ber. **107**, 317 (1974).
[4]W. von Niessen, L. Åsbrink, and G. Bieri, J. Electron Spectrosc. Relat. Phenom. **26**, 173 (1982).

t-CHCl=CHCl$^+$

$\tilde{F},\tilde{G}\ ^2A_g, ^2B_u$ C_{2h}
$T^a \cong$ 53000 gas PE[1-4]

$\tilde{E}\ ^2A_g$ C_{2h}
T^a = 36790(320) gas PE[1-4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g			880(80)	gas	PE	3

$\tilde{D}\ ^2A_u$ C_{2h}
T^a = 33970(320) gas PE[1-4]

$\tilde{C}\ ^2B_g$ C_{2h}
T^a = 24290(320) gas PE[1-4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g			720(80)	gas	PE	3

$\tilde{B}\ ^2B_u$ C_{2h}
$T^a \cong$ 19800 gas PE[1-4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g			640(80)	gas	PE	3

$\tilde{A}\ ^2A_g$ C_{2h}
T^a = 17910(500) gas PE[1-4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g			600(80)	gas	PE	3

$\tilde{X}\ ^2A_u$ C_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g		C=C stretch	1400(80)	gas	PE	1,3
		CCl s–stretch	850(80)	gas	PE	1–3
		CCl s–deform.	340(80)	gas	PE	1,3

[a] From vertical ionization potential.

References

[1]R. F. Lake and H. Thompson, Proc. Roy. Soc. (London) **A315**, 323 (1970).
[2]N. Jonathan, K. Ross, and V. Tomlinson, Int. J. Mass Spectrom. Ion Phys. **4**, 51 (1970).
[3]K. Wittel and H. Bock, Chem. Ber. **107**, 317 (1974).
[4]W. von Niessen, L. Åsbrink, and G. Bieri, J. Electron Spectrosc. Relat. Phenom. **26**, 173 (1982).

HC(O)OOH

$\tilde{X}$ C_s Structure: MW[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3340.7w	gas	IR	1,2
			3334.0m	Ar	IR	5
	2	CH stretch	2977wT	gas	IR	1
			2964.0w	Ar	IR	5
	3	C=O stretch	1744.7vs	gas	IR	1,2
			1737.3s	Ar	IR	5
	4	OH bend	1442sT	gas	IR	1
			1437.4s	Ar	IR	5
	5	Mixed	1340wT	gas	IR	1
			1334.6m	Ar	IR	5
	6	C–O stretch	1124.98vs	gas	IR	1,2,4
			1113.9s	Ar	IR	5
	7	Mixed	859w	gas	IR	1
			857.0m	Ar	IR	5
	8	O–O stretch	810w	gas	IR	1
			810.6m	Ar	IR	5
	9	Skel. deform.	336.3m	Ar	IR	5
a''	11	Torsion	441.3s	Ar	IR	5
	12	Torsion	331.6m	Ar	IR	5

A_0 = 0.676; B_0 = 0.254; C_0 = 0.185 MW^3

DC(O)OOD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2467.5m	Ar	IR	5
	2	CD stretch	2240.0w	Ar	IR	5
	3	C=O stretch	1713.8s	Ar	IR	5
	4	C–O stretch	1143.6s	Ar	IR	5
	5	Mixed	1086.7s	Ar	IR	5
	6	Mixed	986.0w	Ar	IR	5
	7	Mixed	826.2m	Ar	IR	5
	8	O–O stretch	782.6m	Ar	IR	5
	9	COO deform.	322.3m	Ar	IR	5
a''	11	CO torsion	367.6s	Ar	IR	5
	12	OO torsion	274.6s	Ar	IR	5

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[5]M. Tyblewski, J. Dommen, T.-K. Ha, and A. Bauder, Spectrochim. Acta **47A**, 397 (1991).

CH_2COF^-

Dipole–Bound State C_s
T_0 = 17709.646(3) gas PD[1] 547–588 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OCF deform.	571	gas	PD	1
		Torsion	200HT	gas	PD	1

A_0 = 0.382; B_0 = 0.358; C_0 = 0.184 PD[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OCF deform.	694	gas	PD	1
		Torsion	494	gas	PD	1
		OCF deform.	475	gas	PD	1

A_0 = 0.368; B_0 = 0.355; C_0 = 0.180 PD[1]

CD_2COF^-

Dipole–Bound State C_s
T_0 = 17704 gas PD[1] 549–586 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OCF deform.	491	gas	PD	1
		Torsion	172H	gas	PD	1

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OCF deform.	650	gas	PD	1
		OCF deform.	419	gas	PD	1
		Torsion	385	gas	PD	1

References

[1]J. Marks, J. I. Brauman, R. D. Mead, K. R. Lykke, and W. C. Lineberger, J. Chem. Phys. **88**, 6785 (1988).

$CH_2{=}SiCl_2$

In an Ar matrix, absorption maximum at 246 nm.[1]

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1008m	Ar	IR	1
			732s	Ar	IR	1
			593m	Ar	IR	1

References

[1]G. Maier, G. Mihm, and H. P. Reisenauer, Angew. Chem. **93**, 615 (1981); Angew. Chem. Int. Ed. Engl. **20**, 597 (1981).

$CH_2NO_2^-$

Threshold for electron detachment from ground-state $CH_2NO_2^-$ = 19970(80) gas PE[1]

$CD_2NO_2^-$

Threshold for electron detachment from ground-state $CD_2NO_2^-$ = 20010(80) gas PE[1]

References

[1]R. B. Metz, D. R. Cyr, and D. M. Neumark, J. Phys. Chem. **95**, 2900 (1991).

NH_2NO_2

In an Ar or N_2 matrix, photolyzes with a threshold near 250 nm to produce N_2O, H_2O, c-$(NO)_2$, and H_2.[2]

$\tilde{X}$ C_s Structure: MW[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH_2 s–stretch	3359	Ar	IR	2
			3361	N_2	IR	2
	2	NH_2 scissors	1558	Ar	IR	2
			1581	N_2	IR	2
	3	NO_2 s–stretch	1350	Ar	IR	2
			1368	N_2	IR	2
	4	NN stretch	951	Ar	IR	2
	5	NO_2 wag	798	Ar	IR	2
			776	N_2	IR	2
	6	NO_2 bend	692	Ar	IR	2
			714	N_2	IR	2
	7	NH_2 wag	628	Ar	IR	2
			587	N_2	IR	2
a"	8	NH_2 a–stretch	3478	Ar	IR	2
			3474	N_2	IR	2
	9	NO_2 a–stretch	1613	Ar	IR	2
			1610	N_2	IR	2
	10	NH_2 twist	1227	Ar	IR	2
			1238	N_2	IR	2
	11	NO_2 rock	484	Ar	IR	2
	12	Torsion	402	Ar	IR	2
			434	N_2	IR	2

A_0 = 0.422; B_0 = 0.397; C_0 = 0.206 gas MW[1]

ND_2NO_2

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ND_2 s–stretch	2455	Ar	IR	2
			2458	N_2	IR	2
	2	NO_2 s–stretch	1352	Ar	IR	2
			1366	N_2	IR	2
	3	ND_2 scissors	1174	Ar	IR	2
	4	NN stretch	948	Ar	IR	2
	5	NO_2 wag	774	Ar	IR	2
			772	N_2	IR	2
	6	NO_2 bend	662	Ar	IR	2
			671	N_2	IR	2
	7	ND_2 wag	485	Ar	IR	2
			498	Ar	IR	2
a"	8	ND_2 a–stretch	2604	Ar	IR	2
			2603	N_2	IR	2
	9	NO_2 a–stretch	1588	Ar	IR	2
			1583	N_2	IR	2
	10	ND_2 twist	972	Ar	IR	2
			972	N_2	IR	2
	11	NO_2 rock	434	Ar	IR	2
	12	Torsion	287	Ar	IR	2
			318	N_2	IR	2

A_0 = 0.405; B_0 = 0.351; C_0 = 0.190 gas MW[1]

References

[1]J. K. Tyler, J. Mol. Spectrosc. **11**, 39 (1963).
[2]M. Nonella, R. P. Muller, and J. R. Huber, J. Mol. Spectrosc. **112**, 142 (1985).

H_2SiO_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3677s	Ar	IR	2
		Si=O stretch	1270s	Ar	IR	1,2
		Si–O a–stretch	1023m	Ar	IR	2
		Torsion	453vs	Ar	IR	2
		SiO_2 deform.	359wm	Ar	IR	2

D_2SiO_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OD stretch	2710s	Ar	IR	2
		Si=O stretch	1267m	Ar	IR	1,2
		Si–O a–stretch	994ms	Ar	IR	2
		Si–O s–stretch	919m	Ar	IR	2
		Torsion	376s	Ar	IR	2
		SiO_2 deform.	349m	Ar	IR	2

References

[1]R. Withnall and L. Andrews, J. Am. Chem. Soc. **107**, 2567 (1985).
[2]R. Withnall and L. Andrews, J. Phys. Chem. **89**, 3261 (1985).

H_2GeO_3

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3630.7	Ar	IR	1
		Ge=O stretch	971.4	Ar	IR	1
		GeOH deform.	955.1	Ar	IR	1
		GeOH deform.	926.0	Ar	IR	1
		Ge–O a–stretch	749.1	Ar	IR	1
		Ge–O s–stretch	732.3	Ar	IR	1
		OH torsion	396.9	Ar	IR	1

D_2GeO_3

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OD stretch	2677.5	Ar	IR	1
		Ge=O stretch	972.2	Ar	IR	1
		Ge–O a–stretch	748.4	Ar	IR	1
		Ge–O s–stretch	733.8	Ar	IR	1
		OD torsion	295.4	Ar	IR	1
		GeO_2 scissors	243.6	Ar	IR	1
		O_2GeO OPLA	209.5	Ar	IR	1

References

[1]R. Withnall and L. Andrews, J. Phys. Chem. **94**, 2351 (1990).

CH_2FO_2

In the gas phase, an unstructured absorption between 220 and 280 nm, with maximum at 240 nm, has been assigned[1] to CH_2FO_2.

References

[1]T. J. Wallington, J. C. Ball, O. J. Nielsen, and E. Bartkiewicz, J. Phys. Chem. **96**, 1241 (1992).

$HCCl_2OH$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1388	gas	IR	1
			1221	gas	IR	1
			1105	gas	IR	1
			1003	gas	IR	1

References

[1]G. S. Tyndall, T. J. Wallington, M. D. Hurley, and W. F. Schneider, J. Phys. Chem. **97**, 1576 (1993).

$H(C\equiv C)_2F^+$

$\tilde{F}\ ^2\Sigma$ $C_{\infty v}$
T^a = 108100(1000) gas PE[1]

$\tilde{E}\ ^2\Sigma$ $C_{\infty v}$
T^a = 89600(1000) gas PE[1]

$\tilde{D}\ ^2\Sigma$ $C_{\infty v}$
T^a = 75800(1000) gas PE[1]

$\tilde{B},\tilde{C}\ ^2\Pi,^2\Sigma$ $C_{\infty v}$
T^a = 61300(1000) gas PE[1]

$\tilde{A}\ ^2\Pi$ $C_{\infty v}$
T_0 = 20570(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	CF stretch	1370(80)	gas	PE	1
	4	C–C stretch	705(80)	gas	PE	1

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	C≡C stretch	2350(80)	gas	PE	1
	4	C–C stretch	685(80)	gas	PE	1

[a] From vertical ionization potential.

References

[1]G. Bieri, A. Schmelzer, L. Åsbrink, and M. Jonsson, Chem. Phys. **49**, 213 (1980).

$H(C\equiv C)_2Cl^+$

$\tilde{D}$
$T_0 \leqslant$ 61700(560) gas PE[1]

$\tilde{C}$
$T_0 \leqslant$ 57280(320) gas PE[1]

$\tilde{B}\ ^2\Pi_{3/2}$ $C_{\infty v}$
$T_0 \leqslant$ 35100(320) gas PE[1]

$\tilde{A}\ ^2\Pi_{3/2}$ $C_{\infty v}$
T_0 = 19715.0(1) gas EF[2,4]LF[4] $\tilde{A}$–$\tilde{X}$ 445–652 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	C≡C s–stretch	2171(2)	gas	LF	4
	3	C≡C a–stretch	2101(2)	gas	LF	4
	4	C–C stretch	1088(1)	gas	EF,LF	3,4
	5	CCl stretch	523(1)	gas	EF,LF	2–4
Π	8	Skel. deform.	307(1)H	gas	EF,LF	3,4
	9	Skel. deform.	125(2)H	gas	LF	4

τ = 41(2) ns gas EF[2]PEFCO[3]
A = −200(100) gas PE[1]

$\tilde{X}\ ^2\Pi_{3/2}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3101T	gas	EF	4
	2	C≡C stretch	2191(1)	gas	EF	2–4
	3	C≡C stretch	1920(1)	gas	EF	2–4
	4	C–C stretch	1184(1)	gas	EF	2–4
	5	CCl stretch	547(1)	gas	EF	2–4
Π	8	Skel. deform.	309(1)H	gas	EF	3,4
	9	Skel. deform.	124(1)H	gas	EF	4

A = −200(100) gas PE[1]

References

[1]E. Heilbronner, V. Hornung, J. P. Maier, and E. Kloster-Jensen, J. Am. Chem. Soc. **96**, 4252 (1974).
[2]J. P. Maier, O. Marthaler, and E. Kloster-Jensen, J. Electron Spectrosc. Relat. Phenom. **18**, 251 (1980).
[3]J. P. Maier, O. Marthaler, L. Misev, and F. Thommen, J. Chem. Soc., Faraday Disc. **71**, 181 (1981).
[4]D. Klapstein, J. P. Maier, L. Misev, and W. Zambach, Chem. Phys. **72**, 101 (1982).

$H(C\equiv C)_2Br^+$

$\tilde{D}$
$T_0 \leqslant$ 59700(560) gas PE[1]

$\tilde{C}$
$T_0 \leqslant$ 52525(320) gas PE[1]

$\tilde{B}\ ^2\Pi$ $C_{\infty v}$
$T_0 \leq 29130(320)$ gas PE[1]
$A = -800(300)$ gas PE[1]

$\tilde{A}\ ^2\Pi_{3/2}$ $C_{\infty v}$
$T_0 = 18401.9(3)$ gas EF^3LF^3 $\tilde{A}-\tilde{X}$ 467–658 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	C≡C stretch	2138(2)	gas	LF	3
	3	C≡C stretch	2037(2)	gas	LF	3
	4	C–C stretch	918(2)	gas	PE,LF	2,3
	5	CBr stretch	409(1)	gas	EF,LF	2,3
Π	7	Skel. deform.	478(1)H	gas	EF,LF	3
	8	Skel. deform.	348(2)H	gas	LF	3
	9	Skel. deform.	111(2)H	gas	LF	3

$\tau = 27(3)$ ns gas EF^2
$A = -970(80)$ gas $PE^1EF^3LF^3$

$\tilde{X}\ ^2\Pi_{3/2}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3196T	gas	EF	3
	2	C≡C stretch	2155(1)	gas	EF	2,3
	3	C≡C stretch	1914(1)[a]	gas	EF	2,3
	4	C–C stretch	1115(1)	gas	EF	2,3
	5	CBr stretch	440(1)	gas	EF	2,3
Π	7	Skel. deform.	509(1)H	gas	EF	3
	8	Skel. deform.	370(1)H	gas	EF	3
	9	Skel. deform.	112(1)H	gas	EF	3

$A = -650(80)$ gas EF^3L^3

[a] 1906(1) in $\tilde{X}\ ^2\Pi_{1/2}$ state.

References

[1]E. Heilbronner, V. Hornung, J. P. Maier, and E. Kloster-Jensen, J. Am. Chem. Soc. **96**, 4252 (1974).
[2]J. P. Maier, O. Marthaler, and E. Kloster-Jensen, J. Electron Spectrosc. Relat. Phenom. **18**, 251 (1980).
[3]D. Klapstein, J. P. Maier, L. Misev, and W. Zambach, Chem. Phys. **72**, 101 (1982).

$H(C\equiv C)_2I^+$

$\tilde{D}$
$T_0 \leq 62600(560)$ gas PE[1]

$\tilde{B}\ ^2\Pi$ $C_{\infty v}$
$T_0 \leq 27110(320)$ gas PE[1]

$\tilde{A}\ ^2\Pi$ $C_{\infty v}$
$T_0 = 14600(320)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1050(80)	gas	PE	1

$A = -2980(320)$ gas PE[1]

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2100(80)	gas	PE	1

$A = -2020(320)$ gas PE[1]

References

[1]E. Heilbronner, V. Hornung, J. P. Maier, and E. Kloster-Jensen, J. Am. Chem. Soc. **96**, 4252 (1974).

$CHF=CF_2^+$

$\tilde{H},\tilde{I}\ ^2A',^2A'$ C_s
$T^a = 80680(320)$ gas PE[1,2]

$\tilde{G}\ ^2A''$ C_s
$T^a = 68300(1000)$ gas PE[1,2]

$\tilde{F}\ ^2A'$ C_s
$T^a = 63900(320)$ gas PE[1,2]

$\tilde{D},\tilde{E}\ ^2A',^2A''$ C_s
$T^a = 52900(1000)$ gas PE[1,2]

$\tilde{C}\ ^2A''$ C_s
$T^a = 50500(1000)$ gas PE[1,2]

$\tilde{B}\ ^2A'$ C_s
$T^a = 46500(1000)$ gas PE[1,2]

$\tilde{A}\ ^2A'$ C_s
$T^a = 36150(320)$ gas PE[1,2]

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			600(80)	gas	PE	1

[a] From vertical ionization potential.

References

[1]J. A. Sell and A. Kupperman, J. Chem. Phys. **71**, 4703 (1979).
[2]G. Bieri, W. von Niessen, L. Åsbrink, and A. Svensson, Chem. Phys. **60**, 61 (1981).

$CHCl=CF_2^+$

$\tilde{G},\tilde{H}\ ^2A',^2A''$ C_s
$T^a = 65760(320)$ gas PE[1]

$\tilde{F}\ ^2A'$ C_s
$T^a = 49700(320)$ gas PE[1]

$\tilde{E}\ ^2A''$ C_s
$T^a = 46470(320)$ gas PE[1]

$\tilde{D}\ ^2A'$ C_s
$T^a = 40500(320)$ gas PE[1]

$\tilde{B},\tilde{C}\ ^2A'',^2A'$ C_s
T^a = 26380(320) gas PE[1]

$\tilde{A}\ ^2A'$ C_s
T^a = 15570(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1090(80)	gas	PE	1
			570(80)	gas	PE	1

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		C=C stretch	1570(80)	gas	PE	1
		CCl stretch	930(80)	gas	PE	1
		CF_2 scissors	470(80)	gas	PE	1

[a] From vertical ionization potentials.

References

[1]A. W. Potts, J. M. Benson, I. Novak, and W. A. Svensson, Chem. Phys. **115**, 253 (1987).

$CHCl{=}CCl_2^+$

$\tilde{J}\ ^2A'$ C_s
T^a = 74310(320) gas PE[1,2]

$\tilde{I}\ ^2A'$ C_s
T^a = 58740(320) gas PE[1,2]

$\tilde{H}\ ^2A'$ C_s
T^a = 54950(320) gas PE[1,2]

$\tilde{G}\ ^2A''$ C_s
T^a = 41870(320) gas PE[1,2]

$\tilde{F}\ ^2A'$ C_s
T^a = 39620(320) gas PE[1,2]

$\tilde{E}\ ^2A''$ C_s
T^a = 28000(320) gas PE[1,2]

$\tilde{D}\ ^2A'$ C_s
T^a = 26060(320) gas PE[1,2]

$\tilde{C}\ ^2A''$ C_s
T^a = 23600(1000) gas PE[2]

$\tilde{B}\ ^2A'$ C_s
T^a = 21700(320) gas PE[1,2]

$\tilde{A}\ ^2A'$ C_s
T^a = 18150(320) gas PE[1,2]

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		C=C stretch	1390(80)	gas	PE	1
		Deformation	330(80)	gas	PE	1

[a] From vertical ionization potential.

References

[1]R. F. Lake and H. Thompson, Proc. Roy. Soc. (London) **A315**, 323 (1970).
[2]W. von Niessen, L. Åsbrink, and G. Bieri, J. Electron Spectrosc. Relat. Phenom. **26**, 173 (1982).

$HOONO_2$

In the gas phase, the threshold for unstructured absnrption lies near 330 nm. This absorption increases steadily to a maximum at or beyond 190 nm.[4–7,10]

$\tilde{X}$ Structure: MW[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OH stretch	3540.1wm	gas	IR	1,4
	2	NO_2 a-stretch	1728.3vs	gas	IR	1,3,7
	3	OH bend	1396.9wm	gas	IR	1,3,4,7
	4	NO_2 s-stretch	1304.2s	gas	IR	1–4,7
	5	O–O stretch	941.0w	gas	IR	1,3,11
			922.1w	gas	IR	1,3
			919.2w	gas	IR	1,3,11
	6	N–O stretch	802.7m	gas	IR	1–4,7,9
			722T	gas	IR	11
	12	NO_2 torsion	145(6)	gas	MW	8

A_0 = 0.400; B_0 = 0.156; C_0 = 0.113 gas MW[8]

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[1]H. Niki, P. D. Maker, C. M. Savage, and L. P. Breitenbach, Chem. Phys. Lett. **45**, 564 (1977).
[2]S. Z. Levine, W. M. Uselman, W. H. Chan, J. G. Calvert, and J. H. Shaw, Chem. Phys. Lett. **48**, 528 (1977).
[3]R. A. Graham, A. M. Winer, and J. N. Pitts, Jr., Chem. Phys. Lett. **51**, 215 (1977).
[4]R. A. Graham, A. M. Winer, and J. N. Pitts, Jr., Geophys. Res. Lett. **5**, 909 (1978).
[5]R. A. Cox and K. Patrick, Int. J. Chem. Kinet. **11**, 635 (1979).
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[10]R. J. Singer, J. N. Crowley, J. P. Burrows, W. Schneider, and G. K. Moortgat, J. Photochem. Photobiol. A: Chem. **48**, 17 (1989).
[11]R. D. May and D. B. Peterson, J. Mol. Spectrosc. **150**, 647 (1991).

$SiCl_3OH$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3723.8	gas	IR	2
			3693.5	Ar	IR	1
			1330.3wT	Ar	IR	1
		SiO stretch	962.6s	gas	IR	2
			960.5	Ar	IR	1
			798ms	gas	IR	2
	4	SiCl stretch	610vs	gas	IR	2
			621.2	Ar	IR	1
	5	SiCl stretch	462.1	Ar	IR	1
a''	9	SiCl stretch	629.3	Ar	IR	1

$SiCl_3OD$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2722.4	Ar	IR	1
		SiO stretch	937.9[a]	Ar	IR	1
			891.2[a]	Ar	IR	1
	5	SiCl stretch	459.9	Ar	IR	1

[a] Fermi resonance interaction.

References

[1]A. E. Shirk and J. S. Shirk, J. Mol. Spectrosc. **92**, 218 (1982).
[2]H. Niki, P. D. Maker, C. M. Savage, L. P. Breitenbach, and M. D. Hurley, J. Phys. Chem. **89**, 3725 (1985).

Li_6

A prominent absorption maximum at about 20000 (500 nm) and a weaker absorption maximum at 14500 (690 nm), observed in depletion photoionization experiments[1] on gas-phase Li_6, have been assigned to the C_{2v} structure of that species.

References

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Na_6

A prominent absorption maximum at 16800 (596 nm), an absorption maximum at 22800 (438 nm), and relatively weak maxima at 14400 (696 nm) and 19700 (508 nm), observed in depletion photoionization experiments[1,2] on gas-phase Na_6, have been assigned[2] to the D_{3h} structure of that species.

References

[1]K. Selby, V. Kresin, J. Masui, M. Vollmer, W. A. de Heer, A. Scheidemann, and W. D. Knight, Phys. Rev. B **43**, 4565 (1991).
[2]C. R. C. Wang, S. Pollack, T. A. Dahlseid, G. M. Koretsky, and M. M. Kappes, J. Chem. Phys. **96**, 7931 (1992).

C_6

In an argon matrix, the growth behavior of the 1952.5 cm^{-1} infrared absorption on sample warmup has been tentatively correlated with that of an absorption maximum near 246 nm.[4]

$\tilde{X}\ ^3\Sigma_g^-$ $D_{\infty h}$ Structure: ESR[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	2061(10)	gas	TPE	6
	2	Sym. stretch	1322(10)	gas	TPE	5,6
	3	Stretch	489(10)	gas	TPE	6
Σ_u^+	4	Asym. stretch	1952.0	Ar	IR	3,4,7
	5	Asym. stretch	1197.3	Ar	IR	1,3,7
Π_g	7	Bend	240HT	gas	PE	5

References

[1]K. R. Thompson, R. L. DeKock, and W. Weltner, Jr., J. Am. Chem. Soc. **93**, 4688 (1971).
[2]R. J. Van Zee, R. F. Ferrante, K. J. Zeringue, and W. Weltner, Jr., J. Chem. Phys. **88**, 3465 (1988).
[3]M. Vala, T. M. Chandrasekhar, J. Szczepanski, and R. Pellow, High Temp. Sci. **27**, 19 (1988/89).
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C_6^-

Threshold for electron detachment from ground-state C_6^- = 33725(10) gas PE[1,2]TPE[3]

$\tilde{A}\ ^2\Pi_g$? $D_{\infty h}$
T_0 = 33680T gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		2058(5)	gas	PE	3
	2		1307(5)	gas	PE	3
	3		480(2)	gas	PE	3
Σ_u^+	5		837HT	gas	PE	3
Π_g	7		195HT	gas	PE	3
Π_u	8		313HT	gas	PE	3
	9		93HT	gas	PE	3

$\tilde{X}\ ^2\Pi_u$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_g	7		220T	gas	PE	3
Π_u	9		111T	gas	PE	3

A = −29(2) gas PE[3]

References

[1]S. Yang, K. J. Taylor, M. J. Craycraft, J. Conceicao, C. L. Pettiette, O. Cheshnovsky, and R. E. Smalley, Chem. Phys. Lett. **144**, 431 (1988).
[2]D. W. Arnold, S. E. Bradforth, T. N. Kitsopoulos, and D. M. Neumark, J. Chem. Phys. **95**, 8753 (1991).
[3]C. C. Arnold, Y. Zhao, T. N. Kitsopoulos, and D. M. Neumark, J. Chem. Phys. **97**, 6121 (1992).

$NCC{\equiv}CCN^+$

$\tilde{D}\ ^2\Pi_u$ $D_{\infty h}$
T_0 = 25500(160) gas PE[1,3]

$\tilde{C}\ ^2\Sigma_u^+$ $D_{\infty h}$
T_0 = 18720(160) gas PE[1,3]

$\tilde{B}\ ^2\Sigma_g^+$ $D_{\infty h}$
T_0 = 17430(160) gas PE[1,3]

$\tilde{A}\ ^2\Pi_g$ $D_{\infty h}$
T_0 = 16781(1) gas EF^2LF^3 $\tilde{A}$–$\tilde{X}$ 528–720 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡N stretch	2151(3)	gas	LF	3
	2	C≡C stretch	2099(3)	gas	LF	3
	3	C–C stretch	696(3)	gas	LF	3

τ = 13(2) ns gas EF^2PEFCO^3

$\tilde{X}\ ^2\Pi_u$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡N stretch	2210(10)	gas	EF	2,3
	2	C≡C stretch	1930(10)	gas	EF	2,3
	3	C–C stretch	570(10)	gas	EF	2,3

References

[1]G. Bieri, E. Heilbronner, V. Hornung, E. Kloster– Jensen, J. P. Maier, F. Thommen, and W. Von Niessen, Chem. Phys. **36**, 1 (1979).
[2]J. P. Maier, O. Marthaler, and F. Thommen, Chem. Phys. Lett. **60**, 193 (1979).
[3]J. P. Maier, L. Misev, and F. Thommen, J. Phys. Chem. **86**, 514 (1982).

C_5S

$\tilde{X}\ ^1\Sigma^+$ $C_{\infty v}$
B_0 = 0.031 MW[1]

References

[1]Y. Kasai, K. Obi, Y. Ohshima, Y. Hirahara, Y. Endo, K. Kawaguchi, and A. Murakami, Astrophys. J. **410**, L45 (1993).

NCCCNC

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡C stretch	2287.1s	Ar	IR	1
	2	–C≡N stretch	2203.6s	Ar	IR	1
	3	–N≡C stretch	2044.8vs	Ar	IR	1
	4	C–C,C–N a–stretch	1202.3vw	Ar	IR	1
	5	C–C,C–N s–stretch	610.1vw	Ar	IR	1

References

[1]A. M. Smith, G. Schallmoser, A. Thoma, and V. E. Bondybey, J. Chem. Phys. **98**, 1776 (1993).

CNCCNC

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm η1	Med.	Type meas.	Refs.
Σ_u^+	4	C≡N a–stretch	2114.9vs	Ar	IR	1
	5	C–N a–stretch	1287.5m	Ar	IR	1

References

[1]A. M. Smith, G. Schallmoser, A. Thoma, and V. E. Bondybey, J. Chem. Phys. **98**, 1776 (1993).

$CO(CN)_2^+$

T^a = 43100(1000) gas PE[1]

T^a = 33400(1000) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CO stretch	1580(80)	gas	PE	1
		CC stretch	700(80)	gas	PE	1

T^a = 17990(320) gas PE[1]

T^a = 14930(320) gas PE[1]

T^a = 9680(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]R. K. Thomas and H. Thompson, Proc. Roy. Soc. (London) **A327**, 13 (1972).

C_4O_2

In an argon matrix, an absorption maximum has been observed[1] at 212 nm.

In an argon matrix, absorption maxima have been observed[1] at 334 and 340 nm, and irradiation in the 300–440 nm spectral region leads to dissociation forming C_3O + CO.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2130.3vs	Ar	IR	1
			1276.9wm	Ar	IR	1
			467.1w	Ar	IR	1

References

[1]G. Maier, H. P. Reisenauer, H. Balli, W. Brandt, and R. Janoschek, Angew. Chem. **102**, 920 (1990); Angew. Chem. Int. Ed. Engl. **29**, 905 (1990).

C_4OS

$\tilde{B}$

T_0 = 42000 Ar AB[1]

$\tilde{A}$

T_0 = 23470 Ar AB[1] $\tilde{A}$–$\tilde{X}$ 410–426 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			450	Ar	AB	1

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1		2209.6vs	Ar	IR	1
	2		1998.5m	Ar	IR	1
	3		1625.3w	Ar	IR	1
	4		1055.9wm	Ar	IR	1
	5		486.0w	Ar	IR	1
Π	7		428.1w	Ar	IR	1

References

[1]G. Maier, J. Schrot, H. P. Reisenauer, and R. Janoschek, Chem. Ber. **124**, 2617 (1991).

C_4S_2

$\tilde{B}$

T_0 = 36765 Ar AB[1]

$\tilde{A}$

T_0 = 19455 Ar AB[1] $\tilde{A}$–$\tilde{X}$ 440–514 nm

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		2021T[a]	Ar	IR	1
	2		1382T[a]	Ar	IR	1
	3		423T[a]	Ar	IR	1
Σ_u^+	4		1872.1vs	Ar	IR	1
	5		897.7wm	Ar	IR	1
			843.7wmT	Ar	IR	1

[a] From combination bands.

References

[1]G. Maier, J. Schrot, H. P. Reisenauer, and R. Janoschek, Chem. Ber. **124**, 2617 (1991).

$F(C\equiv C)_2F^+$

$\tilde{D}$ $^2\Sigma_g^+$ $D_{\infty h}$

T_0 = 72200(1200) gas PE[1]

$\tilde{C}$ $^2\Pi_{u,3/2}$ $D_{\infty h}$

T_0 = 63700(800) gas PE[1]

$\tilde{B}$ $^2\Pi_{g,3/2}$ $D_{\infty h}$

T_0 = 59700(800) gas PE[1]

$\tilde{A}$ $^2\Pi_{u,3/2}$ $D_{\infty h}$

T_0 = 21230(10) gas EF[2] $\tilde{A}$–$\tilde{X}$ 460–610 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2290(80)	gas	PE	2
	2	CF stretch	1450(80)	gas	PE	2
	3	C–C stretch	520(80)	gas	PE	2

τ = 28(3) ns gas PEFCO[2]

$\tilde{X}$ $^2\Pi_{g,3/2}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2320(10)	gas	EF	2
	2	CF stretch	1550(10)	gas	EF	2
	3	C–C stretch	520(10)	gas	EF	2
Π_g	7	Deformation	300(10)H	gas	EF	2

References

[1]G. Bieri, E. Heilbronner, J.-P. Stadelmann, J. Vogt, and W. von Niessen, J. Am. Chem. Soc. **99**, 6832 (1977).
[2]M. Allan, J. P. Maier, O. Marthaler, and J.-P. Stadelmann, J. Chem. Phys. **70**, 5271 (1979).

$Cl(C\equiv C)_2Cl^+$

$\tilde{E}$
$T_0 \leq 64060(560)$ gas PE[1]

$\tilde{D}$
$T_0 \leq 60600(560)$ gas PE[1]

$\tilde{C}\ ^2\Pi_u$ $D_{\infty h}$
$T_0 \leq 38730(320)$ gas PE[1]

$\tilde{B}\ ^2\Pi_g$ $D_{\infty h}$
$T_0 \leq 35580(320)$ gas PE[1]

$\tilde{A}\ ^2\Pi_{u,3/2}$ $D_{\infty h}$
$T_0 = 19081(0.5)$ gas EF^4LF^4 $\tilde{A}-\tilde{X}$ 460–690 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2125(2)	gas	LF	4
	2	C–C stretch	1179(1)	gas	EF,LF	3,4
	3	CCl stretch	373(1)	gas	EF,LF	3,4
Π_g	7	Skel. deform.	222(2)H	gas	LF	4
Π_u	9	Skel. deform.	78(2)H	gas	LF	4

$\tau_1 = 21(2)$ ns gas EF^2PEFCO^3
$\tau_2 \cong 0.5$ μs gas EF^2
$A \cong -230$ gas LF^4

$\tilde{X}\ ^2\Pi_{g,3/2}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C s–stretch	2214	gas	EF	2–4
	2	C–C stretch	1316	gas	EF	2–4
	3	CCl s–stretch	393	gas	EF	2–4
Σ_u^+	5	CCl a–stretch	657	gas	EF	4

$A \cong -180$ gas LF^4

References

[1]E. Heilbronner, V. Hornung, J. P. Maier, and E. Kloster-Jensen, J. Am. Chem. Soc. **96**, 4252 (1974).
[2]M. Allan, E. Kloster-Jensen, J. P. Maier, and O. Marthaler, J. Electron Spectrosc. Relat. Phenom. **14**, 359 (1978).
[3]J. P. Maier, O. Marthaler, L. Misev, and F. Thommen, J. Chem. Soc., Faraday Disc. **71**, 181 (1981).
[4]D. Klapstein, J. P. Maier, and L. Misev, J. Chem. Phys. **78**, 5393 (1983).

$Br(C\equiv C)_2Br^+$

$\tilde{E}$
$T_0 \leq 56480(560)$ gas PE[1]

$\tilde{D}$
$T_0 \leq 53650(560)$ gas PE[1]

$\tilde{C}\ ^2\Pi_u$ $D_{\infty h}$
$T_0 \leq 32840(320)$ gas PE[1]
$A = -730(320)$ gas PE[1]

$\tilde{B}\ ^2\Pi_g$ $D_{\infty h}$
$T_0 \leq 27670(320)$ gas PE[1]
$A = -1775(320)$ gas PE[1]

$\tilde{A}\ ^2\Pi_{u,3/2}$ $D_{\infty h}$
$T_0 = 16838(0.5)$ gas EF^3LF^3 $\tilde{A}-\tilde{X}$ 510–695 nm

Vib. sym.	No.	Approxhmate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2186(2)	gas	LF	3
	2	C–C stretch	1071(2)	gas	LF	3
	3	CBr stretch	242(1)	gas	EF,LF	3
Π_g	7	Skel. deform.	281HT	gas	LF	3
Π_u	9	Skel. deform.	62(2)H	gas	LF	3

$\tau_1 = 12(2)$ ns gas EF^2
$\tau_2 \cong 0.5$ μs gas EF^2
$A = -1450(80)$ gas $PE^{1,2}$

$\tilde{X}\ ^2\Pi_{g,3/2}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C s–stretch	2186	gas	EF	2,3
	2	C–C stretch	1225	gas	EF	2,3
	3	CBr s–stretch	252	gas	EF	2,3

$A = -950(80)$ gas PE^1LF^3

References

[1]E. Heilbronner, V. Hornung, J. P. Maier, and E. Kloster-Jensen, J. Am. Chem. Soc. **96**, 4252 (1974).
[2]M. Allan, E. Kloster-Jensen, J. P. Maier, and O. Marthaler, J. Electron Spectrosc. Relat. Phenom. **14**, 359 (1978).
[3]D. Klapstein, J. P. Maier, and L. Misev, J. Chem. Phys. **78**, 5393 (1983).

$I(C\equiv C)_2I^+$

$\tilde{E}$
$T_0 \leq 49540(560)$ gas PE[1]

$\tilde{D}$
$T_0 \leq 47120(560)$ gas PE[1]

$\tilde{C}\ ^2\Pi_u$ $D_{\infty h}$
$T_0 \leq 30180(320)$ gas PE[1]
$A = -890(320)$ gas PE[1]

$\tilde{B}\ ^2\Pi_g$ $D_{\infty h}$
$T_0 \leq 21300(320)$ gas PE[1]
$A = -3150(320)$ gas PE[1]

$\tilde{A}\ ^2\Pi_{u,3/2}$ $D_{\infty h}$
$T_0 \cong 12013$ gas PE[1,3]
11973(2) Ne AB[3] $\tilde{A}-\tilde{X}$ 600–840 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2216(3)	Ne	AB	3
	2	C–C stretch	970(80)	gas	PE	1
	3	CI stretch	183(3)	Ne	AB	3
Π_g	7	Skel. deform.	190L	Ne	AB	3

$A = -4280(320)$ gas PE[1]

$\tilde{X}\ ^2\Pi_{u,3/2}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2100(80)	gas	PE	1

A = −2340(320) gas PE[1]

References

[1]E. Heilbronner, V. Hornung, J. P. Maier, and E. Kloster-Jensen, J. Am. Chem. Soc. **96**, 4252 (1974).
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$(SCN)_2^+$

$\tilde{J}\ ^2A$ C_2
T^a = 58500(1000) gas PE[1]

$\tilde{I}\ ^2B$ C_2
T^a = 43250(320) gas PE[1]

$\tilde{H}\ ^2A$ C_2
T^a = 33480(320) gas PE[1]

$\tilde{G}\ ^2B$ C_2
T^a = 25660(320) gas PE[1]

$\tilde{F}\ ^2A$ C_2
T^a = 23480(320) gas PE[1]

$\tilde{E}\ ^2A$ C_2
T^a = 21060(320) gas PE[1]

$\tilde{D}\ ^2B$ C_2
T^a = 19690(320) gas PE[1]

$\tilde{C}\ ^2B$ C_2
T^a = 19040(320) gas PE[1]

$\tilde{B}\ ^2A$ C_2
T^a = 11050(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	CN stretch	1590(60)	gas	PE	1

$\tilde{A}\ ^2B$ C_2
T^a = 2180(320) gas PE[1]

$\tilde{X}\ ^2A$ C_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a			920(80)	gas	PE	1

[a] From vertical ionization potentials.

References

[1]D. C. Frost, C. Kirby, W. M. Lau, C. B. MacDonald, C. A. McDowell, and N. P. C. Westwood, Chem. Phys. Lett. **69**, 1 (1980).

$(SiO)_3$

$\tilde{X}$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	4	Deformation	74T	Ar	IR	2
e'	5	SiO stretch	971.9s	Ar	IR	1–3
			972.6	N_2	IR	1
	6	SiO stretch	629.0w	Ar	IR	1,2
			631.5	N_2	IR	1
	7	Deformation	311.5w	Ar	IR	1,2
			312.0	N_2	IR	1

References

[1]J. S. Anderson and J. S. Ogden, J. Chem. Phys. **51**, 4189 (1969).
[2]J. W. Hastie, R. H. Hauge, and J. L. Margrave, Inorg. Chim. Acta **3**, 601 (1969).
[3]L. Andrews and M. McCluskey, J. Mol. Spectrosc. **154**, 223 (1992).

$(GeO)_3$

$\tilde{X}$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	5	GeO stretch	825.4s	Ar	IR	1,2
			824	N_2	IR	1
	6	GeO stretch	438w	Ar	IR	1
			440	N_2	IR	1

References

[1]J. S. Ogden and M. J. Ricks, J. Chem. Phys. **52**, 352 (1970).
[2]L. Andrews and M. McCluskey, J. Mol. Spectrosc. **154**, 223 (1992).

$(PN)_3$

$\tilde{X}$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	5	PN stretch	1141	Ar	IR	2
			1137s	Kr	IR	1
	6	PN stretch	718w	Kr	IR	1

References

[1]R. M. Atkins and P. L. Timms, Spectrochim. Acta **33A**, 853 (1977).
[2]R. Ahlrichs, M. Bär, H. S. Plitt, and H. Schnöckel, Chem. Phys. Lett. **161**, 179 (1989).

$F_2C{=}C{=}C{=}O$

The gas-phase ultraviolet absorption spectrum[1] shows maxima at 375 and 240 nm.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			2169.1vs	gas	IR	1
			1763.6m	gas	IR	1
			1248.4wm	gas	IR	1
			1194.4wm	gas	IR	1
			821.9w	gas	IR	1
			611.2w	gas	IR	1
			522.9w	gas	IR	1
			486.3w	Ar	IR	1
a''			656.7w	gas	IR	1

References

[1]J. C. Brahms and W. P. Dailey, J. Am. Chem. Soc. **111**, 3071 (1989).

$F_2C{=}C{=}N{=}N$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2104.7	N_2	IR	1
			2085.2	N_2	IR	1
			1672.7	N_2	IR	1
			1650.7	N_2	IR	1
			1262.8	N_2	IR	1
			1143.9	N_2	IR	1
			834.9	N_2	IR	1

References

[1]J. C. Brahms and W. P. Dailey, J. Am. Chem. Soc. **112**, 4046 (1990).

cyc-(CF=CFC)=O

$\tilde{X}$ C_{2v} Structure: MW^2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1919	gas	IR	2
			1914.5m	Ar	IR	1
			1786	gas	IR	2
			1779.9m	Ar	IR	1
			1761.2m	Ar	IR	1
			1283	gas	IR	2
			1285.5s	Ar	IR	1
			1071.4w	Ar	IR	1
			862	gas	IR	2
			860.2w	Ar	IR	1
			699.6w	Ar	IR	1
			656.0w	Ar	IR	1

$A_0 = 0.133$; $B_0 = 0.128$; $C_0 = 0.065$ MW^2

References

[1]J. C. Brahms and W. P. Dailey, J. Am. Chem. Soc. **111**, 8940 (1989).
[2]C. A. Jacobs, J. C. Brahms, W. P. Dailey, K. Beran, and M. D. Harmony, J. Am. Chem. Soc. **114**, 115 (1992).

$S_3N_3^+$

$T^a = 76500(1000)$ gas PE[1]

$T^a = 45000(1000)$ gas PE[1]

$T^a = 39400(1000)$ gas PE[1]

$T^a = 34500(1000)$ gas PE[1]

$T^a = 32100(1000)$ gas PE[1]

$T^a = 20000(1000)$ gas PE[1]

$\tilde{X}\ ^3A_2'$ D_{3h}[b]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			870(50)	gas	PE	1
			630(50)	gas	PE	1

[a] From vertical ionization potentials.
[b] Calculations suggest that this state may experience Jahn–Teller distortion to give a $^3B_2$ state, of C_{2v} symmetry.

References

[1]W. M. Lau, N. P. C. Westwood, and M. H. Palmer, J. Am. Chem. Soc. **108**, 3229 (1986).

$B_2F_4^+$

$\tilde{F}\ ^2E$ D_{2d}
$T_0 = 66890(560)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		BB stretch	600(60)	gas	PE	1

$\tilde{E}\ ^2E$ D_{2d}
$T_0 = 52280(720)$ gas PE[1]

$\tilde{D}\ ^2B_2$ D_{2d}
$T_0 = 40100(560)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		BB stretch	600(100)	gas	PE	1

$\tilde{A},\tilde{B},\tilde{C}\ ^2E,^2A_2,^2B_1$ D_{2d}
$T_0 = 26380(720)$ gas PE[1]

$\tilde{X}\ ^2A_1$ D_{2d}

References

[1]N. Lynaugh, D. R. Lloyd, M. F. Guest, M. B. Hall, and I. H. Hillier, J. Chem. Soc., Faraday Trans. 2 **68**, 2192 (1972).

$B_2Cl_4^+$

$\tilde{I}\ ^2A_1$ D_{2d}
T_0 = 60350(400) gas PE[1]

$\tilde{H}\ ^2B_2$ D_{2d}
T_0 = 49860(240) gas PE[1]

$\tilde{F},\tilde{G}\ ^2E,^2A_1$ D_{2d}
T_0 = 32270(320) gas PE[1]

$\tilde{D},\tilde{E}\ ^2B_2,^2E$ D_{2d}
T_0 = 23560(320) gas PE[1]

$\tilde{A},\tilde{B},\tilde{C}\ ^2E,^2A_2,^2B_1$ D_{2d}
T_0 = 8630(240) gas PE[1]

$\tilde{X}\ ^2A_1$ D_{2d}

References

[1]N. Lynaugh, D. R. Lloyd, M. F. Guest, M. B. Hall, and I. H. Hillier, J. Chem. Soc., Faraday Trans. 2 **68**, 2192 (1972).

t–$(FCO)_2^+$

$\tilde{H}$
T^a = 52360(480) gas PE[1]

$\tilde{G}\ ^2A_u$ C_2
T^a = 46880(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			560(40)	gas	PE	1

$\tilde{F}\ ^2B_u$ C_2
T^a = 39130(480) gas PE[1]

$\tilde{E}\ ^2B_g$ C_2
T^a = 30420(480) gas PE[1]

$\tilde{D}$ C_2
T^a = 27030(480) gas PE[1]

$\tilde{C}\ ^2A_u$ C_2
T_0 = 24690(480) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1130(40)	gas	PE	1

$\tilde{B}\ ^2B_u$ C_2
T_0 = 17190(480) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1410(40)	gas	PE	1
			1280(40)	gas	PE	1

$\tilde{A}\ ^2B_g$ C_2
T_0 = 14040(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1600(30)	gas	PE	1
			380(30)	gas	PE	1

$\tilde{X}\ ^2A_g$ C_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			570(30)	gas	PE	1
			300(30)	gas	PE	1

[a] From vertical ionization potential.

References

[1]D. C. Frost, C. A. McDowell, G. Pouzard, and N. P. C. Westwood, J. Electron Spectrosc. Relat. Phenom. **10**, 273 (1977).

t–$(ClCO)_2^+$

$\tilde{K}$ C_2
T^a = 67300(1200) gas PE[1]

$\tilde{J}$ C_2
T^a = 61800(800) gas PE[1]

$\tilde{I}$ C_2
T^a = 50430(560) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1270(70)	gas	PE	1

$\tilde{H}\ ^2A_u$ C_2
T^a = 48090(800) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1400(70)	gas	PE	1

$\tilde{G}$ C_2
T^a = 41390(800) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1225(70)	gas	PE	1

$\tilde{F}$ ^2B_g C_2
T_0 = 31790(560) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1650(50)	gas	PE	1
			820(50)	gas	PE	1

$\tilde{E}$ ^2B_u C_2
T^a = 21780(560) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1660(50)	gas	PE	1
			600(50)	gas	PE	1

$\tilde{D}$ C_2
T^a = 17190(800) gas PE[1]

$\tilde{C}$ C_2
T^a = 15980(800) gas PE[1]

$\tilde{B}$ C_2
T^a = 13960(800) gas PE[1]

$\tilde{A}$ C_2
T^a = 11860(800) gas PE[1]

$\tilde{X}$ ^2A_g C_2

[a] From vertical ionization potential.

References

[1]D. C. Frost, C. A. McDowell, G. Pouzard, and N. P. C. Westwood, J. Electron Spectrosc. Relat. Phenom. **10**, 273 (1977).

$N_2O_4^+$

$\tilde{G}$ $^2B_{2g}$ D_{2h}
T^a = 58500(1200) gas PE[1-5]

$\tilde{F}$ $^2B_{3g}$ D_{2h}
T^a = 45200(1600) gas PE[1-5]

$\tilde{E}$ $^2B_{1u}$ D_{2h}
T^a = 33900(1600) gas PE[1-5]

$\tilde{C}$,$\tilde{D}$ $^2B_{1g}$, $^2B_{3u}$ D_{2h}
T^a = 16700(1000) gas PE[1-5]

$\tilde{B}$ ^2A_u D_{2h}
T^a = 13200(1000) gas PE[1-5]

$\tilde{A}$ $^2B_{2g}$ D_{2h}
T^a = 7700(900) gas PE[1-5]

$\tilde{X}$ ^2A_g D_{2h}

[a] From vertical ionization potentials.

References

[1]D. L. Ames and D. W. Turner, Proc. Roy. Soc. (London) **A348**, 175 (1976).
[2]D. C. Frost, C. A. McDowell, and N. P. C. Westwood, J. Electron Spectrosc. Relat. Phenom. **10**, 293 (1977).
[3]T. H. Gan, J. B. Peel, and G. D. Willett, J. Chem. Soc., Faraday Trans. 2 **73**, 1459 (1977).
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$N_2S_4^+$

$\tilde{H}$ $^2A'$ C_s
T^a = 47680(320) gas PE[1]

$\tilde{G}$ $^2A'$ C_s
$T^a \cong$ 44500 gas PE[1]

$\tilde{F}$ $^2A''$ C_s
T^a = 37520(320) gas PE[1]

$\tilde{E}$ $^2A'$ C_s
T^a = 31630(320) gas PE[1]

$\tilde{D}$ $^2A''$ C_s
T^a = 28400(320) gas PE[1]

$\tilde{C}$ $^2A'$ C_s
T^a = 20010(320) gas PE[1]

$\tilde{B}$ $^2A''$ C_s
T^a = 17270(320) gas PE[1]

$\tilde{A}$ $^2A'$ C_s
T^a = 6450(320) gas PE[1]

$\tilde{X}$ $^2A''$ C_s

[a] From vertical ionization potentials.

References

[1]M. H. Palmer, W.-M. Lau, and N. P. C. Westwood, Z. Naturforsch. **37a**, 1061 (1982).

PF_2NCO^+

$\tilde{F}$ C_s
T^a = 67400(1000) gas PE[1]

$\tilde{E}$ C_s
T^a = 53700(1000) gas PE[1]

$\tilde{D}$ C_s
T^a = 44800(1000) gas PE[1]

$\tilde{C}$ C_s
T^a = 38300(1000) gas PE[1]

$\tilde{B}$ C_s
T^a = 17300(1000) gas PE[1]

$\tilde{A}$ C_s
T^a = 9280(1000) gas PE[1]

[a] From vertical ionization potentials.

References

[1]S. Cradock and D. W. H. Rankin, J. Chem. Soc., Faraday Trans. 2 **68**, 940 (1972).

PF_2NCS^+

$\tilde{E}$ C_s
T^a = 62900(1600) gas PE[1]

$\tilde{D}$ C_s
T^a = 50000(1600) gas PE[1]

$\tilde{C}$ C_s
T^a = 42800(1600) gas PE[1]

$\tilde{B}$ C_s
T^a = 29900(1600) gas PE[1]

$\tilde{A}$ C_s
T^a = 13700(1600) gas PE[1]

[a] From vertical ionization potentials.

References

[1]S. Cradock and D. W. H. Rankin, J. Chem. Soc., Faraday Trans. 2 **68**, 940 (1972).

N_2O_4

In the gas phase, absorption increases between 300 and 180 nm, with some indication of maxima near 265 and 190 nm.[7]

A broad gas–phase absorption with onset near 380 nm has its maximum near 340 nm.[7]

$\tilde{X}$ D_{2h} Structure: ED[1]IR[10,11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1		1383(3)	Ne	Ra	8
			1383	Ar	Ra	5
			1387(3)	Xe	Ra	8
	2		807(3)	Ne	Ra	8
			813	Ar	Ra	5
			815(3)	Xe	Ra	8
	3		265(3)	Ne	Ra	8
			262	Ar	Ra	5
			257(3)	Xe	Ra	8
a_u	4		82T	gas	IR[a]	6,12
b_{1g}	5		1718(3)	Xe	Ra	8
	6		480T	gas	IR[a]	6,12
			498(3)	Ne	Ra	8
			485(3)	Xe	Ra	8
b_{1u}	7		425	gas	IR	6
b_{2g}	8		657(3)	Xe	Ra	8

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}	9		1756.76	gas	IR	6,10
			1749.2s	Ar	IR	2,3,9
			1735s			
			1761	N_2	IR	4
			1737			
			1750	O_2	IR	3
			1735			
	10		265T	gas	IR	11
b_{3u}	11		1261.08	gas	IR	2,6,11
			1257.0s	Ar	IR	2,3,9
			1261	N_2	IR	4
			1261	O_2	IR	3
	12		751	gas	IR	6
			755sh	Ar	IR	3
			745.8			
			751	N_2	IR	4
			755	O_2	IR	3
			746			

A_0 = 0.217(2); B_0 = 0.122; C_0 = 0.078 IR[10,11]
Barrier to internal rotation = 1900(200) gas IR[12]

[a] From analysis of sequence bands near 540 cm^{-1}.

References

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[2]W. G. Fateley, H. A. Bent, and B. Crawford, Jr., J. Chem. Phys. **31**, 204 (1959).
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[4]E. L. Varetti and G. C. Pimentel, J. Chem. Phys. **55**, 3813 (1971).
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N_2O_4 (V_d)

$\tilde{X}$ V_d ?

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1717	Ar	IR	1,2
			1718	O_2	IR	1,2
			1282	Ar	IR	1
			1282	O_2	IR	1
			752	Ar	IR	1
			752	O_2	IR	1

References

[1]W. G. Fateley, H. A. Bent, and B. Crawford, Jr., J. Chem. Phys. **31**, 204 (1959).
[2]R. V. St. Louis and B. Crawford, Jr., J. Chem. Phys. **42**, 857 (1965).

ONO–NO_2 (D)

In an argon matrix, photolysis is observed[6] at 436 nm, but not at wavelengths longer than 510 nm. The major product is N_2O_4 (V_h), but infrared absorptions of NO, c-$(NO)_2$, O_2N–NO, and N_2O_5 also grow in intensity.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		N=O stretch	1806(3)	Ne	Ra	5
			1828	Ar	IR	1,2,6
			1861	N_2	IR	3
			1829	O_2	IR	1,2,4
		NO_2 a–stretch	1635(3)	Ne	Ra	5
			1644	Ar	IR	1,2,6
			1646(3)	Xe	Ra	5
			1628	N_2	IR	3
			1645	O_2	IR	1,2,4
		NO_2 s–stretch	1295(3)	Ne	Ra	5
			1290	Ar	IR	1,2,6
			1299(3)	Xe	Ra	5
			1279	N_2	IR	3
			1291	O_2	IR	1,2,4
		N–O stretch	903	Ar	IR	6
			905	O_2	IR	2
		NO_2 bend	783(3)	Ne	Ra	5
			787	Ar	IR	1,2,6
			788(3)	Xe	Ra	5
			792	N_2	IR	3
			783	O_2	IR	1,2,4
		O=N–O bend	622(3)	Ne	Ra	5
			626(3)	Xe	Ra	5
			647	N_2	IR	3
			642	O_2	IR	2,4
		NO_2 rock or wag	488	O_2	IR	2,4
			304	O_2	IR	4

References

[1]W. G. Fateley, H. A. Bent, and B. Crawford, Jr., J. Chem. Phys. **31**, 204 (1959).
[2]R. V. St. Louis and B. Crawford, Jr., J. Chem. Phys. **42**, 857 (1965).
[3]E. L. Varetti and G. C. Pimentel, J. Chem. Phys. **55**, 3813 (1971).
[4]G. R. Smith and W. A. Guillory, J. Mol. Spectrosc. **68**, 223 (1977).
[5]F. Bolduan and H. J. Jodl, Chem. Phys. Lett. **85**, 283 (1982).
[6]H. Bandow, H. Akimoto, S. Akiyama, and T. Tezuka, Chem. Phys. Lett. **111**, 496 (1984).

ONO–NO_2 (D′)

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		N=O stretch	1873(3)	Ne	Ra	2
			1899	O_2	IR	1
			1889			

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO_2 a–stretch	1584	O_2	IR	1
		NO_2 s–stretch	1290	O_2	IR	1
		N–O stretch	949(3)	Ne	Ra	2
			953(3)	Xe	Ra	2
			916	O_2	IR	1
		NO_2 bend	794	O_2	IR	1
		O=N–O bend	660	O_2	IR	1
		NO_2 rock or wag	524	O_2	IR	1

References

[1]R. V. St. Louis and B. Crawford, Jr., J. Chem. Phys. **42**, 857 (1965).
[2]F. Bolduan and H. J. Jodl, Chem. Phys. Lett. **85**, 283 (1982).

cyc–N_2S_4

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			882.3	Ar	IR	1
			773.0	Ar	IR	1

References

[1]P. Hassanzadeh and L. Andrews, J. Am. Chem. Soc. **114**, 83 (1992).

P_2S_4

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			748.9T	Ar	IR	1

References

[1]Z. Mielke, G. D. Brabson, and L. Andrews, J. Phys. Chem. **95**, 75 (1991).

$C_2F_4^+$

$\tilde{H}, \tilde{I}\ ^2B_{3g}, ^2B_{3u}$ D_{2h}
T_0 = 73020(320) gas PE[1,4]

$\tilde{G}\ ^2B_{2g}$ D_{2h}
T^a = 65190(320) gas PE[2–4]

$\tilde{F}\ ^2B_{1u}$ D_{2h}
T_0 = 59460(400) gas PE[1–4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g		CF s–stretch	740(80)	gas	PE	1
		CF_2 deform.	330(80)	gas	PE	1

$\tilde{B},\tilde{C},\tilde{D},\tilde{E}\ ^2A_g, ^2B_{2u}, ^2A_u, ^2B_{1g}$ D_{2h}
$T^a \cong 52000$ gas PE[1-4]

$\tilde{A}\ ^2B_{3g}$ D_{2h}
$T^a = 46880(320)$ gas PE[1-4]

$\tilde{X}\ ^2B_{3u}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g		C=C stretch	1710(80)	gas	PE	1–3
		CF s-stretch	820(80)	gas	PE	1–3
			400(80)	gas	PE	2,3

[a] From vertical ionization potential.

References

[1]R. F. Lake and H. Thompson, Proc. Roy. Soc. (London) **A315**, 323 (1970).
[2]C. R. Brundle, M. B. Robin, N. A. Kuebler, and H. Basch, J. Am. Chem. Soc. **94**, 1451 (1972).
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[4]G. Bieri, W. von Niessen, L. Åsbrink, and A. Svensson, Chem. Phys. **60**, 61 (1981).

$CF_2{=}CFCl^+$

$\tilde{H}\ ^2A'$ C_s
$T^a = 72130(320)$ gas PE[3,4]

$\tilde{G}\ ^2A''$ C_s
$T^a = 64060(320)$ gas PE[1,3,4]

$\tilde{F}\ ^2A'$ C_s
$T^a = 57610(320)$ gas PE[1,3,4]

$\tilde{E}\ ^2A''$ C_s
$T^a = 55190(600)$ gas PE[1,3,4]

$\tilde{D}\ ^2A'$ C_s
$T^a = 51960(600)$ gas PE[1,3,4]

$\tilde{C}\ ^2A'$ C_s
$T^a = 42840(320)$ gas PE[1,3,4]

$\tilde{B}\ ^2A''$ C_s
$T^a = 30980(320)$ gas PE[1,3,4]

$\tilde{A}\ ^2A'$ C_s
$T^a = 25900(320)$ gas PE[1,3,4]

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		C=C stretch	1590(80)	gas	PE	1,3,4
		CF stretch	1120(80)	gas	PE	1,3,4
		CCl stretch	680(80)	gas	PE	1,3,4
		CF_2 rock	330(80)	gas	PE	3,4

[a] From vertical ionization potential. The first ionization potential is taken as 9.76 eV, as in the spectroscopic study of Ref. 2.

References

[1]R. F. Lake and H. Thompson, Proc. Roy. Soc. (London) **A315**, 323 (1970).
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$CF_2{=}CCl_2^+$

$\tilde{I}\ ^2A_1$ C_{2v}
$T^a = 68820(400)$ gas PE[1-3]

$\tilde{F},\tilde{G},\tilde{H}\ ^2A_1, ^2B_2, ^2A_2$ C_{2v}
$T^a = 53250(320)$ gas PE[1-3]

$\tilde{E}\ ^2B_2$ C_{2v}
$T^a = 47200(320)$ gas PE[1-3]

$\tilde{D}\ ^2B_1$ C_{2v}
$T^a = 38570(320)$ gas PE[1-3]

$\tilde{C}\ ^2A_1$ C_{2v}
$T_0 = 25660(320)$ gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CCl_2 scissors	250(40)	gas	PE	1–3

$\tilde{B}\ ^2A_2$ C_{2v}
$T_0 = 23240(320)$ gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CF_2 s-stretch	1070(60)	gas	PE	1–3
			600(40)	gas	PE	2
		CCl_2 scissors	190(40)	gas	PE	1–3

$\tilde{A}\ ^2B_2$ C_{2v}
$T^a = 20000(400)$ gas PE[1-3]

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		C=C stretch	1540(40)	gas	PE	1–3
		CF_2 s-stretch	1160(80)	gas	PE	1–3
		CCl_2 s-stretch	530(80)	gas	PE	1–3

[a] From vertical ionization potential.

References

[1]R. F. Lake and H. Thompson, Proc. Roy. Soc. (London) **A315**, 323 (1970).
[2]J. C. Bünzli, D. C. Frost, F. G. Herring, and C. A. McDowell, J. Electron Spectrosc. Relat. Phenom. **9**, 289 (1976).
[3]A. W. Potts, J. M. Benson, I. Novak, and W. A. Svensson, Chem. Phys. **115**, 253 (1987).

$C_2Cl_4^+$

$\tilde{L}\ ^2B_{1u}$ D_{2h}
T^a = 72370(320) gas PE[1,2]

$\tilde{J},\tilde{K}\ ^2B_{2u},^2A_g$ D_{2h}
$T^a \cong$ 59400 gas PE[1,2]

$\tilde{I}\ ^2B_{3u}$ D_{2h}
T^a = 46470(320) gas PE[1,2]

$\tilde{H}\ ^2B_{3g}$ D_{2h}
T^a = 43080(320) gas PE[1,2]

$\tilde{G}\ ^2B_{2g}$ D_{2h}
T^a = 33400(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g			460(80)	gas	PE	1

$\tilde{B},\tilde{C},\tilde{D},\tilde{E},\tilde{F}\ ^2A_u,^2B_{2u},^2B_{1g},^2B_{1u},^2A_g$ D_{2h}
$T^a \cong$ 23000–29500 gas PE[1,2]

$\tilde{A}\ ^2B_{3g}$ D_{2h}
T^a = 16460(320) gas PE[1,2]

$\tilde{X}\ ^2B_{3u}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g		C=C stretch	1320(80)	gas	PE	1

[a] From vertical ionization potential.

References

[1]R. F. Lake and H. Thompson, Proc. Roy. Soc. (London) **A315**, 323 (1970).
[2]W. von Niessen, L. Åsbrink, and G. Bieri, J. Electron Spectrosc. Relat. Phenom. **26**, 173 (1982).

CF_3NO^+

T^a = 73700(1000) gas PE[2]

T^a = 59200(1000) gas PE[2]

T^a = 56000(1000) gas PE[1,2]

T^a = 48700(1000) gas PE[1,2]

T^a = 41500(1000) gas PE[1,2]

T^a = 39000(1000) gas PE[2]

[a] From vertical ionization potentials.

References

[1]H. Bergmann, S. Elbel, and R. Demuth, J. Chem. Soc., Dalton Trans. 401 (1977).
[2]N. P. Ernsting, J. Pfab, J. C. Green, and J. Romelt, J. Chem. Soc., Faraday Trans. 2 **76**, 844 (1980).

CF_2ClNO^+

T^a = 68100(320) gas PE[1]

T^a = 50700(1000) gas PE[1]

T^a = 45100(1000) gas PE[1]

T^a = 36070(320) gas PE[1]

T^a = 17990(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]N. P. Ernsting, J. Pfab, J. C. Green, and J. Romelt, J. Chem. Soc., Faraday Trans. 2 **76**, 844 (1980).

$CFCl_2NO^+$

T^a = 63980(320) gas PE[1]

T^a = 47930(320) gas PE[1]

T^a = 43890(320) gas PE[1]

T^a = 33200(1000) gas PE[1]

T^a = 22910(320) gas PE[1]

T^a = 21540(320) gas PE[1]

T^a = 16940(320) gas PE[1]

T^a = 14040(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]N. P. Ernsting, J. Pfab, J. C. Green, and J. Romelt, J. Chem. Soc., Faraday Trans. 2 **76**, 844 (1980).

CCl_3NO^+

T^a = 58900(1000) gas PE[1]

T^a = 54100(1000) gas PE[1]

T^a = 43810(320) gas PE[1]

T^a = 42800(1000) gas PE[1]

T^a = 40740(320) gas PE[1]

T^a = 24200(1000) gas PE[1]

T^a = 22670(320) gas PE[1]

T^a = 16140(320) gas PE[1]

T^a = 12430(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]N. P. Ernsting, J. Pfab, J. C. Green, and J. Romelt, J. Chem. Soc., Faraday Trans. 2 **76**, 844 (1980).

CF_3CF

In an argon matrix, absorption maxima at 42600 (235 nm) and 21500 (465 nm) have been assigned[1] to CF_3CF.

$\tilde{X}\ ^1A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1286.6wm	Ar	IR	1
			1226.4vs	Ar	IR	1
			1156.9s	Ar	IR	1
			1152.6m	Ar	IR	1
			815.1w	Ar	IR	1
			688.3w	Ar	IR	1
			537.4w	Ar	IR	1

References

[1]J. E. O'Gara and W. P. Dailey, J. Am. Chem. Soc. **114**, 3581 (1992).

CF_3CCl

In an argon matrix, absorption maxima at 42600 (235 nm) and 15600 (640 nm) have been assigned[1] to CF_3CCl.

$\tilde{X}\ ^1A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1238.7ms	Ar	IR	1
			1186.6s	Ar	IR	1
			1154.8vs	Ar	IR	1
			920.0m	Ar	IR	1
			791.7w	Ar	IR	1
			640.3w	Ar	IR	1
			543.6w	Ar	IR	1
			536.7vw	Ar	IR	1

References

[1]J. E. O'Gara and W. P. Dailey, J. Am. Chem. Soc. **114**, 3581 (1992).

CF_3CBr

In an argon matrix, absorption maxima at 42600 (235 nm) and 15000 (665 nm) have been assigned[1] to CF_3CBr.

$\tilde{X}\ ^1A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1229.3s	Ar	IR	1
			1178.0s	Ar	IR	1
			1147.6vs	Ar	IR	1
			858.3wm	Ar	IR	1
			745.2wm	Ar	IR	1
			626.1w	Ar	IR	1
			544.1w	Ar	IR	1
			523.6w	Ar	IR	1

References

[1]J. E. O'Gara and W. P. Dailey, J. Am. Chem. Soc. **114**, 3581 (1992).

CF_3O_2

In the gas phase, an absorption maximum at 255 nm, produced by the pulse radiolysis of CF_3Cl or CF_3Br in the presence of O_2, has been attributed[3] to CF_3O_2.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CF_3 a–stretch	1303.9vs	Ar	IR	2,4,5
	2	C–O stretch	1173.8s	Ar	IR	1,2,4,5
	3	O–O stretch	1092.3m	Ar	IR	1,2,4,5
	4	CF_3 s–stretch	870w	Ar	IR	2
	5	CF_3 s–deform.	692.8m	Ar	IR	2,4,5
	6	CF_3 a–deform.	580w	Ar	IR	2
	7	CF_3 rock	448vw	Ar	IR	2
	8	COO bend	286vw	Ar	IR	2
a''	9	CF_3 a–stretch	1263.2vs	Ar	IR	2,4,5
	10	CF_3 a–deform.	597.2w	Ar	IR	2,5

References

[1]R. R. Smardzewski, R. A. DeMarco, and W. B. Fox, J. Chem. Phys. **63**, 1083 (1975).
[2]R. Butler and A. Snelson, J. Phys. Chem. **83**, 3243 (1979).
[3]R. Cooper, J. B. Cumming, S. Gordon, and W. A. Mulac, Radiat. Phys. Chem. **16**, 169 (1980).
[4]K. C. Clemitshaw and J. R. Sodeau, J. Phys. Chem. **91**, 3650 (1987).
[5]K. C. Clemitshaw and J. R. Sodeau, J. Phys. Chem. **93**, 3552 (1989).

CCl_3O_2

In the gas phase, a broad, unstructured absorption maximum near 255 nm, produced by the pulse radiolysis of CCl_4 in the presence of O_2, has been attributed[1] to CCl_3O_2.

References

[1]R. Cooper, J. B. Cumming, S. Gordon, and W. A. Mulac, Radiat. Phys. Chem. **16**, 169 (1980).

CF_3OF^+

$\tilde{F}$ C_s
T^a = 54500 gas PE[1]

$\tilde{E}$ C_s
T^a = 43000 gas PE[1]

$\tilde{D}$ C_s
T^a = 31000 gas PE[1]

$\tilde{C}$ C_s
T^a = 24000 gas PE[1]

$\tilde{X}\ ^2A''$ C_s

[a] From vertical ionization potentials.

References

[1]M. B. Robin and N. A. Kuebler, J. Electron Spectrosc. Relat. Phenom. **1**, 13 (1972/73).

$P_2F_4^+$

$\tilde{B}$
T^a = 38400(1000) gas PE[1]

$\tilde{A}$
T^a = 22670(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]S. Cradock and D. W. H. Rankin, J. Chem. Soc., Faraday Trans. 2 **68**, 940 (1972).

$OPCl_2OCl$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		P=O stretch	1284	Ar	IR	1
		POCl a–stretch	885	Ar	IR	1
		POCl s–stretch	671	Ar	IR	1
		PCl_2 a–stretch	544	Ar	IR	1

References

[1]B. W. Moores and L. Andrews, J. Phys. Chem. **93**, 1902 (1989).

$PF_3{=}PF$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			967m	Ar	IR	1
			924vs	Ar	IR	1
			898m	Ar	IR	1
			811wm	Ar	IR	1
			751m	Ar	IR	1
			580wm	Ar	IR	1
			408vw	Ar	IR	1
			399w	Ar	IR	1

References

[1]J. K. Burdett, L. Hodges, V. Dunning, and J. H. Current, J. Phys. Chem. **74**, 4053 (1970).

$ClOClO_3$

An unstructured gas–phase absorption with maximum at 42740 (234 nm) has been assigned[4] to $ClOClO_3$.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ClO_2 s–stretch	1283vs	gas	IR	1–3,5
			1287vs	Ar	IR	2
	2	Cl=O stretch	1040s	gas	IR	1,2
			1039s	Ar	IR	2
	3	O–Cl stretch	749wm	gas	IR	1,2
			746m	Ar	IR	2
	4	Cl–O stretch	646vs	gas	IR	1,2
			647vs	Ar	IR	2 5
	5	O=Cl=O bend	580sh	gas	IR	2
			582m	Ar	IR	2
	6	ClO_3 deform.	511wm	gas	IR	2
			513m	Ar	IR	2
	7	O=Cl–O bend	355vw	Ar	IR	2
a''	9	ClO_2 a–stretch	1283vs	gas	IR	1–3,5
			1271vs	Ar	IR	2
	10	O=Cl=O bend	561m	gas	IR	2
			561ms	Ar	IR	2
	11	O=Cl–O bend	382w	Ar	IR	2

References

[1]C. J. Schack and D. Pilipovich, Inorg. Chem. **9**, 1387 (1970).
[2]K. O. Christe, C. J. Schack, and E. C. Curtis, Inorg. Chem. **10**, 1589 (1971).
[3]A. J. Schell–Sorokin, D. S. Bethune, J. R. Lankard, M. M. T. Loy, and P. P. Sorokin, J. Phys. Chem. **86**, 4653 (1982).
[4]M. I. Lopez and J. E. Sicre, J. Phys. Chem. **92**, 563 (1988).
[5]J. B. Burkholder, J. J. Orlando, and C. J. Howard, J. Phys. Chem. **94**, 687 (1990).

CF_3IO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1214	Ar	IR	1
		CF stretch	1202	Ar	IR	1
		IO stretch + CF_3 deform.	732	Ar	IR	1

References

[1]L. Andrews, M. Hawkins, and R. Withnall, Inorg. Chem. **24**, 4234 (1985).

CF_3OI

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1241s[a]	Ar	IR	1,2
		CF stretch	1203s	Ar	IR	1,2
		CO stretch	913	Ar	IR	1,2
		COI bend	320	Ar	IR	1

[a] Moderately intense satellite at 1235 cm^{-1} assigned to 913 + 320 combination band.

References

[1]L. Andrews, M. Hawkins, and R. Withnall, Inorg. Chem. **24**, 4234 (1985).
[2]K. C. Clemitshaw and J. R. Sodeau, J. Phys. Chem. **93**, 3552 (1989).

$SiCl_3OCl$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SiO stretch	929	gas	IR	1

References

[1]H. Niki, P. D. Maker, C. M. Savage, L. P. Breitenbach, and M. D. Hurley, J. Phys. Chem. **89**, 3725 (1985).

CF_3ClF

Threshold for photodecomposition in solid Ar, producing CF_4 + Cl, between 300 and 260 nm.[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1235s	Ar	IR	1
		CF stretch	1224s	Ar	IR	1
		CF stretch	1073vs	Ar	IR	1
		ClF stretch	633m	Ar	IR	1

References

[1]M. E. Jacox, Chem. Phys. **51**, 69 (1980).

CF_3BrF

Threshold for photodecomposition in solid Ar, producing CF_4 + Br, between 345 and 370 nm.[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1251s	Ar	IR	1
		CF stretch	1225s	Ar	IR	1
		CF stretch	1051vs	Ar	IR	1
		BrF stretch	588wm	Ar	IR	1
		CF_3 deform.	454wm	Ar	IR	1

References

[1]M. E. Jacox, Chem. Phys. **51**, 69 (1980).

CF_3IF

Threshold for photodecomposition in solid Ar, producing CF_4 + I, at a wavelength longer than 490 nm.[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1223s	Ar	IR	1
		CF stretch	1197s	Ar	IR	1
		CF stretch	1052vs	Ar	IR	1
		CF_3 deform.	432m	Ar	IR	1,2

References

[1]M. E. Jacox, Chem. Phys. **51**, 69 (1980).
[2]M. E. Jacox, J. Chem. Phys. **83**, 3255 (1985).

PF_5^+

T^a = 42440(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'			702(40)	gas	PE	1

$T^a \cong 32000$ gas PE[1]

$T^a = 28700(1000)$ gas PE[1]

$T^a = 23320(320)$ gas PE[1,2]

$T^a = 18150(320)$ gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	2	PF_2 ax. stretch	480(80)	gas	PE	2

$T^a = 12830(500)$ gas PE[1,2]

$T^a = 9760(500)$ gas PE[1,2]

$T^a = 7420(320)$ gas PE[1,2]

[a] From vertical ionization potentials.

References

[1]P. A. Cox, S. Evans, A. F. Orchard, N. V. Richardson, and P. J. Roberts, Faraday Discuss. Chem. Soc. **54**, 26 (1972).
[2]D. W. Goodman, M. J. R. Dewar, J.R. Schweiger, and A. H. Cowley, Chem. Phys. Lett. **21**, 474 (1973).

PCl_5^+

$T^a = 72800(1000)$ gas PE[1]

$T^a = 43490(320)$ gas PE[1]

$T^a \cong 41300$ gas PE[1]

$T^a \cong 25200$ gas PE[1]

$T^a = 23480(320)$ gas PE[1]

$T^a = 19690(320)$ gas PE[1]

$T^a = 12020(320)$ gas PE[1]

$T^a = 8470(320)$ gas PE[1]

$T^a = 6450(320)$ gas PE[1]

$T^a = 1290(320)$ gas PE[1]

[a] From vertical ionization potentials.

References

[1]P. A. Cox, S. Evans, A. F. Orchard, N. V. Richardson, and P. J. Roberts, Faraday Discuss. Chem. Soc. **54**, 26 (1972).

SiF_5^-

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Ax. SiF stretch	932vs Cs	Ar	IR	1
		Eq. SiF stretch	855s Cs	Ar	IR	1
		Br. SiF stretch	812vs Cs	Ar	IR	1
		Deform.	480s Cs	Ar	IR	1
		Deform.	457wm Cs	Ar	IR	1
		Deform.	444wm Cs	Ar	IR	1

References

[1]B. S. Ault, Inorg. Chem. **18**, 3339 (1979).

SiF_4Cl-

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Ax. SiF stretch	932 Cs	Ar	IR	1
		Eq. SiF stretch	902 Cs	Ar	IR	1
		Eq. SiF stretch	879 Cs	Ar	IR	1
		Br. SiF stretch	802 Cs	Ar	IR	1
		Eq. SiCl str.	579 Cs	Ar	IR	1

References

[1]B. S. Ault, Inorg. Chem. **18**, 3339 (1979).

$SiF_3Cl_2^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Ax. SiF stretch	928 Cs	Ar	IR	1
		Br. SiF stretch	787 Cs	Ar	IR	1
		Eq. SiCl str.	567 Cs	Ar	IR	1

References

[1]B. S. Ault, Inorg. Chem. **18**, 3339 (1979).

$SiF_2Cl_3^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Ax. SiF stretch	925 Cs	Ar	IR	1
		Br. SiF stretch	779 Cs	Ar	IR	1
		Eq. SiCl str.	563 Cs	Ar	IR	1

References

[1]B. S. Ault, Inorg. Chem. **18**, 3339 (1979).

$SiFCl_4^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Br. SiF stretch	769 Cs	Ar	IR	1
		Eq. SiCl str.	558 Cs	Ar	IR	1
		Ax. SiCl str.	499 Cs	Ar	IR	1

References

[1]B. S. Ault, Inorg. Chem. **18**, 3339 (1979).

$SO_2F_3^-$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SO_2 a–stretch	1408w Cs	Ar	IR	1
		SO_2 s–stretch	1130m Cs	Ar	IR	1
		SF_2 a–stretch	925m Cs	Ar	IR	1
		SF eq. stretch	810m Cs	Ar	IR	1
		SF_2 s–stretch	649m Cs	Ar	IR	1

References

[1]K. Garber and B. S. Ault, Inorg. Chem. **22**, 2509 (1983).

XeO_3F_2

$\tilde{X}$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1		806.7	Ar	Ra	1
	2		567.4	Ar	Ra	1
a_2''	3		631.7	Ne	IR	1
	4		375.4	Ne	IR	1
e'	5		895.8	Ne	IR	1
			892	Ar	Ra	1
	6		320.8	Ne	IR	1
			316	Ar	Ra	1
	7		190	Ar	Ra	1
e''	8		361	Ar	Ra	1

References

[1]H. H. Claassen and J. L. Huston, J. Chem. Phys. **55**, 1505 (1971).

SF_5

$\tilde{X}$ C_{4v} Structure: ESR[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Eq. s–stretch	884.5	Ar	IR	5
e	7	SF a–stretch	813.1vs	Ar	IR	3–5
	8	SF stretch	552m	Ar	IR	3,4

References

[1]R. W. Fessenden and R. H. Schuler, J. Chem. Phys. **45**, 1845 (1966).
[2]J. R. Morton and K. F. Preston, Chem. Phys. Lett. **18**, 98 (1973).
[3]R. R. Smardzewski and W. B. Fox, J. Fluorine Chem. **7**, 456 (1976).
[4]R. R. Smardzewski and W. B. Fox, J. Chem. Phys. **67**, 2309 (1977).
[5]P. Hassanzadeh and L. Andrews, J. Phys. Chem. **96**, 79 (1992).

BrF_5^+

$\tilde{I}, \tilde{J}$ $^2A_1, ^2E$ C_{4v}
T^a = 56480(560) gas PE[1]

$\tilde{G}, \tilde{H}$ $^2E, ^2B_2$ C_{4v}
T_0 = 30260(320) gas PE[1]

$\tilde{E}, \tilde{F}$ $^2A_1, ^2B_1$ C_{4v}
T^a = 24690(320) gas PE[1]

$\tilde{C}, \tilde{D}$ $^2E, ^2B_1$ C_{4v}
T^a = 20330(320) gas PE[1]

$\tilde{A}, \tilde{B}$ $^2A_2, ^2E$ C_{4v}
T_0 = 9520(320) gas PE[1]

$\tilde{X}$ $^2A_1$ C_{4v}

[a] From vertical ionization potential.

References

[1]R. L. DeKock, B. R. Higginson, and D. R. Lloyd, Faraday Discuss. Chem. Soc. **54**, 84 (1972).

IF_5^+

$\tilde{I}, \tilde{J}$ $^2A_1, ^2E$ C_{4v}
T_0 = 47520(650) gas PE[1]

$\tilde{G}, \tilde{H}$ $^2E, ^2B_2$ C_{4v}
T_0 = 31870(560) gas PE[1]

$\tilde{E}, \tilde{F}$ $^2A_1, ^2B_1$ C_{4v}
T^a = 26460(320) gas PE[1]

$\tilde{C}, \tilde{D}$ $^2E, ^2B_1$ C_{4v}
T^a = 24040(400) gas PE[1]

$\tilde{A}, \tilde{B}$ $^2A_2, ^2E$ C_{4v}
T_0 = 14200(500) gas PE[1]

$\tilde{X}$ $^2A_1$ C_{4v}

[a] From vertical ionization potential.

References

[1]R. L. DeKock, B. R. Higginson, and D. R. Lloyd, Faraday Discuss. Chem. Soc. **54**, 84 (1972).

$XeOF_4^+$

T^a = 57300(800) gas PE[1]

T^a = 50000(800) gas PE[1]

T^a = 39100(800) gas PE[1]

T^a = 27400(800) gas PE[1]

T^a = 23000(800) gas PE[1]

T^a = 17800(800) gas PE[1]

T^a = 12100(800) gas PE[1]

[a] From vertical ionization potentials.

References

[1]C. R. Brundle and G. R. Jones, J. Electron Spectrosc. Relat. Phenom. **1**, 403 (1972/73).

SF_5^-

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SF a-stretch	795.5m	Ar	IR	2,3
		SF stretch	596s[a]	Ar	IR	1,2
			470w	Ar	IR	2

[a] This absorption was attributed to SF_6^- by Ref. 1. Reassignment to SF_5^- is dictated by the close correspondence, discussed in Ref. 2, of these three absorptions to peaks observed for solid $CsSF_5$.

References

[1]J. E. Barefield, II, and W. A. Guillory, J. Phys. Chem. **81**, 634 (1977).
[2]R. R. Smardzewski and W. B. Fox, J. Chem. Phys. **67**, 2309 (1977).
[3]P. Hassanzadeh and L. Andrews, J. Phys. Chem. **96**, 79 (1992).

6.13. Seven-Atomic Molecules

$B_2H_5^+$

$\tilde{X}$ D_{3h} ?

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1290T	gas	PI	1

References

[1]B. Ruscic, M. Schwarz, and J. Berkowitz, J. Chem. Phys. **91**, 4183 (1989).

$C_2H_5^+$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			400(30)[a]	gas	PE,PI	1-3

[a] The photoionization studies of Ref. 3 suggest that the measured vibrational spacings arise from transitions to higher vibrational states of the bridged ion structure and that $\Delta G(\frac{1}{2})$ may be as great as 730(90).

References

[1]J. M. Dyke, N. Jonathan, and A. Morris, Int. Rev. Phys. Chem. **2**, 3 (1982).
[2]J. M. Dyke, A. R. Ellis, N. Keddar, and A. Morris, J. Phys. Chem. **88**, 2565 (1984).
[3]B. Ruscic, J. Berkowitz, L. A. Curtiss, and J. A. Pople, J. Chem. Phys. **91**, 114 (1989).

C_2H_5

3p Rydberg state

In the gas phase, an absorption with maximum at 205 nm has been assigned[6,7] to the $3p$–$\tilde{X}$ transition of C_2H_5. The detection of this band in MPI studies[9] is consistent with the assignment to a Rydberg state.

3s Rydberg state

In the gas phase, a broad, unstructured absorption with maximum at 246 nm has been assigned[1,3,6,7] to the $3s$–$\tilde{X}$ transition of C_2H_5.

$\tilde{X}$ C_s Structure: MO[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CH_2 s-stretch	3033m	Ar	IR	2,4,5,8
		CH_3 s-stretch	2920m	Ar	IR	4,5
		2-CH stretch	2842s	Ar	IR	2,4,5,8
		CH_2 deform.	1440m	Ar	IR	2,4,5,8
			1383	Ar	IR	8
		CH_3 deform.	1366m	Ar	IR	2,4,5,8
		CC stretch	1138w	Ar	IR	4,5,8
			1025	Ar	IR	8
		CCH_2 umbrella	540vs	Ar	IR	2,4,5,8
a''		CH_2 a-stretch	3112s	Ar	IR	2,4,5,8
		CH_3 a-stretch	2987s	Ar	IR	2,4,5
		CH_3 deform.	1440m	Ar	IR	2,4,5,8
		H deform.	1175m	Ar	IR	4,5,8

C_2D_5

$\tilde{X}$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	CD_2 s–stretch	2199m	Ar	IR	4,5
	CD_3 s–stretch	2094m	Ar	IR	4,5
	2–CD stretch	2048m	Ar	IR	4,5
	CD_3 deform.	1070m	Ar	IR	4,5
	CD_3 deform.	1035m	Ar	IR	4,5
	CCD_2 umbrella	398vs	Ar	IR	4,5
a''	CD_2 a–stretch	2249m	Ar	IR	4,5
	CD_3 a–stretch	2170s	Ar	IR	4,5
	CD_3 deform.	1041m	Ar	IR	4,5

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C_2H_4Li

$\tilde{X}$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CH stretch	3055vw	Ar	IR	1
	CH_2 scissors	1428w	Ar	IR	1
	CC stretch	1176.5s	Ar	IR	1
		704vw	Ar	IR	1
	LiC stretch	369s	Ar	IR	1

C_2D_4Li

$\tilde{X}$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CD stretch	2223vw	Ar	IR	1
	CC stretch	1312s	Ar	IR	1
	CD_2 scissors	931m	Ar	IR	1
	LiC stretch	360s	Ar	IR	1

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SiH_3NH_2

$\tilde{X}$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	NH_2 a–stretch	3547	gas	IR	1
	NH_2 s–stretch	3445	gas	IR	1
	SiH stretch	2172	gas	IR	1
	NH_2 scissors	1564	gas	IR	1
	SiH_3 deform.	996	gas	IR	1
	SiH_3 deform.	983	gas	IR	1
	SiH_3 deform.	970	gas	IR	1
	SiN stretch	845	gas	IR	1
	Deform.	670T	gas	IR	1

SiD_3ND_2

$\tilde{X}$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	ND_2 a–stretch	2599	gas	IR	1
	ND_2 s–stretch	2523	gas	IR	1
	SiD stretch	1574	gas	IR	1
	ND_2 scissors	1118	gas	IR	1
	SiN stretch	815	gas	IR	1
	SiD_3 deform.	702	gas	IR	1

References

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$H_5O_2^+$

$\tilde{X}$ C_2

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	H_2O a–stretch	3684.4	gas	PF	1
	H_2O s–stretch	3608.8	gas	PF	1

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$HFeC_2H_3$

$\tilde{X}$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CH_2 a–stretch	2999.5	Ar	IR	1
	CH stretch	2923.1	Ar	IR	1
		2913.0	Kr	IR	1
	CH_2 s–stretch	2901.6	Ar	IR	1
	FeH stretch	1696.6	Ar	IR	1
		1683.8	Kr	IR	1

$\tilde{X}$ – Continued

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	C=C stretch	1556.3	Ar	IR	1
		1563.0	Kr	IR	1
	CH_2 scissors	1399.1	Ar	IR	1
		1408.3	Kr	IR	1
	CH_2 rock	1019.0	Ar	IR	1
		1020.9	Kr	IR	1
	HCFe bend	972.9	Ar	IR	1
		980.2	Kr	IR	1
	CH_2 wag	944.2	Ar	IR	1
		944.7	Kr	IR	1
	CFe stretch	507.2	Ar	IR	1

$DFeC_2D_3$

$\tilde{X}$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CD_2 a–stretch	2264.5	Ar	IR	1
	CD stretch	2175.3	Ar	IR	1
	CD_2 s–stretch	2150.5	Ar	IR	1
	C=C stretch	1477.4	Ar	IR	1
	FeD stretch	1220.5	Ar	IR	1
	CD_2 scissors	1063.1	Ar	IR	1
	CD_2 wag	737.4	Ar	IR	1
	CD_2 rock	713.5	Ar	IR	1
	CFe stretch	491.0	Ar	IR	1

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AlC_2H_4

$\tilde{X}$ C_{2v}

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CH stretch	3094T	Ar	IR	1
	CH stretch	2980T	Ar	IR	1
	CH_2 deform.	1381ms	Ar	IR	1
	CC stretch	1193s	Ar	IR	1
		781vs	Ar	IR	1
		686m	Ar	IR	1
	AlC_2 s–stretch	352ms	Ar	IR	1
	AlC_2 a–stretch	224m	Ar	IR	1

AlC_2D_4

$\tilde{X}$ C_{2v}

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CD stretch	2337T	Ar	IR	1
	CD stretch	2194T	Ar	IR	1
	CD stretch	2175T	Ar	IR	1
	CC stretch	1289ms	Ar	IR	1
	CD_2 deform.	1041wm	Ar	IR	1
	CD_2 deform.	941wm	Ar	IR	1
		596s	Ar	IR	1
		536w	Ar	IR	1
	AlC_2 s–stretch	337ms	Ar	IR	1
	AlC_2 a–stretch	212m	Ar	IR	1

References

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InC_2H_4

$\tilde{X}$ C_{2v}

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CH stretch	3060wm	Ar	IR	1
	CH_2 s–scissors	1488.5wm	Ar	IR	1
	CH_2 a–scissors	1403.5wm	Ar	IR	1
	Mixed	1201vs	Ar	IR	1
	CH_2 rock	792.5w	Ar	IR	1
	CH_2 wag	762.7w	Ar	IR	1
	InC_2 s–stretch	238w	Ar	IR	1

InC_2D_4

$\tilde{X}$ C_{2v}

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CD stretch	2326wm	Ar	IR	1
	CD stretch	2226m	Ar	IR	1
	CD stretch	2187w	Ar	IR	1
	CC stretch	1313.7s	Ar	IR	1
	CD_2 a–scissors	1054.5wm	Ar	IR	1
	Mixed	944m	Ar	IR	1
	CD_2 rock	560vw	Ar	IR	1
	InC_2 s–stretch	215w	Ar	IR	1

References

[1]L. Manceron and L. Andrews, J. Phys. Chem. **94**, 3513 (1990).

$H_2CCCH_2^+$

$\tilde{B}$
T_a = 61400(800) gas PE[1]

$\tilde{A}\ ^2E$ D_2
T_0 = 35638(32) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_2 scissors	1320(6)	gas	PE	3
	3	C_3 s-stretch	1030(6)	gas	PE	3

$\tilde{X}\ ^2E$ D_2 Structure: PE[2,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_1	4	Torsion	745(5)	gas	PE	3

$D_2CCCD_2^+$

$\tilde{X}\ ^2E$ D_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_1	4	Torsion	565(50)	gas	PE	1

[a] From vertical ionization potential.

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$HNiOCH_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NiH stretch	1868.9	Ar	IR	1
		NiO stretch	569.9	Ar	IR	1

$DNiOCD_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NiD stretch	1347.3	Ar	IR	1
		NiO stretch	546.2	Ar	IR	1

References

[1]M. Park, R. H. Hauge, and J. L. Margrave, High Temp. Sci. **25**, 1 (1988).

CH_3NiOH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3717.6	Ar	IR	1
		NiO stretch	715.0	Ar	IR	1

CD_3NiOD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OD stretch	2738.7	Ar	IR	1
		NiO stretch	686.5	Ar	IR	1
			682.9			

References

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CH_3CNH^+

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NH stretch	3527.29	gas	LD	1,2

B_0 = 0.287 LD[1,2]

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$CH_2{=}CHOH^+$

$\tilde{D}\ ^2A'$ C_s
T_a = 82300(400) gas PE[1,2]

$\tilde{C}\ ^2A'$ C_s
T_a = 61200(400) gas PE[1,2]

$\tilde{B}\ ^2A''$ C_s
T_a = 41300(400) gas PE[1,2]

$\tilde{A}\ ^2A'$ C_s
T_a = 35400(400) gas PE[1,2]

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1400(50)	gas	PE	2

[a] Values for *syn*- rotamer. From vertical ionization potential.

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CH_3CHS^+

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CS stretch	950(50)	gas	PE	1

References

[1]H. W. Kroto, B. M. Landsberg, R. J. Suffolk, and A. Vodden, Chem. Phys. Lett. **29**, 265 (1974).

$CH_2{=}CHOH$

$\tilde{X}$ C_s Structure: MW[1,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3620s	Ar	IR	2,4
	5	C=C stretch[a]	1662vs 1622s	Ar	IR	2,4
	7		1326w	Ar	IR	4
	8		1300m	Ar	IR	4
	9	CO stretch + OH deform.	1121s[b] 1079vs	Ar	IR	2,4
	10		943w	Ar	IR	4
	11		486w	Ar	IR	4
a''	12		960w	Ar	IR	4
	13	H_2C=C OPLA	814s	Ar	IR	2,4
	14		698vw	Ar	IR	4
	15	Torsion	413s	Ar	IR	2,4

$CD_2{=}CDOD$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		OD stretch	2677	Ar	IR	2
		C=C stretch	1590 1584	Ar	IR	2
		CO stretch + OD deform.	926 922	Ar	IR	2

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a''		D_2C=C OPLA	651	Ar	IR	2
		Torsion	310	Ar	IR	2

[a] Fermi resonance between ν_5 and $2\nu_{13}$.
[b] Fermi resonance between ν_9 and $(\nu_{14} + \nu_{15})$.

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HCH_3SiO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Si=O stretch	1207.6	Ar	IR	1,2

References

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CH_3CHS

$\tilde{F}\ ^1A''$ C_s
T_0 = 51560(200) gas AB^2

$\tilde{D}$ or $\tilde{E}\ ^1A'$ C_s
T_0 = 52770(100) gas AB^2

$\tilde{C}\ ^1A'$ C_s
T_0 = 45260(100) gas AB^2

$\tilde{B}\ ^1A'$ C_s
T^a = 47600(100) gas AB^2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		C=S stretch	1154	gas	AB	2

$\tilde{A}\ ^1A''$ C_s
T_0 = 17900(100) gas AB^2
τ_0 = 0.40(5) μs gas LF[4]

$\tilde{a}\ ^3A''$ C_s
T_0 = 16294.9 gas $AB^{2,3}LF^7$ $\tilde{a}-\tilde{X}$ 571–630 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	9	CS stretch	747.2	gas	AB,LF	3,7
	10	CCS deform.	283.9	gas	LF	7
a"	14	Wag	249.4	gas	LF	7
	15	Torsion	52.0	gas	LF	7

$\tau \sim 8.2\ \mu s$ gas LF^4

$\tilde{X}\ ^1A'$ C_s Structure: MW^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3010.4w	Ar	IR	6
		CH stretch	2982.0w	Ar	IR	6
		CH stretch	2944.4m	Ar	IR	6
		CH stretch	2908.7w	Ar	IR	6
			1435.3m	Ar	IR	6
			1433.4wm	Ar	IR	6
			1357.7s	Ar	IR	6
			1345.6vs	Ar	IR	6
		C=S stretch	1240	gas	AB	3
			1140.7s	Ar	IR	6
			1065.0wm	Ar	IR	6
			1020.2wm	Ar	IR	6
			820.1w	Ar	IR	6
			747.8s	Ar	IR	6
	15	Torsion	163.0	gas	LF	7

A_0 = 1.620; B_0 = 0.192; C_0 = 0.177 MW^1

CD_3CDS

$\tilde{a}\ ^3A''$ C_s
T_0 = 16367.2 gas AB^3LF^7 $\tilde{a}-\tilde{X}$ 580–630 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	8	DCS deform.	751.8	gas	LF	7
	9	CS stretch	677.2	gas	AB,LF	3,7
a"	15	Torsion	29.6	gas	LF	7

$\tilde{X}\ ^1A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a"	15	Torsion	122.6	gas	LF	7

[a] Maximum of diffuse absorption with partially resolved structure.

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[1]H. W. Kroto and B. M. Landsberg, J. Mol. Spectrosc. **62**, 346 (1976).
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FCH_2CH_2

$\tilde{X}$ C_s Structure: MO^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		2-CH_2 stretch	2860m	Ar	IR	2
			1372wm	Ar	IR	2
		CF stretch	1047s	Ar	IR	2
		CCF deform.	427wm	Ar	IR	2

FCD_2CD_2

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		2-CD_2 stretch	2090wm	Ar	IR	2
		CF stretch + CD_2 scissors	1211s	Ar	IR	2
			1091m	Ar	IR	2
			1059wm	Ar	IR	2
		CF stretch + CD_2 scissors	969s	Ar	IR	2
		CCF deform.	424w	Ar	IR	2

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[2]M. E. Jacox, Chem. Phys. **58**, 289 (1981).

NH_2NHOH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3198s	Ar	IR	1
		HNOH wag	1329	Ar	IR	1
		NNH deform.	1282	Ar	IR	1
			734s	Ar	IR	1

References

[1]R. Lascola, R. Withnall, and L. Andrews, Inorg. Chem. **27**, 642 (1988).

$CH_3C \equiv CCl^+$

$\tilde{B}\ ^2A_1$ C_{3v}
T_0 = 36790(560) gas PE[1]

$\tilde{A}\ ^2E_{3/2}$ C_{3v}
T_0 = 28334(3) gas EF^3LF^3 $\tilde{A}$–$\tilde{X}$ 335–425 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CH_3 deform.	1196(3)	gas	LF	3
	5	CCl stretch	479(3)	gas	EF,LF	3
e	9	Skel. bend	284H	gas	LF	3
	10	CCl bend	184H	gas	LF	3

τ_1 = 19(3) ns gas EF^2
τ_2 = 600(200) ns gas EF^2

$\tilde{X}\ ^2E_{3/2}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C≡C stretch	2117(3)	gas	EF	3
	3	CH_3 deform.	1260(3)	gas	EF	3
	5	CCl stretch	601(3)	gas	EF	3
e	9	Skel. bend	318T	gas	EF	3
	10	CCl bend	271H	gas	EF	3

$CD_3C \equiv CCl^+$

$\tilde{A}\ ^2E_{3/2}$ C_{3v}
T_0 = 28314(3) gas EF^3LF^3 $\tilde{A}$–$\tilde{X}$ 335–385 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CD_3 deform.	963(3)	gas	LF	3
	5	CCl stretch	464(3)	gas	LF,EF	3
e	9	Skel. bend	263H	gas	LF	3
	10	CCl bend	155H	gas	LF	3

$\tilde{X}\ ^2E_{3/2}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CD_3 deform.	995(3)	gas	EF	3
	5	CCl stretch	566(3)	gas	EF	3
e	9	Skel. bend	311T	gas	EF	3
	10	CCl bend	222T	gas	EF	3

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$CH_3C \equiv CBr^+$

$\tilde{B}\ ^2A_1$ C_{3v}
T_0 = 35820(560) gas PE[1]

$\tilde{A}\ ^2E_{3/2}$ C_{3v}
T_0 = 21849 gas EF^3LF^3 $\tilde{A}$–$\tilde{X}$ 410–580 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CH_3 deform.	1399(2)	gas	LF	3
	5	CBr stretch	392(2)	gas	EF,LF	3
e	10	CBr bend	207H	gas	EF,LF	3

τ_1 = 13(3) ns gas EF^2
τ_2 = 600(200) ns gas EF^2

$\tilde{X}\ ^2E_{3/2}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C≡C stretch	2030(2)	gas	EF	3
	3	CH_3 deform.	1187(2)	gas	EF	3
	5	CBr stretch	486(2)	gas	EF	3
e	9	Skel. bend	335T	gas	EF	3
	10	CBr bend	259H	gas	EF	3

$CD_3C \equiv CBr^+$

$\tilde{A}\ ^2E_{3/2}$ C_{3v}
T_0 = 21824 gas EF^3LF^3 $\tilde{A}$–$\tilde{X}$ 440–525 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	5	CBr stretch	373(2)	gas	EF,LF	3
e	10	CBr bend	195H	gas	EF,LF	3

$\tilde{X}\ ^2E_{3/2}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C≡C stretch	2011(2)	gas	EF	3
	5	CBr stretch	462(2)	gas	EF	3
e	10	CBr bend	243H	gas	EF	3

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[2]J. P. Maier, O. Marthaler, and E. Kloster-Jensen, J. Electron Spectrosc. Relat. Phenom. **18**, 251 (1980).
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CH_3CNO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CN stretch	2309	Ar	IR	1
		CH_3 deform.	1381	Ar	IR	1
		NO stretch	1332	Ar	IR	1
		CC stretch	780	Ar	IR	1

CD_3CNO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CN stretch	2297	Ar	IR	1
		NO stretch	1341	Ar	IR	1

References

[1]Z. Mielke, M. Hawkins, and L. Andrews, J. Phys. Chem. **93**, 558 (1989).

$HOCH_2CN$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3641	Ar	IR	1
		CN stretch	2291	Ar	IR	1
			2262			
			1274	Ar	IR	1
		OH bend	1209m	Ar	IR	1
		CO stretch	1061s	Ar	IR	1
		CH_2 rock	971m	Ar	IR	1
			901	Ar	IR	1
		CC stretch	888	Ar	IR	1
		CCN deform.	355	Ar	IR	1
		OH torsion	256s	Ar	IR	1

$DOCH_2CN$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OD stretch	2688	Ar	IR	1
		CN stretch	2248	Ar	IR	1
			1274	Ar	IR	1
		CD_2 wag	1134	Ar	IR	1
		CO stretch	980	Ar	IR	1
		OD bend	897	Ar	IR	1
		CC stretch	772	Ar	IR	1
		CD_2 rock	724	Ar	IR	1

References

[1]Z. Mielke, M. Hawkins, and L. Andrews, J. Phys. Chem. **93**, 558 (1989).

CH_3OCCl [a]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	2963	Ar	IR	1
			2975	N_2	IR	2
			1475m	N_2	IR	2
			1465m	N_2	IR	2
			1449m	Ar	IR	1
			1445m	N_2	IR	2
			1439m	N_2	IR	2
		COC a–stretch	1300s	Ar	IR	1
			1309vs	N_2	IR	2
		COC a–stretch	1286m	Ar	IR	1
			1280sh	Ar	IR	1
			1299m	N_2	IR	2
			1135vs	Ar	IR	1
			1140s	N_2	IR	2
		COC s–stretch	950s	Ar	IR	1
			947s	N_2	IR	2
			842wm	Ar	IR	1
			840m	N_2	IR	2
			810w	N_2	IR	2
		CCl stretch	777s	Ar	IR	1
			773vs	N_2	IR	2
		CCl stretch	698s	Ar	IR	1
			690m	N_2	IR	2
			451m	Ar	IR	1
			402m	Ar	IR	1
			400m	N_2	IR	2
			394m	N_2	IR	2

CD_3OCCl [a]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD stretch	2178	Ar	IR	1
			2180w	N_2	IR	2
			1370w	Ar	IR	1
			1362m	N_2	IR	2
		COC a–stretch	1330	Ar	IR	1
			1329vs	N_2	IR	2
			1324	Ar	IR	1
			1305vw	N_2	IR	2
			1073	Ar	IR	1
			1071m	N_2	IR	2
			1053	Ar	IR	1
			1050m	N_2	IR	2
			950s	N_2	IR	2
			926	Ar	IR	1
			925w	N_2	IR	2
			807	Ar	IR	1
			805m	N_2	IR	2
			794vw	N_2	IR	2
			777w	N_2	IR	2
			769w	N_2	IR	2

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CCl stretch	755	Ar	IR	1
			749s	N_2	IR	2
		CCl stretch	680	Ar	IR	1
			669m	N_2	IR	2
			434m	N_2	IR	2
			386	Ar	IR	1
			383m	N_2	IR	2
			377w	N_2	IR	2

[a] It has been suggested[2] that *cis*– and *trans*– stereoisomers contribute to the observed spectrum.

References

[1]R. S. Sheridan and M. A. Kesselmayer, J. Am. Chem. Soc. **106**, 436 (1984).
[2]M. A. Kesselmayer and R. S. Sheridan, J. Am. Chem. Soc. **108**, 99 (1986).

c-CH_2(NO)OH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3477m	Ar	IR	1–3
	2	CH stretch	2906w	Ar	IR	2
	3	N=O stretch	1559wm	Ar	IR	1,2
	4	CH_2 scissors	1439m	Ar	IR	2
	5	COH bend	1355m	Ar	IR	2,3
	6	CH_2 wag	1250wm	Ar	IR	2
	7	C–O stretch	1130vs	Ar	IR	1–3
	8	CNO bend + CN stretch	792m	Ar	IR	2
	9	Skel. deform.	755wm	Ar	IR	2
	10	Skel. deform.	334w	Ar	IR	2
a"	11	CH stretch	2916w	Ar	IR	2
	12	CH_2 twist	1202vw	Ar	IR	2
	13	CH_2 rock	888w	Ar	IR	2
	14	OH torsion	346wm	Ar	IR	2
	15	NO torsion	191wm	Ar	IR	2

c–CD_2(NO)OD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2571s	Ar	IR	1–3
	2	CD stretch	2125vw	Ar	IR	2
	3	N=O stretch	1558vs	Ar	IR	2
	4	C–O stretch	1191vs	Ar	IR	2,3
	5	CD_2 wag	1094m	Ar	IR	2
	6	CD_2 scissors	1009m	Ar	IR	2
	7	COD bend	929s	Ar	IR	2,3
	8	CNO bend	765m	Ar	IR	2
	9	CN stretch + OCN scissors	738m	Ar	IR	2
	10	OCN scissors	352w	Ar	IR	2

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a"	12	CD_2 twist	878w	Ar	IR	2
	13	CD_2 rock	702m	Ar	IR	2
	14	OD torsion	285wm	Ar	IR	2

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[1]R. P. Muller and J. R. Huber, J. Phys. Chem. **87**, 2460 (1983).
[2]R. P. Muller, J. R. Huber, and H. Hollenstein, J. Mol. Spectrosc. **104**, 209 (1984).
[3]M. E. Jacox, J. Phys. Chem. **88**, 3373 (1984).

t-CH_2(NO)OH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3638m	Ar	IR	1–3
	2	CH stretch	2906w	Ar	IR	2
	3	N=O stretch	1555s	Ar	IR	1,2
	4	CH_2 scissors	1432wm	Ar	IR	2
	5	COH bend	1352m	Ar	IR	2,3
	6	CH_2 wag	1181w	Ar	IR	2
	7	C–O stretch	1107vs	Ar	IR	1–3
	8	CN stretch	847w	Ar	IR	2
	9	Skel. deform.	542vw	Ar	IR	2
	10	OCN scissors	386m	Ar	IR	2
a"	11	CH stretch	2916w	Ar	IR	2
	13	CH_2 rock	865w	Ar	IR	2
	14	OH torsion	220m	Ar	IR	2

t–CD_2(NO)OD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2687s	Ar	IR	1–3
	3	N=O stretch	1555s	Ar	IR	2
	4	C–O stretch	1173vs	Ar	IR	2,3
	5	CD_2 scissors	1028w	Ar	IR	2,3
	6	COD bend	984m	Ar	IR	2,3
	7	CD_2 wag	906w	Ar	IR	2
	8	CN stretch + COD bend	816wm	Ar	IR	2,3
	9	CN stretch + CNO bend	522w	Ar	IR	2
	10	OCN scissors	369m	Ar	IR	2
a"	11	CD stretch	2170w	Ar	IR	2
	13	CD_2 rock	692wm	Ar	IR	2,3
	14	NO torsion	173m	Ar	IR	2

References

[1]R. P. Muller and J. R. Huber, J. Phys. Chem. **87**, 2460 (1983).
[2]R. P. Muller, J. R. Huber, and H. Hollenstein, J. Mol. Spectrosc. **104**, 209 (1984).
[3]M. E. Jacox, J. Phys. Chem. **88**, 3373 (1984).

$HOCH_2O_2$

In the gas phase, a broad, unstructured absorption with maximum near 43500 (230 nm) has been attributed[1,2] to $HOCH_2O_2$.

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[1]B. Veyret, R. Lesclaux, M.–T. Rayez, J.–C. Rayez, R. A. Cox, and G. K. Moortgat, J. Phys. Chem. **93**, 2368 (1989).
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CH_2ClOOH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3560T	gas	IR	1
		CH stretch	2960	gas	IR	1
			1360	gas	IR	1
			1309.9	gas	IR	1
			1061.0	gas	IR	1
			822	gas	IR	1
			706.7	gas	IR	1

References

[1]H. Niki, P. D. Maker, C. M. Savage, and L. P. Breitenbach, Int. J. Chem. Kinet. **12**, 1001 (1980).

$(HO)_2HPO$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3634.8	Ar	IR	1
		PH stretch	2487.5	Ar	IR	1
		P=O stretch	1298.6	Ar	IR	1
		PO_2 a–stretch	902.0	Ar	IR	1
		PO_2 s–stretch	872.6	Ar	IR	1

References

[1]R. Withnall and L. Andrews, J. Phys. Chem. **91**, 784 (1987).

$(HCO)_2O$

$\tilde{X}$ C_s Structure: MW[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	2987vw	Ar	IR	2
	2	CH stretch	2967w	Ar	IR	2
	3	C=O stretch	1822wm	gas	IR	3
			1812m	Ar	IR	2,4
	4	C=O stretch	1767s	gas	IR	3
			1762s	Ar	IR	2,4
	5	H deformation	1381w	Ar	IR	2
	6	H deformation	1359vw	Ar	IR	2

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	7	C–O stretch + skel. deform.	1105s	gas	IR	3
			1090s	Ar	IR	2,4
	8	C–O stretch	998m	gas	IR	3
			998m	Ar	IR	2,4
	9	C–O stretch	776w	Ar	IR	2
	10	O–C=O bend	540w	Ar	IR	2,4
	11	C–O–C bend	260w	Ar	IR	2
a"	12	H deformation	1067vw	Ar	IR	2
	14	Torsion	227m	Ar	IR	2

$(DCO)_2O$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CD stretch	2260w	Ar	IR	2
	2	CD stretch	2241w	Ar	IR	2
	3	C=O stretch	1774m	Ar	IR	2
	4	C=O stretch	1744s[a]	Ar	IR	2
	5	C–O stretch + CD, OC=O deform.	1101s	Ar	IR	2
	6	C–O stretch + CD, OC=O deform.	1056s	Ar	IR	2
	8	C–O stretch	944m	Ar	IR	2
	9	C–O stretch + skel. deform.	743w	Ar	IR	2
	10	O–C=O bend	532w	Ar	IR	2
	11	C–O–C bend	250w	Ar	IR	2
a"	13	D deformation	865vw	Ar	IR	2
	14	Torsion	205w	Ar	IR	2

[a] Fermi resonance with overtone of 865–cm^{-1} fundamental leads to appearance of a strong absorption at 1700 cm^{-1}.

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[2]H. Kuhne, T.–K. Ha, R. Meyer, and H. H. Gunthard, J. Mol. Spectrosc. **77**, 251 (1979).
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[4]M. Hawkins, C. K. Kohlmiller, and L. Andrews, J. Phys. Chem. **86**, 3154 (1982).

$CHCl_2OOH$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1369	gas	IR	1
			1048	gas	IR	1
			831	gas	IR	1
			766	gas	IR	1

References

[1]H. Niki, P. D. Maker, C. M. Savage, and L. P. Breitenbach, Int. J. Chem. Kinet. **12**, 1001 (1980).

C_6H

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		C≡C stretch	1953.4	Ar	IR	6

$A_{eff} = -15.1$ gas MW^{3-5}
$B_0 = 0.046$ MW^{1-5}

C_6D

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		C≡C stretch	1862.4	Ar	IR	6

References

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$H(C\equiv C)_2CN^+$

$\tilde{C}\ ^2\Pi$ $C_{\infty v}$
$T_0 = 27350(160)$ gas PE[1]

$\tilde{B}\ ^2\Sigma^+$ $C_{\infty v}$
$T_0 = 21860(160)$ gas PE[1]

$\tilde{A}\ ^2\Pi$ $C_{\infty v}$
$T_0 = 17190(5)$ gas EF[1] $\tilde{A}$–$\tilde{X}$ 580–670 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		C≡C stretch	1870(160)	gas	EF	1
	6	C–C stretch	600(160)	gas	EF	1

$\tau_0 = 15(2)$ ns gas EF[1]

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	C≡N,C≡C str.	2190(10)	gas	EF	1
	3	C≡N,C≡C str.	2070(10)	gas	EF	1
	5	C–C stretch	1220(10)	gas	EF	1
	6	C–C stretch	630(10)	gas	EF	1

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[1]G. Bieri, E. Kloster-Jensen, S. Kvisle, J. P. Maier, and O. Marthaler, J. Chem. Soc., Faraday Trans. 2 **76**, 676 (1980).

Li_7

A prominent absorption maximum at about 20800 (480 nm), observed in depletion photoionization experiments[1] on gas-phase Li_7, has been assigned to the D_{5h} structure of that species.

References

[1]V. Bonačić-Koutecký, M. Broyer, J. Chevaleyre, Ph. Dugourd, J. Koutecký, C. Scheuch, J. P. Wolf, and L. Wöste, J. Chem. Phys. **96**, 1793 (1992).

Na_7

A prominent absorption maximum at 19400 (516 nm) and shoulders at 17800 (563 nm) and 21400 (468 nm), observed in depletion photoionization experiments[1,2] on gas-phase Na_7, have been assigned[2] to the D_{5h} structure of that species.

References

[1]K. Selby, V. Kresin, J. Masui, M. Vollmer, W. A. de Heer, A. Scheidemann, and W. D. Knight, Phys. Rev. B **43**, 4565 (1991).
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C_7

$\tilde{X}$ $D_{\infty h}$ Structure: DL[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	3	Sym. stretch	548(90)	gas	PE	4
Σ_u^+	4	Asym. stretch	2138.315	gas	DL	1,2
	5	Asym. stretch	1898.376	gas	DL	3
Π_u	7	Bend	496(110)T	gas	PE	4

$B_0 = 0.031$ DL^{1-3}

References

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C_7^-

Threshold for electron detachment from ground-state C_7^- = 27090(115) gas PE[1,2]

References

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C_6O

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+			2163.8	Ar	IR	1
			1447.8	Ar	IR	1

References

[1]G. Maier, H. P. Reisenauer, and A. Ulrich, Tetrahed. Lett. **32**, 4469 (1991).

C_5O_2

In an argon matrix, photodissociates into C_4O + CO on irradiation at 230 nm, the position of a prominent absorption maximum observed in cyclohexane.[1]

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	4		2242.01	gas	IR	2
			2213.0vs	Ar	IR	1
	5		2065	gas	IR	2
			2058.7m	Ar	IR	1
	6		1152	gas	IR	2
			1144.1w	Ar	IR	1
Π_u	9		542	gas	IR	2
			539.0w	Ar	IR	1
	10		474	gas	IR	2
			470.0vw	Ar	IR	1

B_0 = 0.027 IR[2]

References

[1]G. Maier, H. P. Reisenauer, U. Schäfer, and H. Balli, Angew. Chem. **100**, 590 (1988); Angew. Chem. Int. Ed. Engl. **27**, 566 (1988).
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C_5OS

In an argon matrix, an absorption maximum at 37040 (270 nm) has been assigned[1] to C_5OS.

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1		2227.0vs	Ar	IR	1
	2		2137.8s	Ar	IR	1
	3		1880.8m	Ar	IR	1
	4		1448.3w	Ar	IR	1
	5		945.5wm	Ar	IR	1
	6		463T	Ar	IR	1

References

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C_5S_2

In an argon matrix, absorption maxima at 15100 and 31250 (662 and 320 nm, respectively) have been assigned[1] to C_5S_2.

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	4		2105.0vs	Ar	IR	1
	5		1687.9m	Ar	IR	1
	6		783.5w	Ar	IR	1

References

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$O_2N\text{-}O\text{-}NO_2$

$\tilde{X}$ C_{2v} (C_2 ?)[a] Structure: ED[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NO_2 a-stretch	1720vs	gas	IR	1,2,5,8
			1745	N_2	IR	3
			1752	CO_2	IR	1
	2	NO_2 s-stretch	1338m	gas	IR	2,8
			1305	N_2	IR	3
			1300	O_2	IR	4
			1316	CO_2	IR	1
	3	NO_2 bend	743.4s	gas	IR	2
			737	Ar	IR	7
			739	N_2	IR	3
			736	O_2	IR	4
			737	CO_2	IR	1
	4	NO_2 rock	614mT	gas	IR	2
	5	NON s-stretch	353vsT	gas	IR	2
b_1	9	NO_2 wag	557s	gas	IR	2,5
	10	NO_2 twist	50w,brT	gas	IR	9

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	11	NO_2 a–stretch	1720vs	gas	IR	1,2,5,8
			1704	Ar	IR	7
			1704	N_2	IR	3
			1704	O_2	IR	4
			1700	CO_2	IR	1
	12	NO_2 s–stretch	1245.9s	gas	IR	1,2,5,8
			1245	Ar	IR	7
			1247	N_2	IR	3
			1241	O_2	IR	4
			1248	CO_2	IR	1
	13	NON a–stretch	860m	gas	IR	2,8
	14	NO_2 bend	743.4s	gas	IR	1,2,5,8
			737	Ar	IR	7
			739	N_2	IR	3
			736	O_2	IR	4
			719	CO_2	IR	1
	15	NO_2 rock	353vsT	gas	IR	2,9

$A_0 = 0.221$; $B_0 = 0.063$; $C_0 = 0.060$ MW[10]

[a] Ref. 2 analyzed the spectrum in terms of a C_{2v} structure. No evidence has since been obtained for the appearance of the two infrared–inactive fundamentals expected for that point group. The electron diffraction measurements of Ref. 6, analyzed using a dynamical model, suggest instead a C_2 structure.

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P_2O_5

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		PO_2 a–stretch	1473.2	Ar	IR	1,2
		PO_2 s–stretch	1158.2	Ar	IR	1,2
		POP s–stretch	735.1	Ar	IR	1,2
		PO_2 deform.	479.5	Ar	IR	1

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O_2ClONO_2

An unstructured absorption with onset near 320 nm and maximum at 262 nm has been assigned[1] to gas–phase O_2ClONO_2.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO_2 a–stretch	1658.0vs	gas	IR	1
	2	ClO_2 a–stretch	1275.2s	gas	IR	1
	3	NO_2 s–stretch	1249.7wm	gas	IR	1
	4	ClO_2 s–stretch	1071.8s	gas	IR	1
	5	ClO stretch	838.4s	gas	IR	1
	7	NO_2 wag	718.4wm	gas	IR	1
	8	NO stretch	613.3m	gas	IR	1

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C_2F_5

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CF_3 a–stretch	1273vs	Ar	IR	1,3
		CF_3 s–stretch	1227s	Ar	IR	1,3
		CF_2 s–stretch	1117s	Ar	IR	1,3
		C–C stretch	956vw	Ar	IR	1,3
		CF_3 s–deform.	703m	Ar	IR	1,3
		CF_2 s–deform.	694vw	Ar	IR	1
		CF_3 a–deform.	514w	Ar	IR	1,3
		CF_2 wag	366vw	Ar	IR	1
		CF_3 rock	211vw	Ar	IR	1
a''		CF_3 a–stretch	1398w	Ar	IR	1,3
		CF_2 a–stretch	1184vs	Ar	IR	1,3
		CF_3 a–deform.	604w	Ar	IR	1,3
		CF_2 twist	419vw	Ar	IR	1,3
		CF_3 rock	227vw	Ar	IR	1

[a] Revised assignment offered by Ref. 2, based on more detailed study of infrared and Raman spectrum of C_2F_5I.

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CF_3OSF

$\tilde{X}$ C_1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CF_3 a–stretch	1272.3vs	Ar	IR	1
	2	CF_3 a–stretch	1230.7vs	Ar	IR	1
	3	CF_3 s–stretch	1171.6vs	Ar	IR	1
	4	COS a–stretch	934.1s	Ar	IR	1
	5	COS s–stretch	806.9m	Ar	IR	1
	6	SF stretch	786.4s	Ar	IR	1
	7	CF_3 s–deform.	663.7vw	Ar	IR	1
	8	CF_3 a–deform.	626.2w	Ar	IR	1
	9	CF_3 a–deform.	557.3m	Ar	IR	1
	10	OSF bend	464.9m	Ar	IR	1
	11	CF_3OS deform.	413.3m	Ar	IR	1
	12	CF_3 rock	295.0vw	Ar	IR	1

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6.14. Eight-Atomic Molecules

Ga_2H_6

$\tilde{X}$ D_{2h}[a] Structure: ED[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}	8	GaH_t stretch	1993m	gas	IR	1,2
			2015m	Ar	IR	1,2
			1996m			
			2000m	N_2	IR	1,2
	9	GaH_2 rock	760w	gas	IR	1,2
			773m	Ar	IR	1,2
			761m			
			770m	N_2	IR	1,2
b_{1u}	13	GaH_b stretch	1202s	gas	IR	1,2
			1213m	Ar	IR	1,2
			1208m			
			1195m			
			1220s	N_2	IR	1,2
	14	GaH_2 rock?	659m	Ar	IR	1,2
			655m			
			653m			
			648m			
			655s	N_2	IR	1,2
			647w			
b_{3u}	16	GaH_t stretch	1976m	gas	IR	1,2
			1985s	Ar	IR	1,2
			1968m			
			1985m	N_2	IR	1,2
	17	GaH_b stretch	1273s	gas	IR	1,2
			1283s	Ar	IR	1,2
			1278m			
			1253m			
			1282m	N_2	IR	1,2
	18	GaH_2 bend	671vsT	gas	IR	1,2
			676vs	Ar	IR	1,2
			666s			
			673vs	N_2	IR	1,2

Ga_2D_6

$\tilde{X}$ D_{2h}[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}	8	GaD_t stretch	1439m	gas	IR	1,2
	9	GaD_2 rock	555w	gas	IR	1,2
b_{1u}	13	GaD_b stretch	860s	gas	IR	1,2
	14	GaD_2 rock	439wm	gas	IR	1,2
b_{3u}	16	GaD_t stretch	1416mT	gas	IR	1,2
	17	GaD_b stretch	923s	gas	IR	1,2
	18	GaD_2 bend	484vsT	gas	IR	1,2

[a] As in Ref. 2, the axis definitions and vibrational numbering commonly used for diborane (J. L. Duncan, D. C. McKean, I. Torto, and G. D. Nivellini, J. Mol. Spectrosc. **85**, 16 (1981)) have been adopted.

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$CH_2CHCH_2^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			420(40)	gas	PE	1

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cyc-$C_3H_5^+$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		α–CH bend	1000(70)	gas	PE	1

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CH_2CHCH_2

$\tilde{B}$ $^2B_2$ C_{2v}
T_0 = 41557.8(5) gas MPI[13]Ra[14]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2	9	CH_2 a–twist	596	gas	Ra	14
b_1	12	CH_2 s–twist	564	gas	Ra	14

$\tilde{C}\ ^2B_1$ C_{2v}

T_0 = 40305.5(5) gas AB²MPI[11,13] $\tilde{C}$–$\tilde{X}$ 220–250 nm

In an argon matrix, a very prominent absorption maximum at 213 nm, with a shoulder at 220 nm, has been assigned[5] to this transition of CH_2CHCH_2.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	7	C_3 bend	390T	gas	MPI	11

$A_0 \cong 1.619$; $B_0 \cong 0.351$; $C_0 \cong 0.288$ MPI[11]

$\tilde{B}\ ^2A_1$ (3s) C_{2v}[a]

T_0 = 40056.5(5) gas MPI[7,8,13]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	7	C_3 bend	394(3)T	gas	MPI	7,8
a_2	9	CH_2 a-twist	529(3)T	gas	MPI	8
b_1	12	CH_2 s-twist	491(7)T	gas	MPI	8

$\tilde{A}\ ^2B_1$ C_{2v}

T_0 = 24485 gas AB[1] $\tilde{A}$–$\tilde{X}$ 370–410 nm

24480 Ar AB[5] $\tilde{A}$–$\tilde{X}$ 360–410 nm

Diffuse bands.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1241	gas	AB	1
			1005	gas	AB	1
			908	gas	AB	1
			359	gas	AB	1

$\tilde{X}\ ^2A_2$ C_{2v} Structure: DL[12]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH stretch	3048vw	Ar	IR	4–6
	4	CH_2 scissors	1488(4)	gas	Ra	10,15
			1477w	Ar	IR	4–6
	5	CH_2 rock	1245(3)	gas	Ra	10,15
			1242vw	Ar	IR	4–6
	6	C_3 stretch	1066(4)	gas	Ra	10,15
	7	C_3 bend	427(4)	gas	MPI,Ra	7,8,10,15
a_2	9	CH_2 a-twist	549(4)	gas	MPI,Ra	8,15,16
b_1	10	CH OPLA	968H	gas	Ra	10
			983.6s	Ar	IR	4–6,9
	11	CH_2 s-wag	801.72	gas	DL	12
			801.1vs	Ar	IR	3–6,9
	12	CH_2 s-twist	518(4)	gas	MPI,Ra	7,8,10,15 16
			510.1s	Ar	IR	4–6,9
b_2	13	CH_2 a-stretch	3105w	Ar	IR	4–6
	14	CH stretch	3016w	Ar	IR	4–6
	15	CH_2 scissors	1463vw	Ar	IR	4–6
	16	CH bend	1389m	Ar	IR	4–6
	17	C_3 stretch	1182	Ar	IR	6

A_0 = 1.802; B_0 = 0.346; C_0 = 0.290 DL[12]

CD_2CDCD_2

$\tilde{D}\ ^2B_2$ C_{2v}

T_0 = 41532.1(5) gas MPI[13]

$\tilde{C}\ ^2B_1$ C_{2v}

T_0 = 40286.7(5) gas MPI[13]

$\tilde{B}\ ^2A_1$ (3s) C_{2v}[a]

T_0 = 40096(2) gas MPI[7,13]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		C_3 bend	342(60)T	gas	MPI	7

$\tilde{A}\ ^2B_1$ C_{2v}

T_0 = 24745 gas AB[1] $\tilde{A}$–$\tilde{X}$ 360–405 nm

Diffuse bands.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1155	gas	AB	1
			981	gas	AB	1
			823	gas	AB	1

$\tilde{X}\ ^2A_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD stretch	2285	Ar	IR	6
	3	CD_2 stretch	2214	Ar	IR	6
	4	C_3 stretch	1272(8)	gas	Ra	17
			1263	Ar	IR	6
	5	CD_2 rock	1020(8)	gas	Ra	17
			1018	Ar	IR	6
			1007			
	6	Deform.	822(50)	gas	MPI	7
	7	C_3 deform.	350(8)	gas	MPI,Ra	7,17
a_2	9	CD_2 torsion	372H	gas	Ra	17
b_1	10	Deform.	762H	gas	Ra	17
	11	Deform.	646.5vs	Ar	IR	6,9
	12	Deform.	383H	gas	Ra	17
b_2	14	CD_2 stretch	2209	Ar	IR	6
	16	CD bend	1062	Ar	IR	6

[a] Ref. 14 suggests that this state may be slightly nonplanar, with irregularities in the vibrational energy level pattern resulting from inversion doubling.

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$H_2B{=}OCH_3$

$\tilde{X}$ C_s Structure: MW[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH_3 a–stretch	2994	Ar	IR	2
	2	CH_3 s–stretch	2878	Ar	IR	2
	3	BH_2 a–stretch	2565	Ar	IR	2
	4	BH_2 s–stretch	2482	Ar	IR	2
	5	CH_3 a–deform.	1506	Ar	IR	2
	6	CH_3 s–deform.	1471	Ar	IR	2
	7	B=O stretch	1358vs	Ar	IR	2
	8	BH_2 s–bend	1266	Ar	IR	2
	9	CH_3 rock	1162	Ar	IR	2
	10	CH_3 rock	1115	Ar	IR	2
	11	BH_2 rock	1036	Ar	IR	2
	12	C–O stretch	993	Ar	IR	2
a"	14	CH_3 a–stretch	2956	Ar	IR	2
	15	CH_3 a–deform.	1489	Ar	IR	2
	16	CH_3 rock	1183	Ar	IR	2
	17	H_2BO OPLA	895	Ar	IR	2
	18	Torsion	589	Ar	IR	2

A_0 = 1.691; B_0 = 0.343; C_0 = 0.301 MW[1]

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t–$CH_3CH{=}NH$

$\tilde{X}$ C_s Structure: MW[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH stretch	3264vvw	Ar	IR	1
	2	CH_3 a–stretch	3018m	Ar	IR	1
	3	CH stretch	2954ms	Ar	IR	1
	4	CH_3 s–stretch	2886	gas	IR	3
			2885m	Ar	IR	1
	5	C=N stretch	1651	gas	IR	3
			1659sh	Ar	IR	1
	7	CH_3 s–deform.	1398wm	Ar	IR	1
			1392m			
	8	Mixed	1359T	gas	IR	3
			1358s	Ar	IR	1
	9	CH deform.	1102	gas	IR	3
			1106s	Ar	IR	1

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	10	CNH deform.	1040	gas	IR	3
			1040s	Ar	IR	1
	11	CC stretch	920wm	Ar	IR	1
	12	CCN bend	498wm	Ar	IR	1
a"	13	CH_3 a–stretch	2990m	Ar	IR	1
	14	CH_3 a–deform.	1454	gas	IR	3
			1435s	Ar	IR	1
			1433s			
	15	C=N torsion	1160vw	Ar	IR	1
	16	CH_3 wag	1040s	Ar	IR	1
	17	CH wag	654	gas	IR	3
			668s	Ar	IR	1

A_0 = 1.666; B_0 = 0.328; C_0 = 0.289 MW[2]

t–$CD_3CD{=}ND$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ND stretch	2452vvw	Ar	IR	1
	2	CD_3 a–deform.	2243wm	Ar	IR	1
	3	CD stretch	2209wm	Ar	IR	1
	4	CD_3 s–stretch	2058w	Ar	IR	1
	5	C=N stretch	1613m	Ar	IR	1
	6	CC stretch	1200m	Ar	IR	1
	7	CD_3 s–deform.	1065m	Ar	IR	1
	8	CD_3 a–deform.	1042m	Ar	IR	1
	9	CD deform.	848ms	Ar	IR	1
	10	Mixed	804s	Ar	IR	1
	11	CND deform.	736m	Ar	IR	1
	12	CCN bend	411s	Ar	IR	1
a"	13	CD_3 a–stretch	2243wm	Ar	IR	1
	14	CD_3 a–deform.	1046m	Ar	IR	1
	15	C=N torsion	986m	Ar	IR	1
	16	CD_3 wag	799wm	Ar	IR	1
	17	CD wag	495vs	Ar	IR	1

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c–$CH_3CH{=}NH$

$\tilde{X}$ C_s Structure: MW[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH stretch	3247vvw	Ar	IR	1
	2	CH_3 a–stretch	3018m	Ar	IR	1
	3	CH stretch	2916	gas	IR	3
			2925ms	Ar	IR	1
			2920m			
	4	CH_3 s–stretch	2886	gas	IR	3
			2885m	Ar	IR	1

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	5	C=N stretch	1655	gas	IR	3
			1652vs	Ar	IR	1
	6	CH_3 a–deform.	1438ms	Ar	IR	1
	7	CH_3 s–deform.	1412m	Ar	IR	1
	8	Mixed	1250	gas	IR	3
			1252vs	Ar	IR	1
	9	CH deform.	1107	gas	IR	3
			1114ms	Ar	IR	1
	10	CNH deform.	1052wm	Ar	IR	1
	11	CH_3 rock	950w	Ar	IR	1
	12	CCN deform.	485s	Ar	IR	1
a"	13	CH_3 a–stretch	2988	gas	IR	3
			2990m	Ar	IR	1
	14	CH_3 a–deform.	1454	gas	IR	3
			1435s	Ar	IR	1
			1433s			
	15	C=N torsion	1132vw	Ar	IR	1
	16	CH_3 wag	1045	gas	IR	3
			1045vs	Ar	IR	1
	17	CH wag	678	gas	IR	3
			674w	Ar	IR	1

A_0 = 1.772; B_0 = 0.326; C_0 = 0.290 MW^2

c–CH_3CD=ND

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ND stretch	2425vvw	Ar	IR	1
	2	CD_3 a–stretch	2256wm	Ar	IR	1
	3	CD stretch	2191m	Ar	IR	1
	4	CD_3 s–stretch	2062w	Ar	IR	1
	5	C=N stretch	1631s	Ar	IR	1
			1628vs			
	6	Mixed	1159ms	Ar	IR	1
	7	Mixed	1072m	Ar	IR	1
	8	CD_3 a–deform.	1032wm	Ar	IR	1
	9	Mixed	850w	Ar	IR	1
	10	CD rock	796s	Ar	IR	1
	11	CD_3 rock	736m	Ar	IR	1
	12	CCN bend	405m	Ar	IR	1
a"	13	CD_3 a–stretch	2216wm	Ar	IR	1
	14	CD_3 a–deform.	1039s	Ar	IR	1
	15	CD_3 wag	848ms	Ar	IR	1
	16	C=N torsion	811s	Ar	IR	1
	17	CD wag	527m	Ar	IR	1

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[1]I. Stolkin, T.–K. Ha, and H. H. Gunthard, Chem. Phys. **21**, 327 (1977).
[2]F. J. Lovas, R. D. Suenram, D. R. Johnson, F. O. Clark, and E. Tiemann, J. Chem. Phys. **72**, 4964 (1980).
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$C_2H_3NH_2$

$\tilde{X}$ C_1[a] Structure: $MW^{3-5}IR^5$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	5	CH stretch	2987	gas	IR	2
			2976			
	6	C=C stretch	1672	gas	IR	2
			1668			
	7	NH_2 scissors	1625T	gas	IR	2
	8	CH_2 scissors	1454	gas	IR	2
	10	NH_2 twist	1260	gas	IR	2
			1248			
	11	C–N stretch	1084	gas	IR	2
			1078			
	12	CH wag	1046	gas	IR	2
			1039			
	14	CH_2 wag	812s	gas	IR	2
			805s			
	15	NH_2 wag	615[b]	gas	IR	2,4,5
			570[c]	gas	IR	2,4,5
			470[d]	gas	IR	4,5
			425[e]	gas	IR	4,5
	16	C=C torsion	379[b]	gas	IR	4,5
			333[d]	gas	IR	4,5
			287[e]	gas	IR	4,5

A_0 = 1.879; B_0 = 0.335; C_0 = 0.286 $MW^{1,3,5}$

[a] The barrier to inversion about the N atom is 356(3) cm^{-1},[3–5] leading to splittings in a number of the vibrational band centers. The 0^-–0^+ transition has been observed[5] in the far IR at 45.5 cm^{-1}. Ref. 5 has offered a tentative reassignment of the peaks associated with ν_{15} and ν_{16}.
[b] $1^- - 0^+$.
[c] $1^- - 0^-$.
[d] $1^+ - 0^+$.
[e] $1^+ - 0^-$.

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[4]Y. Hamada, N. Sato, and M. Tsuboi, J. Mol. Spectrosc. **124**, 172 (1987).
[5]R. D. Brown, P. D. Godfrey, B. Kleibömer, A. P. Pierlot, and D. McNaughton, J. Mol. Spectrosc. **142**, 195 (1990).

H_2C=NCH_3

$\tilde{X}$ C_s Structure: MW^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH_2 a–stretch	3024s	gas	IR	3
			3012s	Ar	IR	2–4
	2	CH_3 a–stretch	2962s	gas	IR	3
			2953s	Ar	IR	3
	3	CH_2 s–stretch	2897w	gas	IR	3
			2900s	Ar	IR	2–4
	4	CH_3 s–stretch	2854s	Ar	IR	3,4
			2849s			

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	5	C=N stretch	1661s	gas	IR	3
			1659m	Ar	IR	2,3
	6	CH_2 scissors	1475vs	gas	IR	3
			1470vvs	Ar	IR	2,3
	7	CH_3 a–deform.	1425wT	gas	IR	3
	8	CH_3 s–deform.	1405vw	gas	IR	3
			1402m	Ar	IR	2,3
	9	CH_3 rock	1220s	gas	IR	3
			1221s	Ar	IR	2–4
			1221	N_2	IR	4
	10	C–N stretch	952m	gas	IR	3
			950ms	Ar	IR	2–4
			949	N_2	IR	4
	12	CNC bend	484ms	gas	IR	3
			479ms	Ar	IR	2–4
			484	N_2	IR	4
a″	13	CH_3 a–stretch	2975s	gas	IR	3
			2962ms	Ar	IR	2–4
	14	CH_3 a–deform.	1444s	gas	IR	3
			1441m	Ar	IR	2,3
	15	CH_3 wag	1100vw	Ar	IR	2,3
	16	CH_2 OPLA	1026.14vs	gas	IR,DL	3,5
			1026vvs	Ar	IR	2–4
			1030	N_2	IR	4
	17	C=N torsion	686w	gas	IR	3
	18	CH_3 twist	220wT	Ar	IR	3

A_0 = 1.752; B_0 = 0.356; C_0 = 0.313 MW[1]

References

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[5]G. Yu and G. Duxbury, J. Mol. Spectrosc. **155**, 105 (1992).

C_2H_5O

$\tilde{A}$ $^2A'$ C_s
T_0 = 29204 gas EM[1,2,4]LF[3,5] $\tilde{A}$–$\tilde{X}$ 310–500 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′		CO stretch	596	gas	LF	5

τ_0 = 1.7(2) μs gas LF[3]EM[4]

$\tilde{X}$ $^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_2 wag	1370	gas	LF	3
		C–O stretch	1067	gas	LF,EM	3–5
		C–C stretch	875[a]	gas	LF	3
		CCO bend	442	gas	LF	3

[a] Assignment to overtone of CCO bend cannot be excluded.

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CH_3CHOH

In the gas phase, the onset of continuous absorption has been reported[1] near 33300 (300 nm), with an absorption maximum at 42000 (238 nm).

References

[1]C. Anastasi, J. Munk, P. Pagsberg, and V. J. Simpson, Chem. Phys. Lett. **164**, 18 (1989).

$HOCH_2CH_2$

In the gas phase, the onset of continuous absorption has been reported[1] near 37700 (265 nm), with increasing absorption out to the 210 nm cut-off of the observations.

References

[1]C. Anastasi, V. Simpson, J. Munk, and P. Pagsberg, J. Phys. Chem. **94**, 6327 (1990).

C_2H_5S

$\tilde{A}$ C_s
T_0 = 22720 gas LF[1] $\tilde{A}$–$\tilde{X}$ 390–600 nm
Predissociation occurs.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CS stretch	408(8)	gas	LF	1

τ = 75 ns gas LF[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CS stretch	681(15)	gas	LF	1

References

[1]G. Black and L. E. Jusinski, Chem. Phys. Lett. **136**, 241 (1987).

1,2-$C_2H_4Li_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3036w	Ar	IR	1
		CH stretch	2964vw	Ar	IR	1
			1240vw	Ar	IR	1
		CC stretch	1162w	Ar	IR	1
			695.5s	Ar	IR	1
			583m	Ar	IR	1
		LiC s-stretch	551w	Ar	IR	1
		LiC a-stretch	364w	Ar	IR	1
			360.5m	Ar	IR	1

1,2-$C_2D_4Li_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD stretch	2288w	Ar	IR	1
		CD stretch	2154w	Ar	IR	1
			915w	Ar	IR	1
		LiC s-stretch	595s	Ar	IR	1
			487	Ar	IR	1
			477m	Ar	IR	1
			351w	Ar	IR	1
			279m	Ar	IR	1

References

[1]L. Manceron and L. Andrews, J. Phys. Chem. **90**, 4514 (1986).

CH_3CCHLi

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	2893	Ar	IR	1
		C=C stretch	1738	Ar	IR	1
		H deform.	722	Ar	IR	1
		OPLA deform.	458	Ar	IR	1

References

[1]L. Manceron and L. Andrews, J. Am. Chem. Soc. **107**, 563 (1985).

$H_2C=(cyc-C_3H_2)^+$

$\tilde{F}\ ^2A_1$ C_{2v}
T^a = 80300(1000) gas PE[1]

$\tilde{E}\ ^2A_1$ C_{2v}
T^a = 62500(1000) gas PE[1]

$\tilde{D}\ ^2B_2$ C_{2v}
T^a = 49600(1000) gas PE[1]

$\tilde{B},\tilde{C}\ ^2B_1, ^2A_1$ C_{2v}
T^a = 39900(1000) gas PE[1]

$\tilde{A}\ ^2B_2$ C_{2v}
T^a = 22600(500) gas PE[1]

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1590(20)	gas	PE	1

[a] From vertical ionization potential.

References

[1]S. W. Staley and T. D. Norden, J. Am. Chem. Soc. **111**, 445 (1989).

$cyc-C_4H_4^+$

$\tilde{F}\ ^2A_g$ D_{2h}
T^a = 46500(1000) gas PE[1]

$\tilde{E}\ ^2B_{3u}$ D_{2h}
T^a = 41600(1000) gas PE[1]

$\tilde{C}\ ^2B_{1u}$ D_{2h}
T^a = 32000(1000) gas PE[1]

$\tilde{B}\ ^2B_{2u}$ D_{2h}
T^a = 26300(1000) gas PE[1]

$\tilde{X}\ ^2B_{2g}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g			1129(40)	gas	PE	1

[a] From vertical ionization potentials.

References

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$H_2C=(cyc-C_3H_2)$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1770vs	Ar	IR	1,2
			1519m	Ar	IR	1,2
			754s	Ar	IR	1,2
			664m	Ar	IR	1,2

A_0 = 0.977; B_0 = 0.239; C_0 = 0.192 MW[3,4]

References

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[4]M. Bogey, M. Cordonnier, J.-L. Destombes, J.-M. Denis, and J.-C. Guillemin, J. Mol. Spectrosc. **149**, 230 (1991).

cyc-C_4H_4

$\tilde{X}$ D_{2h} Structure: $IR^{3-5}Ra^{6}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g		CH stretch	3140(5)	Ne,Ar	Ra	6
		C=C stretch	1678(5)	Ne,Ar	Ra	6
		CH deform.	1059(5)	Ne,Ar	Ra	6
		CH deform.	989(5)	Ne,Ar	Ra	6
b_{1u}		CH stretch	3105wm	Ar	IR	5
		C=C stretch	1526w	Ar	IR	4,5
		CH deform.	1028vw	Ar	IR	5
b_{2g}		CH OPLA deform.	531(5)	Ne,Ar	Ra	6
b_{2u}		CH stretch	3073w	Ar	IR	5
		CH deform.	1242s	Ar	IR	1-5
		Ring deform.	719wm	Ar	IR	4,5
b_{3g}		CH stretch	3093(5)	Ne,Ar	Ra	6
		Ring deform.	723(5)	Ne,Ar	Ra	6
b_{3u}		CH OPLA	569vs	Ar	IR	1-5

cyc-C_4D_4

$\tilde{X}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{1u}		C=C stretch	1456w	Ar	IR	4
b_{2u}		CD deform.	1043wm	Ar	IR	4
		Ring deform.	609wm	Ar	IR	4
b_{3u}		CD OPLA	421vs	Ar	IR	4

References

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cyc-C_2H_4OFe

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1457.9	Ar	IR	1
			1259.5	Ar	IR	1
			1138.0	Ar	IR	1
			1134.9			
			836.0	Ar	IR	1
			756.0	Ar	IR	1

cyc-C_2D_4OFe

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1076.1	Ar	IR	1
			1003.1	Ar	IR	1
			924.5	Ar	IR	1
			749.5	Ar	IR	1
			747.5			

References

[1]Z. H. Kafafi, R. H. Hauge, W. E. Billups, and J. L. Margrave, J. Am. Chem. Soc. **109**, 4775 (1987).

CH_2=CHFeOH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3749.7	Ar	IR	1
		CH stretch	2917.1	Ar	IR	1
		C=C stretch	1556.3	Ar	IR	1
		CH_2 rock	1019.0	Ar	IR	1
		CH_2 wag	944.2	Ar	IR	1
		Fe-O stretch	699.6	Ar	IR	1
		Fe-C stretch	541.7	Ar	IR	1

CD_2=CDFeOD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OD stretch	2762.3	Ar	IR	1
		C=C stretch	1484.9	Ar	IR	1
		CD_2 wag	737.6	Ar	IR	1
		Fe-O stretch	681.5	Ar	IR	1
		Fe-C stretch	527.9	Ar	IR	1

References

[1]Z. H. Kafafi, R. H. Hauge, W. E. Billups, and J. L. Margrave, J. Am. Chem. Soc. **109**, 4775 (1987).

cyc-$(H_2COC)=CH_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C=C stretch	1823.4s	Ar	IR	1
			1820.4	Kr	IR	1
		CO stretch + CH_2 deform.	1109.2wm	Ar	IR	1
			1107.3	Kr	IR	1
			1107	Xe	IR	1
		Ring breathing	881.1wm	Ar	IR	1
			879.4	Kr	IR	1
			880.6	Xe	IR	1
		$=CH_2$ deform.	793.8wm	Ar	IR	1
			793.6	Kr	IR	1
			790.1	Xe	IR	1

cyc-$(D_2COC)=CD_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C=C stretch	1765.2	Ar	IR	1
			1760.9	Xe	IR	1
		CO stretch + CD_2 deform.	919.9	Ar	IR	1
		Ring breathing	748.0	Ar	IR	1
		$=CD_2$ deform.	629.2T	Ar	IR	1
			626.0	Xe	IR	1

References

[1]K. A. Singmaster and G. C. Pimentel, J. Mol. Struct. **194**, 215 (1989).

HCH_3(cyc-CCS)

(Methylthiirene)

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3203w	Ar	IR	1,2
		CH stretch	2930vw	Ar	IR	1,2
			1440m	Ar	IR	1,2
			1429m	Ar	IR	1,2
			1036m	Ar	IR	1,2
			897m	Ar	IR	1,2
			650w	Ar	IR	1,2

References

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[2]A. Krantz and J. Laureni, J. Am. Chem. Soc. **103**, 486 (1981).

HO_2CH_2OH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3648	gas	IR	2
		OH stretch	3598	gas	IR	2
		CH stretch	2900T	gas	IR	1
		OOH bend	1350T	gas	IR	1
		CO stretch	1050	gas	IR	1
		OO stretch	820T	gas	IR	1

References

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CH_3COOCa

$\tilde{B}, \tilde{C}\ ^2B_2, ^2B_1$ C_{2v}[a]
T_0 = 15850(20) gas LF[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		Ca··O_2C stretch	341(10)	gas	LF	1

$\tilde{A}\ ^2A_1$ C_{2v}[a]
T_0 = 14573(20) gas LF[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		Ca··O_2C stretch	347(10)	gas	LF	1

$\tilde{X}\ ^2A_1$ C_{2v}[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		Ca··O_2C stretch	332(10)	gas	LF	1

[a] Symmetry of heavy atoms.

References

[1]L. C. O'Brien, C. R. Brazier, S. Kinsey-Nielsen, and P. F. Bernath, J. Phys. Chem. **94**, 3543 (1990).

CH_3COOSr

$\tilde{C}\ ^2B_1$ C_{2v}[a]
T_0 = 14832(20) gas LF[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		Sr··O_2C stretch	292(10)	gas	LF	1

$\tilde{B}\ ^2B_2$ C_{2v}[a]
T_0 = 14643(20) gas LF[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		Sr··O_2C stretch	282(10)	gas	LF	1

$\tilde{A}\ ^2A_1$ C_{2v}[a]
T_0 = 13500(20) gas LF[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		Sr··O_2C stretch	284(10)	gas	LF	1

$\tilde{X}\ ^2A_1$ C_{2v}[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		Sr··O_2C stretch	253(10)	gas	LF	1

[a] Symmetry of heavy atoms.

References

[1]L. C. O'Brien, C. R. Brazier, S. Kinsey-Nielsen, and P. F. Bernath, J. Phys. Chem. **94**, 3543 (1990).

CH_3ONCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NCO a-stretch	2204vs	Ar	IR	1
			2152wm			
			1049m	Ar	IR	1
			828wm	Ar	IR	1
			657wm	Ar	IR	1
			510wm	Ar	IR	1
			425wm	Ar	IR	1

References

[1]J. H. Teles and G. Maier, Chem. Ber. **122**, 745 (1989).

CH_3COO_2

A prominent gas-phase absorption with maximum near 207 nm has been attributed[3,4] to CH_3COO_2.

A weaker, broad gas-phase absorption with maximum near 245 nm has been attributed[2-4] to CH_3COO_2.

$\tilde{A}$
T_0 = 5562(3) gas AB[1] $\tilde{A}$–$\tilde{X}$ 1348–1798 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	932(5)	gas	AB	1
			530	gas	AB	1

References

[1]H. E. Hunziker and H. R. Wendt, J. Chem. Phys. **64**, 3488 (1976).
[2]M. C. Addison, J. P. Burrows, R. A. Cox, and R. Patrick, Chem. Phys. Lett. **73**, 283 (1980).
[3]N. Basco and S. S. Parmar, Int. J. Chem. Kinet. **17**, 891 (1985).
[4]G. Moortgat, B. Veyret, and R. Lesclaux, J. Phys. Chem. **93**, 2362 (1989).

$C_6H_2^+$

$\tilde{B}\ ^2\Pi_u$ $D_{\infty h}$
T_0 = 27350(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			650(80)	gas	PE	1

$\tilde{A}\ ^2\Pi_g$ $D_{\infty h}$
T_0 = 16658 gas EF[2,3]LF[3] $\tilde{A}$–$\tilde{X}$ 485–725 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	CH stretch	3243(2)T	gas	LF	3
	2	C≡C stretch	2053(2)	gas	LF	3
	3	C≡C stretch	1880(2)	gas	LF	3
	4	C–C stretch	617(2)	gas	LF,EF	2,3
Π_g	10	Skel. bend	244T	gas	LF	3

τ_0 = 17(2) ns gas EF[2]

$\tilde{X}\ ^2\Pi_u$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	2	C≡C stretch	2182(2)	gas	EF	2,3
	3	C≡C stretch	1903(2)	gas	EF	2,3
	4	C–C stretch	632(2)	gas	EF	2,3
Π_g	10	Skel. bend	228(2)T	gas	LF	3

References

[1]F. Brogli, E. Heilbronner, V. Hornung, and E. Kloster-Jensen, Helv. Chim. Acta **56**, 2171 (1973).
[2]M. Allan, E. Kloster-Jensen, and J. P. Maier, Chem. Phys. **17**, 11 (1976).
[3]D. Klapstein, R. Kuhn, J. P. Maier, M. Ochsner, and W. Zambach, J. Phys. Chem. **88**, 5176 (1984).

HON=CHCNO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3621vs	Ar	IR	1
		CNO a-stretch	2301vs	Ar	IR	1
		CNO s-stretch	1453m	Ar	IR	1
			1346w	Ar	IR	1
			1258m	Ar	IR	1
			1241wm	Ar	IR	1
			989ms	Ar	IR	1
			940wm	Ar	IR	1
			914wm	Ar	IR	1
			425s	Ar	IR	1
			423m			

References

[1]G. Maier and J. H. Teles, Angew. Chem. **99**, 152 (1987); Angew. Chem. Int. Ed. Engl. **26**, 155 (1987).

HON=CHNCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3638	Ar	IR	1
		NCO a-stretch	2276	Ar	IR	1
			1646	Ar	IR	1
			976	Ar	IR	1

References

[1]G. Maier and J. H. Teles, Angew. Chem. **99**, 152 (1987); Angew. Chem. Int. Ed. Engl. **26**, 155 (1987).

CF_3H(cyc-CCS)

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3210w	Ar	IR	1
			1240s	Ar	IR	1
			1190s	Ar	IR	1
			1180s	Ar	IR	1
			720w	Ar	IR	1

References

[1]M. Torres, A. Clement, J. E. Bertie, H. E. Gunning, and O. P. Strausz, J. Org. Chem. **43**, 2490 (1978).

Li_8

A prominent absorption maximum at about 20800 (480 nm) and a much weaker absorption maximum at 14700 (680 nm), observed in depletion photoionization experiments[1] on gas-phase Li_8, have been assigned to the T_d and/or the D_{2d} structures of that species.

References

[1]V. Bonačić-Koutecký, M. Broyer, J. Chevaleyre, Ph. Dugourd, J. Koutecký, C. Scheuch, J. P. Wolf, and L. Wöste, J. Chem. Phys. **96**, 1793 (1992).

Na_8

A prominent absorption maximum at 20400 (490 nm), weaker absorption maxima at 16900 (ca. 600 nm) and 13500 (740 nm), and possibly an absorption maximum at 19600 (510 nm), observed[1,2,4] in depletion photoionization experiments on gas-phase Na_8, have been assigned[3,4] to the T_d and/or the D_{2d} structures of that species.

References

[1]K. Selby, M. Vollmer, J. Masui, V. Kresin, W. de Heer, and W. Knight, Phys. Rev. B **40**, 5417 (1989).
[2]C. R. C. Wang, S. Pollack, and M. M. Kappes, Chem. Phys. Lett. **166**, 26 (1990).
[3]V. Bonačić-Koutecký, M. M. Kappes, P. Fantucci, and J. Koutecký, Chem. Phys. Lett. **170**, 26 (1990).
[4]C. R. C. Wang, S. Pollack, D. Cameron, and M. M. Kappes, J. Chem. Phys. **93**, 3787 (1990).

C_8

In an argon matrix, the growth behavior of the 1998 cm^{-1} infrared absorption on sample warmup has been correlated with that of the maximum of a structured absorption near 308 nm.[3,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			411	Ar	AB	4

$\tilde{X}\ ^3\Sigma$ $D_{\infty h}$ Structure: ESR[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	4	Sym. stretch	565T	gas	PE	5
Σ_u^+		Asym. stretch	1998	Ar	IR	2–4

References

[1]R. J. Van Zee, R. F. Ferrante, K. J. Zeringue, and W. Weltner, Jr., J. Chem. Phys. **88**, 3465 (1988).
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[5]D. W. Arnold, S. E. Bradforth, T. N. Kitsopoulos, and D. M. Neumark, J. Chem. Phys. **95**, 8753 (1991).

C_8^-

Threshold for electron detachment from ground-state C_8^- = 35330(50) gas PE[1,2]

References

[1]S. Yang, K. J. Taylor, M. J. Craycraft, J. Conceicao, C. L. Pettiette, O. Cheshnovsky, and R. E. Smalley, Chem. Phys. Lett. **144**, 431 (1988).
[2]D. W. Arnold, S. E. Bradforth, T. N. Kitsopoulos, and D. M. Neumark, J. Chem. Phys. **95**, 8753 (1991).

$CF_2{=}PCF_3$

$\tilde{X}$ C_s Structure: ED[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	C=P stretch	1365.3vs	gas	IR	1,3
	2	CF_2 a-stretch	1248.9s	gas	IR	1,3
	3	CF_3 a-stretch	1149.1vs	gas	IR	1,3
	4	CF_3 s-stretch	1095w	gas	IR	3
	5	CF_2 s-stretch	746vw	gas	IR	1,3
	6	Mixed	737w	gas	IR	1,3
	7	Mixed	484vw	gas	IR	3
	8	CF_3 a-deform.	470w	gas	IR	1,3
	9	CF_2 scissors	432vw	gas	IR	3
a"	13	CF_3 a-stretch	1134.5m	gas	IR	1,3
	14	CF_2 wag	551vw	gas	IR	1,3
	15	CF_3 a-deform.	475w	gas	IR	1,3

References

[1]A. B. Burg, Inorg. Chem. **22**, 2573 (1983).
[2]B. Steger, H. Oberhammer, J. Grobe, and D. Le Van, Inorg. Chem. **25**, 3177 (1986).
[3]K. Ohno, E. Kurita, M. Kawamura, and H. Matsuura, J. Am. Chem. Soc. **109**, 5614 (1987).

CF_3ONO_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO_2 a-stretch	1735.5	Ar	IR	1
			1345.2	Ar	IR	1
		NO_2 s-stretch	1327.1	Ar	IR	1
		CF_3 stretch	1260.8s	Ar	IR	1
		CF_3 stretch	1249.5vs	Ar	IR	1
			1142.5vs	Ar	IR	1
		C-O stretch	924.1w	Ar	IR	1
		NO_2 scissors	785.2	Ar	IR	1
		ONO_2 OPLA	752.9	Ar	IR	1
			519.0	Ar	IR	1

References

[1]K. C. Clemitshaw and J. R. Sodeau, J. Phys. Chem. **91**, 3650 (1987).

$SiCl_3ONO_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1683	gas	IR	1
			1290	gas	IR	1
			870	gas	IR	1

References

[1]H. Niki, P. D. Maker, C. M. Savage, L. P. Breitenbach, and M. D. Hurley, J. Phys. Chem. **89**, 3725 (1985).

$O_3ClOClO_2$

In the gas phase,[2,3] there is a very broad, unstructured absorption with maximum at 268 nm (37300). A second absorption maximum near 215 nm has also been reported.[3] In an argon matrix,[2] the threshold for dissociation into O_2 and $ClOClO_3$ lies at a wavelength longer than 400 nm. These same products were observed on irradiation in the 400–250 nm spectral range.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ClO_3 a-stretch	1249.5	Ne	IR	2
			1245.9	Ar	IR	2
	2	ClO_2 s-stretch	1080	gas	IR	1
			1082.3	Ne	IR	2
			1081.5	Ar	IR	2
	3	ClO_3 s-stretch	1024	gas	IR	1
			1026.3	Ne	IR	2
			1026.0	Ar	IR	2
	4	O_3Cl-O stretch	691	gas	IR	1
			693.0	Ne	IR	2
			695.7	Ar	IR	2
	5	O_2Cl-O stretch	629	gas	IR	1
			625.2	Ne	IR	2
			624.0	Ar	IR	2
	6	ClO_3 a-deform.	578.2	Ne	IR	2
			580.0	Ar	IR	2
	7	ClO_2 deform.	544	gas	IR	1
			543.6	Ne	IR	2
			542.5	Ar	IR	2
	8	ClO_3 s-deform.	486.6	Ne	IR	2
			486.0	Ar	IR	2
	9	ClO_2 rock	374.6	Ar	IR	2
	10	ClO_3 rock	371.2	Ar	IR	2
	11	ClOCl deform.	238.0	Ar	IR	2
a"	12	ClO_3 a-stretch	1284.1	Ne	IR	2
			1278.1	Ar	IR	2
	13	ClO_2 a-stretch	1265	gas	IR	1
			1263.1	Ne	IR	2
	14	ClO_2 a-deform.	579	gas	IR	1
			585.5	Ne	IR	2
			585.9	Ar	IR	2
	15	ClO_2 rock	374.6	Ar	IR	2
	16	ClO_3 rock	371.2	Ar	IR	2

References

[1]M. Jansen, K. M. Tobias, and H. Willner, Naturwiss. **73**, 734 (1986).
[2]M. Jansen, G. Schatte, K. M. Tobias, and H. Willner, Inorg. Chem. **27**, 1703 (1988).
[3]M. I. Lopez and J. E. Sicre, J. Phys. Chem. **94**, 3860 (1990).

6.15. Hydrocarbons with More Than Eight Atoms

$C_2H_7^+$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	HH stretch	3964.0	gas	PF	1
		CH stretch	2683	gas	PF	1
		CH stretch	2601	gas	PF	1
		CH stretch	2521	gas	PF	1

References

[1]L. I. Yeh, J. M. Price, and Y. T. Lee, J. Am. Chem. Soc. **111**, 5597 (1989).

br–$C_2H_7^+$

$\tilde{X}$ C_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a		CH stretch	3128	gas	PF	1
b		CH stretch	3082	gas	PF	1
		CH stretch	2945.4	gas	PF	1

References

[1]L. I. Yeh, J. M. Price, and Y. T. Lee, J. Am. Chem. Soc. **111**, 5597 (1989).

1–$C_3H_7^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Skel. bend	700(30)	gas	PE	1,2

References

[1]J. C. Schultz, F. A. Houle, and J. L. Beauchamp, J. Am. Chem. Soc. **106**, 3917 (1984).
[2]J. Dyke, A. Ellis, N. Jonathan, and A. Morris, J. Chem. Soc., Faraday Trans. 2 **81**, 1573 (1985).

2–$C_3H_7^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		Skel. bend	600(30)	gas	PE	1

References

[1]J. Dyke, A. Ellis, N. Jonathan, and A. Morris, J. Chem. Soc., Faraday Trans. 2 **81**, 1573 (1985).

$CH_3CH_2CH_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3100	Ar	IR	1
		CH stretch	3018	Ar	IR	1
		2–CH stretch	2812	Ar	IR	1
		RCH_2 deform.	530vs	Ar	IR	1

References

[1]J. Pacansky, D. E. Horne, G. P. Gardini, and J. Bargon, J. Phys. Chem. **81**, 2149 (1977).

$(CH_3)_2CH$

3d Rydberg state

A gas–phase absorption maximum at 207 nm has been assigned[3] to the $3d$–$\tilde{X}$ transition of $(CH_3)_2CH$.

3p Rydberg state

An unstructured gas–phase absorption between 225 and 260 nm, with maximum at 236 nm, has been assigned[1,3] to the $3p$–$\tilde{X}$ transition of $(CH_3)_2CH$.

3s Rydberg state

In gas–phase absorption studies, a shoulder at 270 nm has been tentatively assigned[3] to the $3s$–$\tilde{X}$ transition of $(CH_3)_2CH$.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3052	Ar	IR	2,4
		CH_3 stretch	2920	Ar	IR	2
		CH_3 stretch	2850	Ar	IR	2
		CH_3 stretch	2830	Ar	IR	2
		CH_3 deform.	1468	Ar	IR	2
		CH_3 deform.	1440	Ar	IR	2
		CH_3 deform.	1388	Ar	IR	2
		CH_3 deform.	1378	Ar	IR	2
		CH_3 rock	1165	Ar	IR	4
		CC stretch	879	Ar	IR	4
		$HC(CH_3)_2$ OPLA	364s	Ar	IR	2,4

References

[1]D. A. Parkes and C. P. Quinn, J. Chem. Soc., Faraday Trans. 1 **72**, 1952 (1976).
[2]J. Pacansky and H. Coufal, J. Chem. Phys. **62**, 3298 (1980).
[3]H. R. Wendt and H. E. Hunziker, J. Chem. Phys. **81**, 717 (1984).
[4]G. Chettur and A. Snelson, J. Phys. Chem. **91**, 913 (1987).

t–$C_4H_9^+$

$\tilde{X}$ C_{3h}[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C–C s–stretch[b]	760(30)	gas	PE	1,2
		C_4 OPLA[b]	460(30)	gas	PE	1–3

[a] Probable symmetry of carbon skeleton; see Ref. 2.
[b] Presumes C_{3v} structure for t–C_4H_9.

References

[1]T. Koenig, T. Balle, and W. Snell, J. Am. Chem. Soc. **97**, 662 (1975).
[2]J. Dyke, N. Jonathan, E. Lee, A. Morris, and M. Winter, Phys. Scr. **16**, 197 (1977).
[3]F. A. Houle and J. L. Beauchamp, J. Am. Chem. Soc. **101**, 4067 (1979).

n–C_4H_9

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		1–CH_2 stretch	3105	Ar	IR	1,2
		1–CH_2 stretch	3024	Ar	IR	1,2
			2886	Ar	IR	2
		2–CH_2 stretch	2835	Ar	IR	2
		2–CH_2 stretch	2809	Ar	IR	1,2
			1471	Ar	IR	2
			1463	Ar	IR	2
		2–CH_2 deform.	1425	Ar	IR	2
			1183	Ar	IR	2
			1098	Ar	IR	2
		$(C_3H_7)CH_2$ OPLA	520s	Ar	IR	1

References

[1]J. Pacansky, D. E. Horne, G. P. Gardini, and J. Bargon, J. Phys. Chem. **81**, 2149 (1977).
[2]J. Pacansky and A. Gutierrez, J. Phys. Chem. **87**, 3074 (1983).

i–C_4H_9

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		1–CH stretch	3023	Ar	IR	1
		1–CH stretch	3115	Ar	IR	1
		2–CH stretch	2820	Ar	IR	1
		$(C_3H_7)CH_2$ OPLA	557s	Ar	IR	1
			546s			

References

[1]J. Pacansky, D. W. Brown, and J. S. Chang, J. Phys. Chem. **85**, 2562 (1981).

t–C_4H_9

3d Rydberg state

In the gas phase, an absorption with maximum at 233 nm has been assigned[1,2,5] to the $3d$–$\tilde{X}$ transition of t–C_4H_9.

3p Rydberg state

In the gas phase, an absorption with maximum at 253 nm has been assigned[2,5] to the $3p$–$\tilde{X}$ transition of t–C_4H_9.

3s Rydberg state

In the gas phase, a broad absorption with maximum at 333 nm has been assigned[5] to the $3s$–$\tilde{X}$ transition of t–C_4H_9.

$\tilde{X}$ C_{3v} Structure: IR[3,6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CH stretch	2931	Ar	IR	3,6
		CH stretch	2833[b]	gas	IR	4
			2825vs	Ar	IR	3,6
		CH_3 deform.	1455	Ar	IR	3,6
		CH_3 deform.	1367	Ar	IR	3,6
		CH_3 rock	992	Ar	IR	3,6
		CC stretch	733	Ar	IR	3,6
e		CH stretch	2931	Ar	IR	3,6
		CH stretch	2825vs	Ar	IR	3,6
		CH_3 deform.	1455	Ar	IR	3,6
		CH_3 deform.	1371	Ar	IR	3,6
		CC stretch	1279	Ar	IR	3,6
		CH_3 rock	811	Ar	IR	3,6
		C_3 bend	541	Ar	IR	3,6

[a] Unassigned absorptions, attributed to combination bands or impurities, were also observed at 1252, 1205, 1184, and 1129 cm^{-1}.
[b] Time–resolved infrared spectral photography (TRISP); resolution 3 cm^{-1}.

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[3]J. Pacansky and J. S. Chang, J. Chem. Phys. **74**, 5539 (1981).
[4]D. S. Bethune, J. R. Lankard, P. P. Sorokin, A. J. Schell-Sorokin, R. M. Plecenik, and Ph. Avouris, J. Chem. Phys. **75**, 2231 (1981).
[5]H. R. Wendt and H. E. Hunziker, J. Chem. Phys. **81**, 717 (1984).
[6]B. Schrader, J. Pacansky, and U. Pfeiffer, J. Phys. Chem. **88**, 4069 (1984).

$CH_3(C\equiv C)_2H^+$

$\tilde{A}\ ^2E$ C_{3v}
T_0 = 20374.5(5) gas EF[1,4]LF[2] $\tilde{A}$–$\tilde{X}$ 450–630 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	C≡C stretch	2135(10)	gas	LF	2
	4	C≡C stretch	2000(10)	gas	LF	2
	5	CH_3 deform.	1272(10)	gas	LF	2
	6	C–C a-stretch	1130	gas	EF,LF	1,2,4
	7	C–C s-stretch	664[a]	gas	EF,LF	1,2,4
e	13	Skel. deform.	303H[a] 306	gas	EF,LF	1,2,4

τ_0 = 50(3) ns gas EF[1]PEPICO[3]

$\tilde{X}\ ^2E$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	C≡C stretch	2212	gas	EF	1,4
	4	C≡C stretch	1921	gas	EF	4
	6	C–C a-stretch	1203	gas	EF	1,4
	7	C–C s-stretch	685[a] 691	gas	EF	1,4
e	13	Skel. deform.	313H[a] 324	gas	EF	4

$CD_3(C\equiv C)_2D^+$

$\tilde{A}\ ^2E$ C_{3v}
T_0 = 20374.7(5) gas EF[1,4] $\tilde{A}$–$\tilde{X}$ 460–570 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	5	C–C a-stretch	1157	gas	EF	4
	6	CD_3 deform.	1019[a]	gas	EF	4
	7	C–C s-stretch	617[a]	gas	EF	1,4
e	13	Skel. bend	284H[a]	gas	EF	4

τ_0 = 53(3) ns gas EF[1]PEPICO[3]

$\tilde{X}\ ^2E$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	C≡C stretch	2186	gas	EF	1,4
	4	C≡C stretch	1884	gas	EF	4
	5	C–C a-stretch	1219	gas	EF	1,4
	6	CD_3 deform.	1020[a]	gas	EF	1,4
	7	C–C s-stretch	634[a]	gas	EF	1,4
e	13	Skel. deform.	283H[a] 292	gas	EF	4

[a] Uncorrected for Fermi resonance.

References

[1]J. P. Maier, O. Marthaler, and E. Kloster-Jensen, J. Chem. Phys. **72**, 701 (1980).
[2]J. P. Maier and L. Misev, Chem. Phys. **51**, 311 (1980).
[3]P. Forster, J. P. Maier, and F. Thommen, Chem. Phys. **59**, 85 (1981).
[4]S. Leutwyler, D. Klapstein, and J. P. Maier, Chem. Phys. **78**, 151 (1983).

cyc–C_5H_4

(Cyclopentadienylidine)

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1345w	N_2	IR	1
			1335m	N_2	IR	1
			1101w	N_2	IR	1
			1074w	N_2	IR	1
			922w	N_2	IR	1
			703s	N_2	IR	1
			577w	N_2	IR	1

References

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cyc–C_5H_5

$\tilde{A}\ ^2A_2''$ D_{5h} Structure: LF[9]
T_0 = 29572.166(2) gas AB[1,3,4]LF[6,8] $\tilde{A}$–$\tilde{X}$ 306–395 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e_2'			798	gas	AB,LF	4,9
e_2''		CH bend	331	gas	AB,LF	1,3,4,9

τ_0 = 64.9(5) ns gas LF[7]
B_0 = 0.286; C_0 = 0.144 LF[8,9]

$\tilde{X}\ ^2E_1''$ D_{5h} Structure: ESR[2]AB[4]LF[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e_2'	10	C–C stretch	1690(40)[a]	gas	PD	5
	11	CH deform.	1170(40)	gas	PD	5
	12		880	gas	PD,LF	5,6,9
	13	Ring deform.	475	gas	LF	6
e_2''	14	Ring deform.	380	gas	LF	6

B_0 = 0.296; C_0 = 0.148 LF[8,9]

cyc–C_5D_5

$\tilde{A}\ ^2A_2''$ D_{5h}
T_0 = 29819.434(2) gas AB[4]LF[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e_2''		CD bend	233	gas	AB	4

B_0 = 0.233; C_0 = 0.117 LF[9]

$\tilde{X}\ ^2E_1''$ D_{5h}
$B_0 = 0.240$; $C_0 = 0.120$ LF[9]

[a] Alternatively, may be contributed by $2\nu_{12}$.

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n-C_5H_{11}

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		1-CH_2 stretch	3103	Ar	IR	1
		1-CH_2 stretch	3025	Ar	IR	1
		2-CH_2 stretch	2838	Ar	IR	1
		2-CH_2 stretch	2802	Ar	IR	1
		2-CH_2 deform.	1425	Ar	IR	1
			1181	Ar	IR	1
			1096	Ar	IR	1
		$(C_4H_9)CCH_2$ OPLA	519s	Ar	IR	1

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$(CH_3)_3CCH_2$

(Neopentyl)

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		1-CH stretch	3105	Ar	IR	1
		1-CH stretch	3020	Ar	IR	1
		$(C_4H_9)CCH_2$ OPLA	565vs	Ar	IR	1
			555vs			

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$C_6H_4^+$

T^a = 23880(160) gas PE[1]

T^a = 2820(160) gas PE[1]

$T^a \cong 2000$ gas PE[1]

[a] From vertical ionization potentials.

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C_6H_4

(o-Benzyne)

Absorption maxima at 40650 and 50250 (246 and 199 nm) have been reported[6,7] for *o*-benzyne isolated in an argon matrix.

An absorption maximum at 26320 (380 nm) has been assigned[6,7] to *o*-benzyne isolated in an argon matrix. In a neon matrix, this absorption maximum appears at 28730 (348 nm).[8]

$\tilde{a}\ ^3B_2$ C_{2v}
T_0 = 13210(200) gas PE[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1440(30)	gas	PE	4
			570(30)	gas	PE	4

$\tilde{X}\ ^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	3094wm	Ne	IR	8
			3088	N_2	IR	2
	2	CH stretch	3071w	Ne	IR	8
	3	C≡C stretch	1860(15)	gas	PE	4
			1846w	Ne	IR	8
	4	Mixed	1415vw	Ne	IR	8
	5	Mixed	1271w	Ne	IR	8
	6	CH deform.	1055wm	Ne	IR	8
			1053m	Ar	IR	1
			1056	N_2	IR	2,5
	7	Ring stretch	1040(20)	gas	PE	4
			1039m	Ne	IR	8
			1038m	Ar	IR	1
			1039	N_2	IR	2,5
	8	Ring stretch	982wm	Ne	IR	8
	9	Ring deform.	605(15)	gas	PE	4
			589vw	Ne	IR	8
b_1	14	CH wag	838vw	Ne	IR	8
	15	CH wag	737s	Ne	IR	8
			736vs	Ar	IR	1
			743	N_2	IR	2,5
	16	Ring torsion	388wm	Ne	IR	8

$\tilde{X}\ ^1A_1$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	17	CH stretch	3086m	Ne	IR	8
	18	CH stretch	3049vw	Ne	IR	8
	19	Ring stretch	1451m	Ne	IR	8
			1451m	Ar	IR	1
			1448	N_2	IR	2,5
	20	Mixed	1394wm	Ne	IR	8
			1395	N_2	IR	5
			1355	N_2	IR	5
	21	Mixed	1307vw	Ne	IR	8
	22	Mixed	1094w	Ne	IR	8
	23	Ring deform.	849ms	Ne	IR	8
			849s	Ar	IR	1
			847	N_2	IR	2,5
	24	Ring deform.	472vs	Ne	IR	8
			469vs	Ar	IR	1
			472	N_2	IR	2,5

$A_0 = 0.233$; $B_0 = 0.190$; $C_0 = 0.105$ MW[3]

C_6D_4

$\tilde{a}\ ^3B_2$ C_{2v}

T_0 = 13250(200) gas PE[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1330(30)	gas	PE	4
			550(30)	gas	PE	4

$\tilde{X}\ ^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD stretch	2311wm	Ne	IR	8
			2293	N_2	IR	2
	2	CD stretch	2295vw	Ne	IR	8
	3	C≡C stretch	1860(15)	gas	PE	4
			1844vw	Ne	IR	8
	4	Mixed	1364w	Ne	IR	8
	5	Mixed	1198w	Ne	IR	8
	6	Ring stretch	980(20)	gas	PE	4
			995wm	Ne	IR	8
	7	CD deform.	853w	Ne	IR	8
	8	Ring stretch	792wm	Ne	IR	8
	9	Ring deform.	585(15)	gas	PE	4
			579vw	Ne	IR	8
b_1	14	CD wag	679vw	Ne	IR	8
	15	CD wag	571m	Ne	IR	8
	16	Ring torsion	336w	Ne	IR	8
b_2	17	CD stretch	2314wm	Ne	IR	8
	18	CD stretch	2285vw	Ne	IR	8
	19	Ring stretch	1411w	Ne	IR	8
	20	Mixed	1293w	Ne	IR	8
			1293	N_2	IR	2
	21	Mixed	1112vw	Ne	IR	8
			1108	N_2	IR	2
	22	Mixed	875vw	Ne	IR	8
	23	Ring deform.	790m	Ne	IR	8
			792	N_2	IR	2
	24	Ring deform.	469vs	Ne	IR	8
			471	N_2	IR	2

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$C_6H_4^-$

Threshold for electron detachment from ground-state $C_6H_4^-$ = 4520(80) gas PE[1]

$\tilde{X}\ ^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			600(30)	gas	PE	1

$C_6D_4^-$

Threshold for electron detachment from ground-state $C_6D_4^-$ = 4450(80) gas PE[1]

$\tilde{X}\ ^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			580(30)	gas	PE	1

References

[1]D. G. Leopold, A. E. S. Miller, and W. C. Lineberger, J. Am. Chem. Soc. **108**, 1379 (1986).

$C_6H_5^+$

$\tilde{a}\ ^3B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CH stretch	2790(100)	gas	PE	1

$C_6D_5^+$

$\tilde{a}\ ^3B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CD stretch	2370(110)	gas	PE	1

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C_6H_5

A broad gas–phase absorption with maximum near 245 nm has been attributed[6] to C_6H_5.

A prominent absorption near 288 nm in argon–matrix studies of photolyzed benzene samples has also been attributed[4] to C_6H_5.

$\tilde{A}\ ^2B_1$ C_{2v}
T_0 = 18908 gas AB[1] $\tilde{A}$–$\tilde{X}$ 440–530 nm
18716 Ar AB[4] $\tilde{A}$–$\tilde{X}$ 530–535 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			896	gas	AB	1
			722	gas	AB	1
			571	gas	AB	1

Gas–phase photoelectron spectra[7] suggest that there is an excited electronic state of C_6H_5 at or below 13700.

$\tilde{X}\ ^2A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			968(15)	gas	PE	7
			600(10)	gas	PE	7
b_1		CH deform.	707s	Ar	IR	2–5

C_6D_5

A prominent absorption at 286 nm in argon–matrix studies of photolyzed benzene samples has been attributed[4] to C_6D_5.

$\tilde{A}\ ^2B_1$ C_{2v}
T_0 = 18840 Ar AB[4] $\tilde{A}$–$\tilde{X}$ 530–535 nm

$\tilde{X}\ ^2A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			960(20)	gas	PE	7
			588(10)	gas	PE	7
b_1		CD deform.	519s	Ar	IR	2,5

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$C_6H_5^-$

Threshold for electron detachment from ground–state $C_6H_5^-$ = 8840(50) gas PE[1]

References

[1]R. F. Gunion, M. K. Gilles, M. L. Polak, and W. C. Lineberger, Int. J. Mass Spectrom. Ion Proc. 117, 601 (1992).

$C_6H_6^+$

$\tilde{G}\ ^2A_{1g}$ D_{6h}
T_a = 61290(100) gas PE[1,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1[b] (2)	CH stretch	2790(100)	gas	PE	1
	2 (1)	Ring stretch	930(100)	gas	PE	1

$\tilde{F}\ ^2B_{1u}$ D_{6h}
T_a = 50160(100) gas PE[1,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1[b] (2)	CH stretch	2340(100)	gas	PE	1

$\tilde{E}\ ^2B_{2u}$ D_{6h}
T_a = 45320(100) gas PE[5]

$\tilde{D}\ ^2E_{1u}$ D_{6h}
T_a = 38220(100) gas PE[5]

$\tilde{C}\ ^2A_{2u}$ D_{6h}
T_a = 25310(100) gas PE[5]

In the gas phase, the mass–selected ion–dip spectrum of $C_6H_6^+$ shows a broad, unstructured absorption with onset near 19000 and increasing in intensity up to the detection limit of 24000.[10]

A broad, unstructured absorption near 24000 may have been contributed by the $\tilde{C}$–$\tilde{X}$ transition of $C_6H_6^+$ produced by vacuum–ultraviolet photolysis of benzene isolated in a neon matrix.[2]

$T_0 \cong 19840$ Ar LF^3AB^4 $\tilde{C}-\tilde{X}$ 420–547 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e_{2g}	18[b] (6)	Ring deform.	600(30)T	Ar	AB	4

$\tilde{B}\ ^2E_{2g}$ D_{6h}
$T_0 = 18113$ gas PF[9]

In an argon matrix, a weak, sharp absorption at 18100 has been attributed[3] to a vibronically allowed transition in the excitation of $C_6H_6^+$ to the $\tilde{B}$ state.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1[b] (2)	CH stretch	2850(100)	gas	PE	1
	2 (1)	Ring stretch	990[c]	gas	PF	9
e_{2g}	16 (8)	Ring stretch	1520(100)T	gas	PE	1
	17 (9)	CH bend	1140[c]	gas	PF	9
	18 (6)	Ring deform.	645(100)[d]	gas	PE	1
e_{2u}	19 (17)	CH bend	574	gas	PF	9
	20 (16)	Ring deform.	224	gas	PF	9

$\tilde{X}\ ^2E_{1g}$ D_{6h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1[b] (2)	CH stretch	2960(100)T	gas	PE	1
	2 (1)	Ring stretch	975(15)	gas	PE,MPI	1,6,8
b_{2g}	8 (4)	Ring deform.	415(20)	gas	PE	6
e_{1g}	11 (10)	CH bend	835(15)	gas	MPI	8
e_{2g}	16 (8)	Ring stretch	1561(20)[d]	gas	PE	1,6
			1480(10)T	Ar	LF	3
	17 (9)	CH bend	1230(15)[d]	gas	PE,MPI	1,6,8
	18 (6)	Ring deform.	660(15)[d]	gas	PE,MPI	1,6,8
			630(10)T	Ar	LF	3
			340(10)[e]	gas	PE	6
e_{2u}	20 (16)	Ring deform.	295(5)	gas	PE,MPI	6,8

$B_0 \cong 0.2$ gas PE[7]

$C_6D_6^+$

$\tilde{G}\ ^2A_{1g}$ D_{6h}
$T^a \cong 62000$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1[b] (2)	CD stretch	2240(100)	gas	PE	1
	2 (1)	Ring stretch	920(100)	gas	PE	1

$\tilde{F}\ ^2B_{1u}$ D_{6h}
$T^a \cong 50000$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1[b] (2)	CD stretch	1610T	gas	PE	1

$\tilde{C}\ ^2A_{2u}$ D_{6h}
$T_0 \cong 19930^c$ Ar LF^3AB^4 $\tilde{C}-\tilde{X}$ 470–545 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e_{2g}	18[b] (6)	Ring deform.	590(60)T	Ar	AB	4

$\tilde{B}\ ^2E_{2g}$ D_{6h}
$T^a \cong 18600$ gas PE[1]

In an argon matrix, a weak, sharp absorption at 18215 has been attributed[3] to a vibronically allowed transition in the excitation of $C_6D_6^+$ to the $\tilde{B}$ state.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1[b] (2)	CD stretch	2140(100)	gas	PE	1
e_{2g}	16 (8)	Ring stretch	1450(100)	gas	PE	1
	17 (9)	CD bend	870(100)	gas	PE	1
	18 (6)	Ring deform.	600(100)	gas	PE	1

$\tilde{X}\ ^2E_{1g}$ D_{6h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1[b] (2)	CD stretch	2330(100)	gas	PE	1
	2 (1)	Ring stretch	928(20)	gas	PE	1,6
b_{2g}	8 (4)	Ring deform.	351(20)	gas	PE	6

$\tilde{X}\ ^2E_{1g}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e_{2g}	16	Ring stretch	1565(100)	gas	PE	1
	(8)		1460(10)T	Ar	LF	3
	18	Ring deform.	637(20)[d]	gas	PE	1,6
	(6)		590(10)T	Ar	LF	3
			343(20)[e]	gas	PE	6
e_{2u}	20	Ring deform.	278(20)	gas	PE	6
	(12)					

[a] From vertical ionization potentials. The first ionization potential of benzene is taken to equal 74555.0(4), or 9.2405 eV, from Ref. 7.
[b] In order to be consistent with other vibrational numberings in these tables, the vibrational numbering of Herzberg is used here. However, many authors use instead the vibrational numbering of Wilson (E. B. Wilson, Jr., Phys. Rev. **45**, 706 (1934)). This latter numbering is indicated in parentheses.
[c] From analysis of combination bands.
[d] j = 1/2.
[e] j = 3/2.

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$CH_3(C\equiv C)_2CH_3^+$

$\tilde{A}\ ^2E_u$ D_{3d}
T_0 = 20556 gas EF[1,4,7]LF[3,5] $\tilde{A}$–$\tilde{X}$ 425–625 nm
20499 Ne LF[2] $\tilde{A}$–$\tilde{X}$ 425–555 nm
≅ 20190 Ar LF[2]
The emission spectrum in an argon matrix is highly perturbed.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	2	C≡C stretch	2126(2)	gas	LF	3,5
			2137	Ne	LF	2
			2118(10)	Ar	LF	2
	4	C–C stretch	1219	gas	LF,EF	3,5,7
			1231	Ne	LF	2
			1220	Ar	LF	2
	5	C–C stretch	524	gas	LF,EF	3–5,7
			531	Ne	LF	2
			518	Ar	LF	2
e_g	20	Skel. bend	248H	gas	EF	7

τ_0 = 25(3) ns gas EF[1,4]PEPICO[6]

$\tilde{X}\ ^2E_g$ D_{3d}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	2	C≡C stretch	2247	gas	EF	1,4,7
			2246	Ne	LF	2
	4	C–C stretch	1323	gas	EF	1,7
			1322	Ne	LF	2
	5	C–C stretch	555	gas	EF,LF	1,3,4,7
			558	Ne	LF	2
e_u	14	Skel. deform.	327H	gas	EF	7
e_g	20	Skel. deform.	237H	gas	EF	7

$CD_3(C\equiv C)_2CD_3^+$

$\tilde{A}\ ^2E_u$ D_{3d}
T_0 = 20575 gas EF[4,7]LF[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}		C≡C stretch	2137(10)	gas	LF	5
			1236	gas	LF,EF	5,7
	5	C–C stretch	483	gas	EF,LF	4,5,7
e_g	20	Skel. bend	230H	gas	EF	7

τ_0 = 32(3) ns gas EF[4]PEPICO[6]

$\tilde{X}\ ^2E_g$ D_{3d}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	2	C≡C stretch	2248	gas	EF	4,7
	4	C–C stretch	1335	gas	EF	4,7
	5	C–C stretch	509	gas	EF,LF	4,5,7
e_g	20	Skel. deform.	217H	gas	EF	7

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$CH_3(cyc\text{-}C_5H_4)$

$\tilde{B}\ ^2B_2$ C_{2v} Structure: LF^2
T_0 = 29765.309 gas $LF^{1,2}$ $\tilde{B}\text{-}\tilde{X}$ 328–337 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1163	gas	LF	1
			999	gas	LF	1
			338	gas	LF	1
			103	gas	LF	1
			88	gas	LF	1

τ_0 = 69.6(1.5) ns gas LF^1
A_0 = 0.285T; B_0 = 0.111; C_0 = 0.080 LF^2

$\tilde{X}\ ^2B_2$ C_{2v} Structure: LF^2
A_0 = 0.286T; B_0 = 0.115; C_0 = 0.082 LF^2

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$t\text{-}CH_2(CH)_4CH_2^+$

$\tilde{A}\ ^2B_g$ C_{2h}
T_0 = 15868(5) gas EF^1 $\tilde{A}\text{-}\tilde{X}$ 610–730 nm
15810 Ne LF^2 $\tilde{A}\text{-}\tilde{X}$ 575–730 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	6	C=C stretch	1486	Ne	LF	2
	7	CH deform.	1434	Ne	LF	2
	8	CH deform.	1373	Ne	LF	2
	9	Mixed	1245	Ne	LF	2
	10	Mixed	1071	Ne	LF	2
	12	Skel. deform.	443	Ne	LF	2
	13	Skel. deform.	350(10)	gas	EF	1
			343	Ne	LF	2

τ_0 = 17(3) ns gas EF^1

$\tilde{X}\ ^2A_u$ C_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	5	C=C stretch	1610(10)	gas	EF	1
			1622	Ne	LF	2
	6	C=C stretch	1513	Ne	LF	2
	7	CH deform.	1376	Ne	LF	2
	8	CH deform.	1293	Ne	LF	2
	9	Mixed	1239	Ne	LF	2
	10	Mixed	1115	Ne	LF	2
	11	Mixed	951	Ne	LF	2
	12	Skel. deform.	442	Ne	LF	2
	13	Skel. deform.	350(10)	gas	EF	1
			350	Ne	LF	2

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C_6H_5CH

In an argon matrix, absorption maxima have been observed[2] at 240 and 245 nm.

In an argon matrix, structured absorption has been observed[1,2] between 372 and 430 nm.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			3078ms	Ar	IR	1,2
			1505(5)m	Ar	IR	1
			1460(5)m	Ar	IR	1
			1430(5)m	Ar	IR	1
			1390(5)m	Ar	IR	1
			1210(5)wm	Ar	IR	1
			1020(5)m	Ar	IR	1
			945(5)wm	Ar	IR	1
			885(5)m	Ar	IR	1
			740vs	Ar	IR	1,2
			670vs	Ar	IR	1,2
			550(5)wm	Ar	IR	1
			445s	Ar	IR	1,2

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$cyc\text{-}C_7H_6$

(1,2,4,6-Cycloheptatetraene)

In an argon matrix, the onset of absorption occurs near 390 nm, with increasing absorption out to the limit of the measurements, near 220 nm.[2]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			3040s	Ar	IR	1,2
			3010s	Ar	IR	1,2
			1824m	Ar	IR	1–3
			1816w	Ar	IR	1–3
			1500(5)wm	Ar	IR	1
			1425(5)wm	Ar	IR	1
			1380vs	Ar	IR	1–3
			1365(5)wm	Ar	IR	1
			1270m	Ar	IR	1,2
			1190(5)m	Ar	IR	1
			965(5)m	Ar	IR	1
			912m	Ar	IR	1,2

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			771vs	Ar	IR	1–3
			690s	Ar	IR	1–3
			679vs	Ar	IR	1,2
			582ms	Ar	IR	1,2
			410(5)m	Ar	IR	1

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[3]O. L. Chapman and C. J. Abelt, J. Org. Chem. **52**, 1218 (1987).

cyc–C_7H_6:

(Cycloheptatrienylidene)

In an argon matrix, absorption maxima have been observed[1] between 460 and 530 nm, between 282 and 307 nm, and at 220 nm.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			638	Ar	IR	1

References

[1]R. J. McMahon and O. L. Chapman, J. Am. Chem. Soc. **108**, 1713 (1986).

$C_6H_5CH_2^+$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	13	Ring deform.	526	gas	PE,TPE	1,2
b_1	28	Ring deform.	598	gas	TPE	2

$C_6H_5CD_2^+$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	13	Ring deform.	500	gas	PE,TPE	1,2
b_1	28	Ring deform.	575	gas	TPE	2

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cyc–$C_7H_7^+$

$\tilde{X}$ $^1A_1$ D_{7h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Ring stretch	1424(100)T	gas	PE	1

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$C_6H_5CH_2$

$\tilde{E}$

A gas-phase absorption maximum near 230 nm has been attributed[9] to the first Rydberg transition of $C_6H_5CH_2$.

$\tilde{D}$

A gas-phase absorption between 260 and 245 nm, with maximum near 255 nm, has been attributed[9] to the $\tilde{D}$–$\tilde{X}$ transition of $C_6H_5CH_2$. This band may have been excited in the MPI studies of Ref. 16. In a neon matrix, the counterpart of this absorption maximum has been observed near 245 nm.[6]

$\tilde{C}$ $^2A_2$ C_{2v}

T_0 = 32760 gas AB[2,5,7] $\tilde{C}$–$\tilde{X}$ 291–309 nm
32730 Ne AB[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	7a	C–CH_2 stretch	1145	gas	AB	7
	18a	CH deform.	968	gas	AB	7
	1	Ring breathing	931	gas	AB	7
	12a	Ring deform.	804	gas	AB	7
	6a	Ring deform.	432	gas	AB	7
b_2	6b	Ring deform.	525	gas	AB	7
	18b	CH deform.	276	gas	AB	7

$\tilde{B}$ $^2B_1$ [a] C_{2v}

T_0 = 22850T gas AB[11]EM[11]LF[22,24]
Vibronically coupled to modes of b_2 symmetry in the $\tilde{A}$ state.[11,22,24]
A^b = 0.179; B^b = 0.088; C^b = 0.059 gas LF[24]

$\tilde{A}$ $^2A_2$ C_{2v}

T_0 = 22001.5 gas EM[1,3,5,10]AB[4]LF[12,20–22] $\tilde{A}$–$\tilde{X}$ 429–455 nm
22003 Ne AB[6] $\tilde{A}$–$\tilde{X}$ 429–455 nm
21862 Ar LF[13] $\tilde{A}$–$\tilde{X}$ 430–510 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			910	Ar	LF	13
			770T	gas	LF	20
			798	Ar	LF	13

$\tilde{A}\ ^2A_2$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	6a	Ring deform.	437	gas	AB,LF	11,18,20 22
			433	Ne	AB	6
			456	Ar	LF	13
	6b	Ring deform.	388[c]	gas	AB	11,17,18
					LF	22
			402	Ne	AB	6
	6b	Ring deform.	328[c]	gas	AB	11,17,18
					LF	22
			344	Ne	AB	6

$\tau_{0(1)}$ = 0.4 μs; $\tau_{0(2)}$ = 1.85 μs gas LF[15,20,21]
A^d = 0.180; B^d = 0.088; C^d = 0.059 EM[10,17,19]LF[22,24]

$\tilde{X}\ ^2B_1$ [a] C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	8a	Ring stretch	1603	gas	EM	5,8,18
		C–CH_2 stretch	1510(25)T	gas	PE	23
	19a	Ring stretch	1431	gas	EM	5,8,18
			1423	Ar	LF	13
	7a		1258	gas	EM,LF	5,7,18,20
	9a	CH deform.	1181	gas	EM	5,8
	18a	CH deform.	1046	gas	EM	18
	1	Ring breathing	987.4	gas	EM,LF	5,8,10,18 20
			982	Ar	LF	13
	12a	Ring deform.	830	gas	EM,LF	5,8,18,20
	6a	Ring deform.	524	gas	EM,LF	5,8,10,20
					PE	23
			520	Ar	LF	13
a_2	17a	CH deform.	963	gas	EM	18
	10a	CH deform.	860	gas	EM	8,18
	16a	Ring deform.	393	gas	EM	8
b_1	16b	Ring deform.	430	gas	EM	8
b_2	8b	Ring stretch	1549	gas	EM	5,8,18
			1530	Ar	LF	13
	9b	CH deform.	1152	gas	EM	5,8,18
	15	CH deform.	1089	gas	EM	5,8
	6b	Ring deform.	615	gas	EM,LF	5,8,10,18 20
			612	Ar	LF	13
	18b	CH deform.	356	gas	EM,LF	5,8,18,20
			357	Ar	LF	13

A_0 = 0.184; B_0 = 0.090; C_0 = 0.060 EM[10,17,19]LF[24]

$C_6D_5CD_2$

$\tilde{B}\ ^2B_1$ [a] C_{2v}
T_0 = 22455(10) gas AB[11]EM[11]

$\tilde{A}$ C_{2v}
T_0 = 22093.7 gas EM[5,10]
21962 Ar LF[13] $\tilde{A}$–$\tilde{X}$ 434–502 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			844	Ar	LF	13
			731	Ar	LF	13
	6a	Ring deform.	404	Ar	LF	13

$\tau \cong$ 1340 ns gas LF[14]

$\tilde{X}\ ^2B_1$ [a] C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	8a	Ring stretch	1593	gas	EM	5,8
	19a	Ring stretch	1327	gas	EM	5,8
			1323	Ar	LF	13
	7a	C–CD_2 stretch	1204	gas	EM	5,8
	1	Ring breathing	945.7	gas	EM	5,8,10
			945	Ar	LF	13
	9a	CD deform.	895	gas	EM	5,8
	18a	CD deform.	848	gas	EM	8
	12a	Ring stretch	791	gas	EM	5,8
	6a	Ring deform.	497.5	gas	EM	5,8,10
			495	Ar	LF	13
a_2	10a	CD deform.	750	gas	EM	8
	16a	Ring deform.	305	gas	EM	8
b_1	16b	Ring deform.	376	gas	EM	8
b_2	8b	Ring stretch	1495	gas	EM	5,8
			1490	Ar	LF	13
	15	CD deform.	848	gas	EM	5,8
	6b	Ring deform.	589.1	gas	EM	5,8,10
			588	Ar	LF	13
	18b	CD deform.	305	gas	EM	5,8
			303	Ar	LF	13

[a] In many of the references concerned with this molecule, the x axis is chosen in the molecular plane, resulting in an interchange of the B_1 and B_2 representations. However, the international convention established in 1955 is followed in the symmetry designations given here. In all of the references, the vibrational numbering follows that introduced by Wilson (E. B. Wilson, Jr., Phys. Rev. **45**, 706 (1934).) In view of this unanimity, the common vibrational numbering is retained.
[b] From analysis of band at 22326.368(2).
[c] Data presented in Ref. 22 suggest that this level is mixed with a nearby a_1 level of the $\tilde{B}\ ^2B_1$ state.
[d] From analysis of band at 22432.395(2).

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cyc-C_7H_7

7f Rydberg state D_{7h}
T_0 = 47888 gas MPI[2]

6f Rydberg state D_{7h}
T_0 = 47060 gas MPI[2]

5d Rydberg state D_{7h}
T_0 = 45991 gas AB[1]

5f Rydberg state D_{7h}
T_0 = 45696 gas MPI[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	2	Ring breathing	861	gas	MPI	2
e_3'	18	CCC deform.	763H	gas	MPI	2
e_3''	20	OPLA	635H	gas	MPI	2

5p Rydberg state D_{7h}
T_0 = 45138 gas MPI[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e_3'	18	CCC deform.	764H	gas	MPI	2

4d Rydberg state D_{7h}
T_0 = 43654 gas AB[1]

4f Rydberg state D_{7h}
T_0 = 43135 gas MPI[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	2	Ring breathing	859	gas	MPI	2
e_3'	18	CCC deform.	768H	gas	MPI	2
e_3''	20	OPLA	643H	gas	MPI	2

4p Rydberg state D_{7h}
T_0 = 41920 gas MPI[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	2	Ring breathing	861	gas	MPI	2
e_3'	18	CCC deform.	762H	gas	MPI	2
e_3''	20	OPLA	642H	gas	MPI	2

3d Rydberg state D_{7h}
T_0 = 38500 gas AB[1]

3p Rydberg state D_{7h}
T_0 = 35186 gas MPI[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	2	Ring breathing	866	gas	MPI	2
e_3'	18	CCC deform.	775H	gas	MPI	2
e_3''	20	OPLA	648H	gas	MPI	2

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$C_6H_5CH_2^-$

Threshold for electron detachment from ground-state $C_6H_5CH_2^-$ = 7360(50) gas PE[2]

X̃

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			945	gas	MPD	1

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$C_6H_5CH_3^+$

C̃
T^a = 25420(160) gas PE[1]

B̃
T_0 = 17590(160) gas PE[1]
Threshold for H-atom photodetachment near 19000 gas PF[2,3]
In an argon matrix, a broad absorption with maximum at 23300 (430 nm) has been assigned[4,5] to $C_6H_5CH_3^+$. Irradiation in the spectral region of this absorption leads to a decrease in its intensity. In a krypton-matrix study,[4] the counterpart of this absorption maximum appeared at 23000 (435 nm).

Ã
T^a = 4200(160) gas PE[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1694(40)	gas	PE	1
			986	gas	TPE	7
		In-plane deform.	976	gas	TPE	6,7
			564(40)	gas	PE	1
		In-plane deform.	498	gas	TPE	6,7
			430T	gas	PE	6

[a] From vertical ionization potential.

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o-$CH_3C_6H_4CH$:

Ar $AB^{1,2}$ 244–249 nm

Ar $AB^{1,2}$ 292–305 nm

Ar $AB^{1,2}$ 413–450 nm

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			742	Ar	IR	1

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m-$CH_3C_6H_4CH$:

Ar $AB^{1,2}$ 394–448 nm

Irradiation in this spectral region results in isomerization to 4- and 5-methylcycloheptatetraene.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			3072w	Ar	IR	1,2
			3047w	Ar	IR	1,2
			3029w	Ar	IR	1,2
			2991w	Ar	IR	1,2
			2985w	Ar	IR	1,2

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2962w	Ar	IR	1,2
			2933w	Ar	IR	1,2
			2876w	Ar	IR	1,2
			1570m	Ar	IR	1,2
			1567m	Ar	IR	1,2
			1520w	Ar	IR	1,2
			1462m	Ar	IR	1,2
			1379w	Ar	IR	1,2
			927w	Ar	IR	1,2
			922w	Ar	IR	1,2
			873w	Ar	IR	1,2
			852w	Ar	IR	1,2
			786m	Ar	IR	1,2
			764s	Ar	IR	1,2
			761s	Ar	IR	1,2
			747w	Ar	IR	1,2
			697m	Ar	IR	1,2
			687m	Ar	IR	1,2
			669s	Ar	IR	1,2
			540w	Ar	IR	1,2
			471w	Ar	IR	1,2
			463m	Ar	IR	1,2
			457m	Ar	IR	1,2
			421m	Ar	IR	1,2

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[1]O. L. Chapman, R. J. McMahon, and P. R. West, J. Am. Chem. Soc. **106**, 7973 (1984).
[2]O. L. Chapman, J. W. Johnson, R. J. McMahon, and P. R. West, J. Am. Chem. Soc. **110**, 501 (1988).

p-$CH_3C_6H_4CH$:

Ar $AB^{1,2}$ 395–444 nm

Irradiation in this spectral region results in isomerization to 5-methylcycloheptatetraene.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			3073w	Ar	IR	1,2
			3053vw	Ar	IR	1,2
			3021vw	Ar	IR	1,2
			2987w	Ar	IR	1,2
			2957w	Ar	IR	1,2
			2925w	Ar	IR	1,2
			2891vw	Ar	IR	1,2
			2871w	Ar	IR	1,2
			2847vw	Ar	IR	1,2
			2736vw	Ar	IR	1,2
			1881vw	Ar	IR	1,2
			1573m	Ar	IR	1,2
			1522w	Ar	IR	1,2
			1518w	Ar	IR	1,2
			1512w	Ar	IR	1,2
			1467m	Ar	IR	1,2
			1454w	Ar	IR	1,2
			1449m	Ar	IR	1,2
			1380w	Ar	IR	1,2
			1116w	Ar	IR	1,2

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1089w	Ar	IR	1,2
			1035w	Ar	IR	1,2
			1029w	Ar	IR	1,2
			1018w	Ar	IR	1,2
			1000w	Ar	IR	1,2
			992w	Ar	IR	1,2
			983w	Ar	IR	1,2
			953w	Ar	IR	1,2
			948w	Ar	IR	1,2
			798s	Ar	IR	1,2
			779w	Ar	IR	1,2
			494w	Ar	IR	1,2
			446s	Ar	IR	1,2

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[1]O. L. Chapman, R. J. McMahon, and P. R. West, J. Am. Chem. Soc. **106**, 7973 (1984).
[2]O. L. Chapman, J. W. Johnson, R. J. McMahon, and P. R. West, J. Am. Chem. Soc. **110**, 501 (1988).

o-$(CH_2)_2C_6H_4$

Ar AB^{1-3} 326–403 nm

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			3105w	Ar	IR	1
			3070w	Ar	IR	1
			3045w	Ar	IR,Ra	1
			2950w	Ar	IR	1
			1741w	Ar	IR	1
			1576w	Ar	IR,Ra	1–3
			1552m	Ar	IR,Ra	1–3
			1542w	Ar	IR	1
			1529m	Ar	Ra	1
			1493m	Ar	IR	1–3
			1471w	Ar	IR	1–3
			1465w	Ar	IR	1
			1427w	Ar	IR	1
			1333w	Ar	IR	1
			1303w	Ar	IR	1
			1293m	Ar	Ra	1
			1158w	Ar	IR	1
			1000w	Ar	IR	1
			953w	Ar	IR	1
			870s	Ar	IR,Ra	1–3
			866w	Ar	IR,Ra	1
			779w	Ar	IR,Ra	1
			776s	Ar	IR	1–3
			754m	Ar	IR	2,3
			742m	Ar	IR	1
			737m	Ar	IR	1
			675m	Ar	IR	1
			638m	Ar	IR	1–3
			442m	Ar	IR	1–3

References

[1]K. L. Tseng and J. Michl, J. Am. Chem. Soc. **99**, 4840 (1977).
[2]R. J. McMahon and O. L. Chapman, J. Am. Chem. Soc. **109**, 683 (1987).
[3]O. L. Chapman, J. W. Johnson, R. J. McMahon, and P. R. West, J. Am. Chem. Soc. **110**, 501 (1988).

$C_6H_5CCH_3$

Ar AB^{1-3} 244–251 nm

Ar AB^{1-3} 302 nm

Ar AB^{1-3} 381–449 nm

In an argon matrix, irradiation in this spectral region results in isomerization to styrene.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			3090w	Ar	IR	1–3
			3075m	Ar	IR	1–3
			3038w	Ar	IR	1–3
			2942w	Ar	IR	1–3
			2920w	Ar	IR	1–3
			2893w	Ar	IR	1–3
			2862m	Ar	IR	1–3
			2807w	Ar	IR	1–3
			2690vw	Ar	IR	1–3
			1468m	Ar	IR	1–3
			1018m	Ar	IR	1–3
			1007w	Ar	IR	1–3
			875w	Ar	IR	1–3
			740s	Ar	IR	1–3
			670s	Ar	IR	1–3
			480m	Ar	IR	1–3

References

[1]O. L. Chapman, R. J. McMahon, and P. R. West, J. Am. Chem. Soc. **106**, 7973 (1984).
[2]R. J. McMahon and O. L. Chapman, J. Am. Chem. Soc. **109**, 683 (1987).
[3]O. L. Chapman, J. W. Johnson, R. J. McMahon, and P. R. West, J. Am. Chem. Soc. **110**, 501 (1988).

1-CH_3(cyc-C_7H_5)

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1386m	Ar	IR	1
			790s	Ar	IR	1
			710s	Ar	IR	1
			655m	Ar	IR	1
			588m	Ar	IR	1
			503w	Ar	IR	1

References

[1]O. L. Chapman, J. W. Johnson, R. J. McMahon, and P. R. West, J. Am. Chem. Soc. **110**, 501 (1988).

4–CH_3(*cyc*–C_7H_5)

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			3070w	Ar	IR	1,2
			3042m	Ar	IR	1,2
			3025m	Ar	IR	1,2
			3012m	Ar	IR	1,2
			2985m	Ar	IR	1,2
			2958m	Ar	IR	1,2
			2924m	Ar	IR	1,2
			1827vw	Ar	IR	1,2
			1816w	Ar	IR	1,2
			1491m	Ar	IR	1,2
			1458w	Ar	IR	1,2
			1445w	Ar	IR	1,2
			1436m	Ar	IR	1,2
			1427w	Ar	IR	1,2
			1401w	Ar	IR	1,2
			1374m	Ar	IR	1,2
			1342w	Ar	IR	1,2
			1280w	Ar	IR	1,2
			1269w	Ar	IR	1,2
			1153m	Ar	IR	1,2
			1095w	Ar	IR	1,2
			1072w	Ar	IR	1,2
			1033w	Ar	IR	1,2
			942w	Ar	IR	1,2
			893w	Ar	IR	1,2
			888w	Ar	IR	1,2
			831w	Ar	IR	1,2
			812w	Ar	IR	1,2
			781s	Ar	IR	1,2
			771m	Ar	IR	1,2
			748w	Ar	IR	1,2
			706s	Ar	IR	1,2
			686w	Ar	IR	1,2
			636w	Ar	IR	1,2
			610m	Ar	IR	1,2
			590m	Ar	IR	1,2
			518w	Ar	IR	1,2
			419w	Ar	IR	1,2
			397w	Ar	IR	1,2
			392w	Ar	IR	1,2

References

[1]O. L. Chapman, R. J. McMahon, and P. R. West, J. Am. Chem. Soc. **106**, 7973 (1984).
[2]O. L. Chapman, J. W. Johnson, R. J. McMahon, and P. R. West, J. Am. Chem. Soc. **110**, 501 (1988).

5–CH_3(*cyc*–C_7H_5)

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			3042m	Ar	IR	1,2
			3020m	Ar	IR	1,2
			2998w	Ar	IR	1,2
			2960w	Ar	IR	1,2
			2929m	Ar	IR	1,2
			2901vw	Ar	IR	1,2
			2896vw	Ar	IR	1,2
			2868vw	Ar	IR	1,2
			1819w	Ar	IR	1,2
			1811w	Ar	IR	1,2
			1581w	Ar	IR	1,2
			1519w	Ar	IR	1,2
			1512w	Ar	IR	1,2
			1454m	Ar	IR	1,2
			1448w	Ar	IR	1,2
			1416m	Ar	IR	1,2
			1386w	Ar	IR	1,2
			1379m	Ar	IR	1,2
			1367m	Ar	IR	1,2
			1350vw	Ar	IR	1,2
			1334w	Ar	IR	1,2
			1276w	Ar	IR	1,2
			1210w	Ar	IR	1,2
			1180vw	Ar	IR	1,2
			1170vw	Ar	IR	1,2
			1111vw	Ar	IR	1,2
			1057w	Ar	IR	1,2
			1038w	Ar	IR	1,2
			960w	Ar	IR	1,2
			891w	Ar	IR	1,2
			862m	Ar	IR	1,2
			829vw	Ar	IR	1,2
			819w	Ar	IR	1,2
			809w	Ar	IR	1,2
			795s	Ar	IR	1,2
			744m	Ar	IR	1,2
			734w	Ar	IR	1,2
			698s	Ar	IR	1,2
			660m	Ar	IR	1,2
			598m	Ar	IR	1,2
			485w	Ar	IR	1,2
			407m	Ar	IR	1,2
			378w	Ar	IR	1,2

References

[1]O. L. Chapman, R. J. McMahon, and P. R. West, J. Am. Chem. Soc. **106**, 7973 (1984).
[2]O. L. Chapman, J. W. Johnson, R. J. McMahon, and P. R. West, J. Am. Chem. Soc. **110**, 501 (1988).

C_9

In an argon matrix, the growth behavior of the 2004 cm^{-1} infrared absorption on sample warmup has been correlated with that of the maximum of a structured absorption near 247.1 nm.[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1146	Ar	AB	2
			622	Ar	AB	2

$\tilde{X}\ ^1\Sigma_g^+$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	3	Sym. stretch	1258(50)	gas	PE	3
	4	Sym. stretch	484(48)	gas	PE	3
Σ_u^+	6		2014.28	gas	DL	1,4
			2004	Ar	IR	2

B_0 = 0.0143 DL[1,4]

References

[1]J. R. Heath and R. J. Saykally, J. Chem. Phys. **93**, 8392 (1990).
[2]J. Szczepanski and M. Vala, J. Phys. Chem. **95**, 2792 (1991).
[3]D. W. Arnold, S. E. Bradforth, T. N. Kitsopoulos, and D. M. Neumark, J. Chem. Phys. **95**, 8753 (1991).
[4]A. Van Orden, H. J. Hwang, E. W. Kuo, and R. J. Saykally, J. Chem. Phys. **98**, 6678 (1993).

C_9^-

Threshold for electron detachment from ground-state C_9^- = 29720(80) gas PE[1,2]

References

[1]S. Yang, K. J. Taylor, M. J. Craycraft, J. Conceicao, C. L. Pettiette, O. Cheshnovsky, and R. E. Smalley, Chem. Phys. Lett. **144**, 431 (1988).
[2]D. W. Arnold, S. E. Bradforth, T. N. Kitsopoulos, and D. M. Neumark, J. Chem. Phys. **95**, 8753 (1991).

C_{11}

$\tilde{X}\ ^1\Sigma_g^+$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+		Sym. stretch	440T	gas	PE	1

References

[1]D. W. Arnold, S. E. Bradforth, T. N. Kitsopoulos, and D. M. Neumark, J. Chem. Phys. **95**, 8753 (1991).

C_{11}^-

Threshold for electron detachment from ground-state C_{11}^- = 31570(65) gas PE[1,2]

References

[1]S. Yang, K. J. Taylor, M. J. Craycraft, J. Conceicao, C. L. Pettiette, O. Cheshnovsky, and R. E. Smalley, Chem. Phys. Lett. **144**, 431 (1988).
[2]D. W. Arnold, S. E. Bradforth, T. N. Kitsopoulos, and D. M. Neumark, J. Chem. Phys. **95**, 8753 (1991).

6.16. Non–Hydrocarbons with More Than Eight Atoms

$B_2H_5NH_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NH a–stretch	3472	Ar	IR	1
			3430			
		NH s–stretch	3401	Ar	IR	1
			3362			
		BH a–stretch	2568	Ar	IR	1
		BH s–stretch	2494	Ar	IR	1
		BH br. s–stretch	1912	Ar	IR	1
		BH br. a–stretch	1663	Ar	IR	1
		NH_2 a–bend	1105	Ar	IR	1
		BH_2 a–bend	1075	Ar	IR	1
		BN stretch	1069	Ar	IR	1
		BH_2 wag	1030	Ar	IR	1
		BH_2 wag	995	Ar	IR	1

References

[1]J. D. Carpenter and B. S. Ault, J. Phys. Chem. **95**, 3502 (1991).

$H_2B{=}NHCH_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NH stretch	3447	Ar	IR	1
		CH_3 stretch	2960	Ar	IR	1
		CH_3 stretch	2939	Ar	IR	1
		CH_3 stretch	2887	Ar	IR	1
		BH_2 a–stretch	2561	Ar	IR	1
		BH_2 s–stretch	2471	Ar	IR	1
			1521	Ar	IR	1
			1511	Ar	IR	1
		CH_3 deform.	1458	Ar	IR	1
		CH_3 deform.	1424	Ar	IR	1
		B=N stretch	1314	Ar	IR	1
		BH_2 s–bend	1155	Ar	IR	1
		BH_2 OPLA	984	Ar	IR	1

References

[1]J. D. Carpenter and B. S. Ault, J. Phys. Chem. **95**, 3507 (1991).

$H_2B{=}N(CH_3)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BH a–stretch	2560	Ar	IR	1
		BH s–stretch	2502	Ar	IR	1
			1523	Ar	IR	1
		CH_3 deform.	1420	Ar	IR	1
		B=N stretch	1224	Ar	IR	1
		BH_2 deform.	1104	Ar	IR	1
		CN stretch	1052	Ar	IR	1
		CN stretch	984	Ar	IR	1

References

[1]J. D. Carpenter and B. S. Ault, J. Phys. Chem. **95**, 3507 (1991).

$cyc{-}(FBNH)_3^+$

$\tilde{X}\ ^2E''$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	2	B–F stretch	1260(10)	gas	EF	1
	3	Ring breathing	840(10)	gas	EF	1
	4	Ring breathing	430(10)	gas	EF	1

References

[1]T. B. Jones, J. P. Maier, and O. Marthaler, Inorg. Chem. **18**, 2140 (1979).

$(CH_3)_2Si$

In an argon or a nitrogen matrix,[1,2,4,5] an absorption maximum at 450 nm is associated with photoisomerization of $(CH_3)_2Si$ to $CH_3SiH{=}CH_2$.

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4	CH_3 s–deform.	1222s	Ar	IR	1,4,6
	5	In–plane CH_3 rock	844vs	Ar[a]	IR	3–6
	6	Si–C stretch	690w	Ar[a]	IR	4,6
b_1	12	CH_3 stretch	2942m	Ar	IR	6
	13	CH_3 a–deform.	1435m	Ar	IR	2,4,6
b_2	17	CH_3 stretch	2977s	Ar	IR	6
	19	CH_3 s–deform.	1212s	Ar[a]	IR	4,6
	20	In–plane CH_3 rock	803vs	Ar[a]	IR	4,6
	21	Si–C stretch	735mT	Ar[a]	IR	4

[a] Observed by Ref. 4 in both Ar and N_2; frequencies in these two matrices were not distinguished.

References

[1]T. J. Drahnak, J. Michl, and R. West, J. Am. Chem. Soc. **101**, 5427 (1979).
[2]T. J. Drahnak, J. Michl, and R. West, J. Am. Chem. Soc. **103**, 1845 (1981).
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[4]C. A. Arrington, K. A. Klingensmith, R. West, and J. Michl, J. Am. Chem. Soc. **106**, 525 (1984).
[5]G. Maier, G. Mihm, H. P. Reisenauer, and D. Littmann, Chem. Ber. **117**, 2369 (1984).
[6]G. Raabe, H. Vancik, R. West, and J. Michl, J. Am. Chem. Soc. **108**, 671 (1986).

$CH_3SiH{=}CH_2$

In an argon matrix, an absorption maximum at 260 nm has been assigned[1,3,4] to $CH_3SiH{=}CH_2$.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CH stretch	3018w	Ar	IR	5
		CH stretch	2976w	Ar	IR	5
	5	SiH stretch	2187s	Ar[a]	IR	1–5
	6	CH_3 a–deform.	1394w	Ar[a]	IR	3,5
	7	CH_2 scissors	1297w	Ar[a]	IR	1,3–5
	8	CH_3 s–deform.	1255s	Ar[a]	IR	1–5
	9	Si=C stretch	989s	Ar[a]	IR	1–5
	10	Deform.	880s	Ar[a]	IR	1–3,5
	11	CH_3 rock	811s	Ar[a]	IR	1–5
	12	Si–C stretch	729w	Ar[a]	IR	3,5
	13	Deform.	678m	Ar[a]	IR	3,5
a''	16	CH_3 a–deform.	1412w	Ar[a]	IR	3,5
	17	CH_2 OPLA wag	830w	Ar[a]	IR	3,5
	18	CH_3 rock	711m	Ar[a]	IR	1–5
	19	CH_2 torsion	614m	Ar[a]	IR	1,3–5

[a] Observed by Ref. 3 in both Ar and N_2; frequencies in these two matrices were not distinguished.

References

[1]T. J. Drahnak, J. Michl, and R. West, J. Am. Chem. Soc. **103**, 1845 (1981).
[2]H. P. Reisenauer, G. Mihm, and G. Maier, Angew. Chem. **94**, 864 (1982); Angew. Chem. Int. Ed. Engl. **21**, 854 (1982).
[3]C. A. Arrington, K. A. Klingensmith, R. West, and J. Michl, J. Am. Chem. Soc. **106**, 525 (1984).
[4]G. Maier, G. Mihm, H. P. Reisenauer, and D. Littmann, Chem. Ber. **117**, 2369 (1984).
[5]G. Raabe, H. Vancik, R. West, and J. Michl, J. Am. Chem. Soc. **108**, 671 (1986).

$(CH_3)_2Ge$

In an argon matrix, an absorption maximum has been observed[1,2] at 420 nm.

$\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	2987w	Ar	IR	2
		CH stretch	2974s	Ar	IR	2
		CH stretch	2957s	Ar	IR	2
		CH stretch	2897w	Ar	IR	2
		CH_3 deform.	1234m	Ar	IR	2
		CH_3 deform.	1217w	Ar	IR	2
		CH_3 deform.	1205m	Ar	IR	2
		CH_3 deform.	1195w	Ar	IR	2
		CH_3 rock	882m	Ar	IR	2
		CH_3 rock	817m	Ar	IR	2
		GeC stretch	541w	Ar	IR	2
		GeC stretch	527vs	Ar	IR	2

References

[1]S. Tomoda, M. Shimoda, Y. Takeuchi, Y. Kajii, K. Obi, I. Tanaka, and K. Honda, J. Chem. Soc., Chem. Commun. 910 (1988).
[2]J. Barrau, D. L. Bean, K. M. Welsh, R. West, and J. Michl, Organometallics **8**, 2606 (1989).

$(CH_3)_2Sn$

$\bar{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_3 stretch	2990	Ar	IR	1
		CH_3 stretch	2924	Ar	IR	1
		CH_3 deform.	1187	Ar	IR	1
			1182sh			
		CH_3 rock	774	Ar	IR	1
			745sh			
			739	Ar	IR	1
		SnC a-stretch	518	Ar	IR	1
		SnC s-stretch	504	Ar	IR	1

$(CD_3)_2Sn$

$\bar{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD_3 stretch	2240	Ar	IR	1
		CD_3 stretch	2123	Ar	IR	1
		CD_3 deform.	1032	Ar	IR	1
		CD_3 deform.	932	Ar	IR	1
			927sh			
		CD_3 rock	596	Ar	IR	1
			569sh			
			565	Ar	IR	1
		SnC a-stretch	476	Ar	IR	1
		SnC s-stretch	462	Ar	IR	1

References

[1]P. Bleckmann, H. Maly, R. Minkwitz, W. P. Neumann, and B. Watta, Tetrahedron Lett. **23**, 4655 (1982).

$(CH_3)_3Al$

$\bar{X}$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	CH_3 s-stretch	2920	gas	Ra	1
	2	CH_3 deform.	1200	gas	Ra	1
	3	AlC_3 s-stretch	530	gas	Ra	1
a_2''	7	CH_3 a-stretch	2948s	Ar	IR	2
	9	CH_3 rock	744vs	gas	IR	3
			742s	Ar	IR	2
e'	11	CH_3 a-stretch	2982m	gas	IR,Ra	1,3
			2971s	Ar	IR	2
	12	CH_3 s-stretch	2901m	gas	IR,Ra	1,3
			2905m	Ar	IR	2
	13	CH_3 a-deform.	1430vwT	gas	IR,Ra	1,3
			1430vwT	Ar	IR	2
	14	CH_3 s-deform.	1202s	gas	IR	3
			1196s	Ar	IR	2
	15	CH_3 rock	754sT	gas	IR,Ra	1,3
	16	AlC_3 a-stretch	691m,sh	gas	IR	3
			689s	Ar	IR	2
	17	AlC_3 deform.	170	gas	Ra	1
e''	18	CH_3 a-stretch	2951	gas	Ra	1
	19	CH_3 a-deform.	1440	gas	Ra	1
	20	CH_3 rock	717vw	Ar	IR	2

$(CD_3)_3Al$

$\bar{X}$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD_3 a-stretch	2227m	gas	IR	3
		CD_3 s-stretch	2113m	gas	IR	3
		CD_3 a-deform.	1036vw	gas	IR	3
		CD_3 s-deform.	953s	gas	IR	3
		CD_3 rock	658vsT	gas	IR	3
		CD_3 rock	574m	gas	IR	3

References

[1]R. J. O'Brien and G. A. Ozin, J. Chem. Soc. A 1136 (1971).
[2]S. Kvisle and E. Rytter, Spectrochim. Acta **40A**, 939 (1984).
[3]G. A. Atiya, A. S. Grady, D. K. Russell, and T. A. Claxton, Spectrochim. Acta **47A**, 467 (1991).

$(CH_3)_2Si–CH_2^+$

$\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		H_2C-Si stretch	760(30)	gas	PE	1

References

[1]J. M. Dyke, G. D. Josland, R. A. Lewis, and A. Morris, J. Phys. Chem. **86**, 2913 (1982).

$(CH_3)_2Si{=}CH_2$ [a]

$\tilde{X}$ Structure: ED[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1251	Ar	IR	1,4,5
			1260w			
			1004m	Ar	IR	1,2,4,5
		HCSi deform.	818w	Ar	IR	1,4,5
		Si–C stretch	643m	Ar	IR	1,2,4,5
b_1		HCSi deform.	825m	Ar	IR	1,2,4,5

$(CD_3)_2Si{=}CD_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Si=C stretch	1112	Ar	IR	6
			1028	Ar	IR	6
		CD_3 deform.	1005	Ar	IR	6
			1002			
			866	Ar	IR	6
			732	Ar	IR	6
			651	Ar	IR	6
			502	Ar	IR	6

[a] Peaks at 696, 932, and 992 cm^{-1} have also been attributed to $(CH_3)_2Si{=}CH_2$ in an argon matrix in Ref. 5. However, Ref. 4, in which the product yield was higher and very dilute samples were used, presents evidence for the assignment of the peaks at 696 and 932 cm^{-1} to the dimer and of the 992-cm^{-1} peak to propylene.

References

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[5]L. E. Gusel'nikov, V. V. Volkova, V. G. Avakyan, and N. S. Nametkin, J. Organomet. Chem. **201**, 137 (1980).
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$(CH_3)_2Si{=}CHCH_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			3020m	Ar	IR	1,2
			2980m	Ar	IR	1,2
			2965m	Ar	IR	1,2
			2940s	Ar	IR	1,2
			2900s	Ar	IR	1,2
			2870s	Ar	IR	1,2
			1450m	Ar	IR	1,2
			1410s	Ar	IR	1,2
			1370ms	Ar	IR	1,2
			1315m	Ar	IR	1,2
			1255vs	Ar	IR	1,2
			1120m	Ar	IR	1,2
			978s	Ar	IR	1,2
			883vs	Ar	IR	1,2
			808s	Ar	IR	1,2
		=CH deform.	795vs	Ar	IR	1–3
			712m	Ar	IR	1,2
			708sh	Ar	IR	1,2
		=CH deform.	645s	Ar	IR	1–3
			608ms	Ar	IR	1–3
			358m	Ar	IR	1,2

References

[1]O. L. Chapman, C.-C. Chang, J. Kolc, M. E. Jung, J. A. Lowe, T. J. Barton, and M. L. Tumey, J. Am. Chem. Soc. **98**, 7844 (1976).
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[3]A. K. Mal'tsev, V. A. Korolev, V. N. Khabashesku, and O. M. Nefedov, Dokl. Akad. Nauk SSSR **251**, 1166 (1980); Dokl. Phys. Chem. **251**, 295 (1980).

MgC_5H_5

$\tilde{A}\ ^2E_1$ C_{5v}
T_0 = 20216 gas LF[1] $\tilde{A}$–$\tilde{X}$ 464–525 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4	Mg··C_5 stretch	339	gas	LF	1
e_1	10	Mg··C_5 bend	133	gas	LF	1
e_2	14	Ring deform.	391	gas	LF	1
	16	Ring torsion	172	gas	LF	1

$\tilde{X}\ ^2A_1$ C_{5v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C–C stretch	1014	gas	LF	1
	4	Mg··C_5 stretch	330	gas	LF	1
e_2	14	Ring deform.	376	gas	LF	1
	16	Ring torsion	211	gas	LF	1

MgC_5D_5

$\tilde{A}\ ^2E_1$ C_{5v}
T_0 = 20216 gas LF[1] $\tilde{A}$–$\tilde{X}$ 469–495 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4	Mg··C_5 stretch	334	gas	LF	1
e_1	10	Mg··C_5 bend	124	gas	LF	1
e_2	14	Ring deform.	346	gas	LF	1
	16	Ring torsion	152	gas	LF	1

References

[1]E. S. J. Robles, A. M. Ellis, and T. A. Miller, J. Phys. Chem. **96**, 8791 (1992).

CaC_5H_5

$\tilde{B}\ ^2A_1$ C_{5v}
T_0 = 16772(5)T gas LF[1,3] $\tilde{B}$–$\tilde{X}$ 585–607 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		Ca··C_5 stretch	300(5)T	gas	LF	1

$\tilde{A}\ ^2E_1$ C_{5v}
T_0 = 14536 gas LF[1–3] $\tilde{A}$–$\tilde{X}$ 645–745 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CH wag	738	gas	LF	3
	4	Ca··C_5 stretch	329(2)	gas	LF	1–3
e_1	10	Ca··C_5 bend	222H	gas	LF	3
e_2	13	CH deform.	1039T	gas	LF	3
	15	CH wag	869T	gas	LF	3

A = 56 gas LF[1–3]

$\tilde{X}\ ^2A_1$ C_{5v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4	Ca··C_5 stretch	311	gas	LF	1,3

CaC_5D_5

$\tilde{A}\ ^2E_1$ C_{5v}
T_0 = 14536 gas LF[3] $\tilde{A}$–$\tilde{X}$ 645–690 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CD wag	512	gas	LF	3
	4	Ca··C_5 stretch	316	gas	LF	3
e_1	10	Ca··C_5 bend	221H	gas	LF	3
e_2	13	CD deform.	727T	gas	LF	3
	15	CD wag	614T	gas	LF	3

A = 56 gas LF[3]

References

[1]L. C. O'Brien and P. F. Bernath, J. Am. Chem. Soc. **108**, 5017 (1986).
[2]A. M. Ellis, E. S. J. Robles, and T. A. Miller, J. Chem. Phys. **94**, 1752 (1991).
[3]E. S. J. Robles, A. M. Ellis, and T. A. Miller, J. Am. Chem. Soc. **114**, 7171 (1992).

SrC_5H_5

$\tilde{B}\ ^2A_1$ C_{5v}
T_0 = 14846(5) gas LF[1] $\tilde{B}$–$\tilde{X}$ 660–685 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		Sr··C_5 stretch	260(5)	gas	LF	1

$\tilde{A}\ ^2E_1$ C_{5v}
T_0 = 13395(5) gas LF[1] $\tilde{A}$–$\tilde{X}$ 695–780 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		Sr··C_5 stretch	259(5)	gas	LF	1

A = 258(5) gas LF[1]

$\tilde{X}\ ^2A_1$ C_{5v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		Sr··C_5 stretch	223(5)	gas	LF	1

References

[1]L. C. O'Brien and P. F. Bernath, J. Am. Chem. Soc. **108**, 5017 (1986).

ZnC_5H_5

$\tilde{A}\ ^2E_1$ C_{5v}
T_0 = 22739 gas LF[1] $\tilde{A}$–$\tilde{X}$ 410–480 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CC stretch	953	gas	LF	1
	3	CH wag	737	gas	LF	1
	4	Zn··C_5 stretch	279	gas	LF	1
e_1	10	Zn··C_5 bend	133H	gas	LF	1
e_2	15	CH wag	188HT[a] 171HT	gas	LF	1
	16	Ring torsion	635T	gas	LF	1

$\tilde{X}\ ^2A_1$ C_{5v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CC stretch	1001	gas	LF	1
	3	CH wag	772	gas	LF	1
	4	Zn··C_5 stretch	254	gas	LF	1
e_1	10	Zn··C_5 bend	117H	gas	LF	1
e_2	15	CH wag	133HT	gas	LF	1
	16	Ring torsion	542T	gas	LF	1

[a] Presumed to be split by vibronic interaction.

References

[1]E. S. J. Robles, A. M. Ellis, and T. A. Miller, J. Phys. Chem. **96**, 3247 (1992).

CdC_5H_5

$\tilde{A}\ ^2E_1$ C_{5v}
T_0 = 22261 gas LF[1,2] $\tilde{A}$–$\tilde{X}$ 420–485 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CC stretch	1123	gas	LF	2
	3	CH wag	748	gas	LF	2
	4	Cd··C_5 stretch	220	gas	LF	1,2
e_1	10	Cd··C_5 bend	124H	gas	LF	2
e_2	15	CH wag	186HT[a] 165HT	gas	LF	2
	16	Ring torsion	620T	gas	LF	2

$\tilde{X}\ ^2A_1$ C_{5v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CC stretch	1188	gas	LF	2
	3	CH wag	793	gas	LF	2
	4	Cd··C_5 stretch	199	gas	LF	2
e_1	10	Cd··C_5 bend	108H	gas	LF	2
e_2	15	CH wag	123HT	gas	LF	2
	16	Ring torsion	530T	gas	LF	2

[a] Presumed to be split by vibronic interaction.

References

[1]A. M. Ellis, E. S. J. Robles, and T. A. Miller, J. Chem. Phys. **94**, 1752 (1991).
[2]E. S. J. Robles, A. M. Ellis, and T. A. Miller, J. Phys. Chem. **96**, 3247 (1992).

$MgC_5H_4CH_3$

$\tilde{A}$ C_s
T_0 = 20150 gas LF[1] $\tilde{A}$–$\tilde{X}$ 480–522 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	17	C–CH_3 deform.	187	gas	LF	1
	18	Ring torsion	169	gas	LF	1
	19	Mg··C_5 stretch	323	gas	LF	1
	20	Mg··C_5 bend	125	gas	LF	1
a''	34	C–CH_3 deform.	242H	gas	LF	1
	36	Mg··C_5 bend	126H	gas	LF	1

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	18	Ring torsion	203	gas	LF	1
	19	Mg··C_5 stretch	321	gas	LF	1
	20	Mg··C_5 bend	95T	gas	LF	1

References

[1]E. S. J. Robles, A. M. Ellis, and T. A. Miller, J. Phys. Chem. **96**, 8791 (1992).

$CaC_5H_4CH_3$

$\tilde{B}$ C_s
T_0 = 14567 gas LF[1] $\tilde{B}$–$\tilde{X}$ 657–687 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	19	Ca··C_5 stretch	304	gas	LF	1
	20	Ca··C_5 bend	150	gas	LF	1
a''	36	Ca··C_5 bend	175H	gas	LF	1

$\tilde{A}$ C_s
T_0 = 14465 gas LF[1] $\tilde{A}$–$\tilde{X}$ 660–692 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	19	Ca··C_5 stretch	307	gas	LF	1
	20	Ca··C_5 bend	139	gas	LF	1
a''	36	Ca··C_5 bend	175H	gas	LF	1

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	19	Ca··C_5 stretch	297	gas	LF	1
	20	Ca··C_5 bend	143	gas	LF	1
a''	36	Ca··C_5 bend	169H	gas	LF	1

References

[1]E. S. J. Robles, A. M. Ellis, and T. A. Miller, J. Am. Chem. Soc. **114**, 7171 (1992).

$ZnC_5H_4CH_3$

$\tilde{B}$ C_s [a]
T_0 = 22661 gas LF[1] $\tilde{B}$–$\tilde{X}$ 420–470 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	19	Zn··C_5 stretch	260	gas	LF	1
a″	36	Zn··C_5 bend	138H	gas	LF	1

$\tilde{A}$ C_s [a]
T_0 = 21324 gas LF[1] $\tilde{A}$–$\tilde{X}$ 440–500 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′			311T	gas	LF	1
			278T	gas	LF	1
	19	Zn··C_5 stretch	260	gas	LF	1
	20	Zn··C_5 bend	127	gas	LF	1
a″	36	Zn··C_5 bend	128H	gas	LF	1

$\tilde{X}$ $^2A'$ C_s [a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′		Zn··C_5 stretch	250	gas	LF	1
			188T	gas	LF	1
	20	Zn··C_5 bend	117	gas	LF	1
a″	36	Zn··C_5 bend	112H	gas	LF	1

[a] Considering CH_3 group as a structureless ball. In the $\tilde{X}$ and $\tilde{B}$ states, low frequency structure has been assigned[1] to torsion of the CH_3 group.

References

[1]E. S. J. Robles, A. M. Ellis, and T. A. Miller, J. Chem. Soc., Faraday Trans. **88**, 1927 (1992).

$CdC_5H_4CH_3$

$\tilde{C}$ C_s [a]
T_0 = 22325 gas LF[1] $\tilde{C}$–$\tilde{X}$ 435–448 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	19	Cd··C_5 stretch	206	gas	LF	1

$\tilde{B}$ C_s [a]
T_0 = 22176 gas LF[1] $\tilde{B}$–$\tilde{X}$ 438–467 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	19	Cd··C_5 stretch	218	gas	LF	1
a″	36	Cd··C_5 bend	123H	gas	LF	1

$\tilde{A}$ C_s [a]
T_0 = 21057 gas LF[1] $\tilde{A}$–$\tilde{X}$ 450–505 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	19	Cd··C_5 stretch	215	gas	LF	1
	20	Cd··C_5 bend	124	gas	LF	1
a″	36	Cd··C_5 bend	113H	gas	LF	1

$\tilde{X}$ $^2A'$ C_s [a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′			222T	gas	LF	1
	19	Cd··C_5 stretch	192	gas	LF	1
	20	Cd··C_5 bend	104	gas	LF	1
a″	36	Cd··C_5 bend	105H	gas	LF	1

[a] Considering CH_3 group as a structureless ball. In the $\tilde{X}$ and $\tilde{B}$ states, low frequency structure has been assigned[1] to torsion of the CH_3 group.

References

[1]E. S. J. Robles, A. M. Ellis, and T. A. Miller, J. Chem. Soc., Faraday Trans. **88**, 1927 (1992).

$C_5SiH_6^+$

(Silabenzene Cation)

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Ring deform.	800(50)	gas	PE	1

References

[1]H. Bock, P. Rosmus, B. Solouki, and G. Maier, J. Organomet. Chem. **271**, 145 (1984).

C_5SiH_6

(Silabenzene)

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SiH stretch	2244sh	Ar	IR	2
			2217s	Ar	IR	1,2
			1526m	Ar	IR	1,2
			1502s	Ar	IR	1,2
			1409wm	Ar	IR	2
			1354vs	Ar	IR	1,2
			1259vs	Ar	IR	1,2
			1069wm	Ar	IR	2
			886m	Ar	IR	1,2
			720wm	Ar	IR	2

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			716			
			700vs	Ar	IR	2
			698			
			568vs	Ar	IR	1,2
			565			
			419s	Ar	IR	1,2

References

[1]G. Maier, G. Mihm, and H. P. Reisenauer, Angew. Chem. **92**, 58 (1980); Angew. Chem. Int. Ed. Engl. **19**, 52 (1980).
[2]G. Maier, G. Mihm, R. O. W. Baumgartner, and H. P. Reisenauer, Chem. Ber. **117**, 2337 (1984).

C_5SiH_6 (Dewar)

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SiH stretch	2142vs	Ar	IR	1,2
			1890ms	Ar	IR	1,2
			1263ms	Ar	IR	1,2
			1084m	Ar	IR	1,2
			818vs	Ar	IR	1,2
			761vs	Ar	IR	1,2
			728ms	Ar	IR	1,2
			689s	Ar	IR	1,2
			591s	Ar	IR	1,2
			559s	Ar	IR	1,2

References

[1]G. Maier, G. Mihm, and H. P. Reisenauer, Angew. Chem. **92**, 58 (1980); Angew. Chem. Int. Ed. Engl. **19**, 52 (1980).
[2]G. Maier, G. Mihm, R. O. W. Baumgartner, and H. P. Reisenauer, Chem. Ber. **117**, 2337 (1984).

$1\text{-}CH_3C_5SiH_5$

(1-Methylsilabenzene)

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1530	Ar	IR	1
			1500	Ar	IR	1
			1410	Ar	IR	1
			1360	Ar	IR	1
			1268	Ar	IR	1
			980	Ar	IR	1
			965	Ar	IR	1
			900	Ar	IR	1
			890	Ar	IR	1
			883	Ar	IR	1
			842	Ar	IR	1
			770	Ar	IR	1
			697	Ar	IR	1
			655	Ar	IR	1
			563	Ar	IR	1

References

[1]C. L. Kreil, O. L. Chapman, G. T. Burns, and T. J. Barton, J. Am. Chem. Soc. **102**, 841 (1980).

$C_3F_6^+$

(Perfluoropropene Cation)

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C=C stretch	1543	Ar	IR	1
		$=CF_2$ a-stretch	1414	Ar	IR	1
		$=CF_2$ s-stretch	1062	Ar	IR	1

References

[1]B. J. Kelsall and L. Andrews, J. Phys. Chem. **85**, 1288 (1981).

$n\text{-}C_3F_7$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CF_3 a-stretch	1354m	Ar	IR	1
	2	CF_3 s-stretch	1231s	Ar	IR	1
	3	CF_2 s-stretch	1222vs	Ar	IR	1
	4	CF_2 · s-stretch	1116s	Ar	IR	1
	5	C_3 s-stretch	1016m	Ar	IR	1
	6	C_3 a-stretch	888m	Ar	IR	1
	7	CF_3 s-deform.	750m	Ar	IR	1
	8	CF_2 s-deform.	703w	Ar	IR	1
	9	CF_2 s-deform.	638m	Ar	IR	1
	10	CF_3 a-deform.	520w	Ar	IR	1
	11	CF_2 wag	395vw	Ar	IR	1
	12	CF_2 wag	306w	Ar	IR	1
	13	CF_3 rock	220vw	Ar	IR	1
	14	C_3 bend	273w	Ar	IR	1
a''	16	CF_2 a-stretch	1285vs	Ar	IR	1
	17	CF_3 a-stretch	1260m	Ar	IR	1
	18	CF_2 · a-stretch	1191s	Ar	IR	1
	19	CF_3 a-deform.	608vw	Ar	IR	1
	20	CF_2 twist	472vw	Ar	IR	1
	21	CF_2 twist	401vw	Ar	IR	1
	22	CF_2 rock	265vw	Ar	IR	1
	23	CF_3 rock	248vw	Ar	IR	1

[a] Revised assignment offered by Ref. 2, based on more detailed study of infrared and Raman spectrum of $n\text{-}C_3F_7I$.

References

[1]R. Butler and A. Snelson, J. Fluorine Chem. **16**, 33 (1980).
[2]D. A. C. Compton and D. M. Rayner, J. Phys. Chem. **86**, 1628 (1982).

l-C_3F_7

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CF_3 s-stretch	1365s 1362s	Ar	IR	1
	2	CF_3 s-stretch	1242vs	Ar	IR	1
	3	CF_3 a-stretch	1192m	Ar	IR	1
	4	CF_3 a-stretch	1157vs 1152s	Ar	IR	1
	5	·CF stretch	1137m 1141w	Ar	IR	1
	6	C_3 a-stretch	986vs	Ar	IR	1
	7	CF_3 s-deform.	775w	Ar	IR	1
	8	CF_3 s-deform.	731w	Ar	IR	1
	9	CCF deform.	703m	Ar	IR	1
	10	CF_3 a-deform.	499vw	Ar	IR	1
	11	CF_3 a-deform.	489vw	Ar	IR	1
	12	CF_3 rock	347vw	Ar	IR	1
	13	C_3 s-stretch	321vw	Ar	IR	1
	14	CF_3 rock	293vw	Ar	IR	1
a"	16	CF_3 a-stretch	1249vs	Ar	IR	1
	17	CF_3 a-stretch	1206vs	Ar	IR	1
	18	CF_3 a-deform.	684w	Ar	IR	1
	19	CF_3 a-deform.	543w	Ar	IR	1
	20	CF_3 rock	456w	Ar	IR	1
	21	CF_3 rock	255vw	Ar	IR	1
	22	CCF deform.	207vw	Ar	IR	1

References

[1]R. Butler and A. Snelson, J. Fluorine Chem. **16**, 33 (1980).

$CH_3(C\equiv C)_2Cl^+$

$\tilde{B}$ C_{3v}
T^a = 37200(320) gas PE[1]

$\tilde{A}$ $^2E_{3/2}$ C_{3v}
T_0 = 19820 gas $EF^{2,3}LF^3$ $\tilde{A}$–$\tilde{X}$ 445–650 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C≡C s-stretch	2123(2)	gas	LF	3
	4	CH_3 s-deform.	1296(2)	gas	LF	3
	5	C–C a-stretch	1207(2)	gas	LF	3
	6	C–C s-stretch	888(2)	gas	LF	3
	7	CCl stretch	424(2)	gas	EF,LF	2,3
e	12	Skel. s-bend	319T	gas	LF	3
	13	CCCl bend	235(2)	gas	LF	3
	14	Skel. bend	87T	gas	LF	3

τ_0 = 22(2) ns gas EF^2

$\tilde{X}$ $^2E_{3/2}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C≡C s-stretch	2232(2)	gas	EF	2,3
	4	CH_3 deform.	1334(2)	gas	EF	3
	5	C–C a-stretch	1320(2)	gas	EF	2,3
	7	C–Cl stretch	503(2)	gas	EF	3
e	13	C≡CCl bend	228(2)	gas	EF	3
	14	Skel. bend	92(2)T	gas	EF	3

[a] From vertical ionization potential.

References

[1]E. Heilbronner, V. Hornung, J. P. Maier, and E. Kloster-Jensen, J. Am. Chem. Soc. **96**, 4252 (1974).
[2]J. P. Maier, O. Marthaler, and E. Kloster-Jensen, J. Electron Spectrosc. Relat. Phenom. **18**, 251 (1980).
[3]D. Klapstein, R. Kuhn, J. P. Maier, L. Misev, and M. Ochsner, Helv. Chim. Acta **67**, 1222 (1984).

$CH_3(C\equiv C)_2Br^+$

$\tilde{B}$ C_{3v}
T^a = 30740(320) gas PE[1]

$\tilde{A}$ $^2E_{3/2}$ C_{3v}
T_0 = 18553 gas $EF^{2,3}LF^3$ $\tilde{A}$–$\tilde{X}$ 480–710 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C≡C s-stretch	2141T	gas	LF	3
	5	C–C a-stretch	1151(2)	gas	LF,EF	3
	6	C–C s-stretch	780(2)	gas	LF	3
	7	CBr stretch	350(2)	gas	EF,LF	2,3
e	12	Skel. s-bend	306T	gas	LF	3
	13	CCBr bend	203(2)	gas	LF	3
	14	Skel. bend	76(2)	gas	LF	3

A = −720(80) gas PE^1EF^3
τ_0 = 10(2) ns gas EF^2

$\tilde{X}$ $^2E_{3/2}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C≡C s-stretch	2216(2)	gas	EF	2,3
	3	C≡C a-stretch	1989(2)	gas	EF	2,3
	5	C–C a-stretch	1276(2)	gas	EF	2,3
	6	C–C s-stretch	795(2)	gas	EF	3
	7	C–Br stretch	368(2)	gas	EF	2,3
e	13	C≡CBr bend	226(2)	gas	EF	3
	14	Skel. bend	101(2)T	gas	EF	3

A = −400(80) gas PE^1EF^3

[a] From vertical ionization potential.

References

[1]E. Heilbronner, V. Hornung, J. P. Maier, and E. Kloster-Jensen, J. Am. Chem. Soc. **96**, 4252 (1974).
[2]J. P. Maier, O. Marthaler, and E. Kloster-Jensen, J. Electron Spectrosc. Relat. Phenom. **18**, 251 (1980).
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cyc-C_5H_4F

$\tilde{B}\ ^2B_2$ C_{2v} Structure: LF^2
T_0 = 30758.170(3) gas AB^1LF^2 $\tilde{B}$–$\tilde{X}$ 310–326 nm
A_0 = 0.280(2); B_0 = 0.113; C_0 = 0.081 LF^2

$\tilde{X}\ ^2B_2$ C_{2v} Structure: LF^2
A_0 = 0.280(2); B_0 = 0.119; C_0 = 0.084 LF^2

References

[1]G. Porter and B. Ward, Proc. Roy. Soc. (London) **A303**, 139 (1968).
[2]D. W. Cullin, L. Yu, J. M. Williamson, and T. A. Miller, J. Phys. Chem. **96**, 89 (1992).

cyc-C_5H_4Cl

$\tilde{B}\ ^2B_2$ C_{2v} Structure: LF^2
T_0 = 29192.726(3) gas AB^1LF^2 $\tilde{B}$–$\tilde{X}$ 329–345 nm
A_0 = 0.28(2); B_0 = 0.068; C_0 = 0.055 LF^2

$\tilde{X}\ ^2B_2$ C_{2v} Structure: LF^2
A_0 = 0.283(2); B_0 = 0.070; C_0 = 0.057 LF^2

References

[1]G. Porter and B. Ward, Proc. Roy. Soc. (London) **A303**, 139 (1968).
[2]D. W. Cullin, L. Yu, J. M. Williamson, and T. A. Miller, J. Phys. Chem. **96**, 89 (1992).

$CF_3(C\equiv C)_2F^+$

$\tilde{A}\ ^2E$ C_{3v}
T_0 = 20400(10) gas EF^2 $\tilde{A}$–$\tilde{X}$ 480–635 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4	CF stretch	1160(40)	gas	PE	1,2
	6	C–C stretch	760(40)	gas	PE	1,2
	7	CF_3 deform.	340(10)	gas	EF	2

τ_0 = 30(3) ns gas EF^2

$\tilde{X}\ ^2E$ C_{3v} Structure: PE^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	C≡C stretch	2280(10)	gas	EF	2
	3	C–C a-stretch	1440(10)	gas	EF	2
	4	CF stretch	1140(10)	gas	EF	2
	5	CF stretch	880(10)	gas	EF	2
	6	C–C stretch	710(10)	gas	EF	2
	7	CF_3 deform.	340(10)	gas	EF	2

References

[1]G. Bieri, E. Heilbronner, J.-P. Stadelmann, J. Vogt, and W. von Niessen, J. Am. Chem. Soc. **99**, 6832 (1977).
[2]M. Allan, J. P. Maier, O. Marthaler, and J.-P. Stadelmann, J. Chem. Phys. **70**, 5271 (1979).

$CF_3(C\equiv C)_2CF_3^+$

$\tilde{B}$
T_0 = 33160(240) gas PE[1]

$\tilde{A}\ ^2E_u$ D_{3d}
T_0 = 19534(3) gas $EF^{2,3}LF^3$ $\tilde{A}$–$\tilde{X}$ 448–595 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1	C≡C stretch	2085(5)	gas	LF	3
	3	C–C stretch	1033(5)	gas	LF	3
	4	C–C stretch	743(5)	gas	LF	3
	5	CF_3 deform.	232(2)	gas	EF	2,3

τ_0 = 46(2) ns gas EF^2PEPCO^3

$\tilde{X}\ ^2E_g$ D_{3d}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1	C≡C stretch	2239(2)	gas	EF	2,3
	2	C–F stretch	1262(2)	gas	EF	2,3
	3	C–C stretch	1095(2)	gas	EF	2,3
	4	C–C stretch	752(2)	gas	EF	3
	5	CF_3 deform.	235(2)	gas	EF	3

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[1]J. P. Delwiche, M.-Th. Praet, G. Caprace, M.-J. Hubin-Franskin, P. Natalis, and J. E. Collin, J. Electron Spectrosc. Relat. Phenom. **12**, 395 (1977).
[2]M. Allan, J. P. Maier, O. Marthaler, and J.-P. Stadelmann, J. Chem. Phys. **70**, 5271 (1979).
[3]D. Klapstein, J. P. Maier, L. Misev, F. Thommen, and W. Zambach, J. Chem. Soc., Faraday Trans. 2 **78**, 1765 (1982).

cyc-1-C_7H_5F

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			3060w	Ar	IR	1
			3025w	Ar	IR	1
			1810m	Ar	IR	1
			1528w	Ar	IR	1
			1502m	Ar	IR	1
			1460w	Ar	IR	1
			1443m	Ar	IR	1
			1403s	Ar	IR	1
			1388m	Ar	IR	1
			1248m	Ar	IR	1
			1228m	Ar	IR	1
			1188s	Ar	IR	1
			1182s	Ar	IR	1

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			937m	Ar	IR	1
			839w	Ar	IR	1
			823m	Ar	IR	1
			789m	Ar	IR	1
			759m	Ar	IR	1
			732s	Ar	IR	1
			661w	Ar	IR	1
			598w	Ar	IR	1
			532w	Ar	IR	1
			474w	Ar	IR	1

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[1]R. J. McMahon, C. J. Abelt, O. L. Chapman, J. W. Johnson, C. L. Kreil, J.-P. LeRoux, A. M. Mooring, and P. R. West, J. Am. Chem. Soc. **109**, 2456 (1987).

cyc-1-C_7H_5Cl

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1809m	Ar	IR	1,2
			1425w	Ar	IR	1
			1387m	Ar	IR	2
			1360w	Ar	IR	1
			1222w	Ar	IR	1
			1061s	Ar	IR	1,2
			920m	Ar	IR	1
			881w	Ar	IR	1
			798s	Ar	IR	1,2
			726s	Ar	IR	1,2
			714s	Ar	IR	1,2
			590w	Ar	IR	1
			553w	Ar	IR	1
			497w	Ar	IR	1

References

[1]R. J. McMahon, C. J. Abelt, O. L. Chapman, J. W. Johnson, C. L. Kreil, J.-P. LeRoux, A. M. Mooring, and P. R. West, J. Am. Chem. Soc. **109**, 2456 (1987).
[2]W. Sander, Spectrochim. Acta **43A**, 637 (1987).

$H_2B{=}OC_2H_5$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	2995	Ar	IR	1
		CH stretch	2915	Ar	IR	1
		BH_2 a–stretch	2575	Ar	IR	1
		BH_2 s–stretch	2470	Ar	IR	1
			1491	Ar	IR	1
			1464	Ar	IR	1
			1446	Ar	IR	1
			1420	Ar	IR	1

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		B=O stretch	1349	Ar	IR	1
		BH_2 scissors	1287	Ar	IR	1
			1166	Ar	IR	1
			1123	Ar	IR	1
			1112	Ar	IR	1
			1105	Ar	IR	1
		BH_2 rock	1036	Ar	IR	1
		C–O stretch	1000	Ar	IR	1
		H_2BO OPLA	900	Ar	IR	1

References

[1]J. D. Carpenter and B. S. Ault, J. Phys. Chem. **96**, 4288 (1992).

$H_2C{=}CH{-}CH{=}NH$ [a]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	4	CH_2 s–stretch	2955	gas	IR	2
	5	CH stretch	2885T	gas	IR	2
	6	C=N stretch	1651	gas	IR	2
	7	C=C stretch	1600	gas	IR	2
	8	CH_2 scissors	1416T	gas	IR	2
	9	CH bend	1368	gas	IR	2
	10	CH bend	1260	gas	IR	2
	11	CNH bend	1251	gas	IR	2
	12	CH_2 rock	1089	gas	IR	2
	13	C–C stretch	855T	gas	IR	2
a"	16	C=N torsion	1096	gas	IR	2
	17	CH OPLA	991	gas	IR	2
	18	CH_2 OPLA	979	gas	IR	2
	19	CH OPLA	839	gas	IR	2
	20	C=C torsion	568	gas	IR	2

A_0 = 1.527; B_0 = 0.152; C_0 = 0.138 MW[1]

[a] Two or more rotational isomers contribute to the observed microwave and infrared spectra.

References

[1]R. E. Penn, J. Mol. Spectrosc. **69**, 373 (1978).
[2]Y. Hamada, M. Tsuboi, T. Matsuzawa, K. Yamanouchi, K. Kuchitsu, Y. Koga, and S. Kondo, J. Mol. Spectrosc. **105**, 453 (1984).

$H_2C{=}C{=}NCH_3$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH_2 s–stretch	2984	gas	IR	1
	2	CH_3 stretch	2941T	gas	IR	1
	3	CH_3 s–stretch	2889	gas	IR	1
	4	CCN a–stretch	2060vs	gas	IR	1
	5	CH_3 deform.	1470	gas	IR	1
	6	CH_2 scissors	1410	gas	IR	1
	7	CH_3 s–deform.	1363	gas	IR	1

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	8	CCN s–stretch	1233	gas	IR	1
	10	N–C stretch	875	gas	IR	1
	11	CH_2 wag	693s	gas	IR	1
	12	C=C=N bend	595	gas	IR	1
	13	C=N–C bend	207	gas	IR	1
a"	14	CH_2 a–stretch	3050	gas	IR	1
	16	CH_3 deform.	1464	gas	IR	1
	18	CH_2 rock	1015	gas	IR	1

References

[1]Y. Amatatsu, Y. Hamada, and M. Tsuboi, J. Mol. Spectrosc. **123**, 476 (1987).

$H_2C{=}CHN{=}CH_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CH_2 a–stretch	3035	gas	IR	1
	4	CH stretch	2871	gas	IR	1
	5	CH_2 s–stretch	2832	gas	IR	1
	6	C=N stretch	1635	gas	IR	1
	7	C=C stretch	1618	gas	IR	1
	8	CH_2 scissors	1452wT	gas	IR	1
	9	CH_2 scissors	1382	gas	IR	1
	10	CH bend	1298	gas	IR	1
	11	CH_2 rock	1233	gas	IR	1
	14	CNC bend	523wT	gas	IR	1
a"	16	CH_2 OPLA	1015	gas	IR	1
	17	CH OPLA	965	gas	IR	1
	18	CH_2 OPLA	913	gas	IR	1
	20	C=C torsion	585	gas	IR	1

References

[1]Y. Amatatsu, Y. Hamada, and M. Tsuboi, J. Mol. Spectrosc. **123**, 276 (1987).

cyc–C_3H_5N

(1–Azetine)

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	3015T	gas	IR	2
	3	CH_2 s–stretch	2870	gas	IR	2
	4	C=N stretch	1575s	gas	IR	1,2
	5	CH_2 scissors	1460	gas	IR	2
	6	CH_2 scissors	1430T	gas	IR	1,2
	7	CH_2 wag	1279s	gas	IR	1,2
	8	CH bend	1220	gas	IR	2
	9	CH_2 wag	1208	gas	IR	1,2
	10	C–N stretch	1020	gas	IR	1,2
	11	Ring deform.	895	gas	IR	2
	12	C–C stretch	888s	gas	IR	1,2
	13	C–C stretch	866	gas	IR	1,2

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a"	16	CH_2 twist	1142	gas	IR	2
	17	CH_2 twist	1102s	gas	IR	1,2
	18	CH_2 rock	1038T	gas	IR	2
	19	CH OPLA	873	gas	IR	2
	20	CH_2 rock	711s	gas	IR	1,2

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[1]R. Dammel, H. Bock, and J. M. Denis, Chem. Phys. Lett. **102**, 239 (1983).
[2]Y. Amatatsu, Y. Hamada, and M. Tsuboi, J. Mol. Spectrosc. **123**, 267 (1987).

$CH_3CH{=}CHNH_2$

$\tilde{X}$ C_s (approximate)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH_2 a–stretch	3500	gas	IR	1
	2	NH_2 s–stretch	3415	gas	IR	1
	3	1–CH stretch	3070	gas	IR	1
	5	CH_3 stretch	2970	gas	IR	1
	6	CH_3 s–stretch	2877	gas	IR	1
	7	C=C stretch	1666s	gas	IR	1
	8	NH_2 scissors	1615mT	gas	IR	1
	10	CH_3 s–deform.	1375	gas	IR	1
	11	2–CH bend	1280	gas	IR	1
	12	1–CH bend	1270	gas	IR	1
	13	CH_3 rock	1078	gas	IR	1
	14	CN stretch	1067	gas	IR	1
	15	C–C stretch	920	gas	IR	1
	16	C_3 bend	480	gas	IR	1
a"	18	CH_3 stretch	2935	gas	IR	1
	19	CH_3 deform.	1457	gas	IR	1
	20	NH_2 twist	1210	gas	IR	1
	21	CH_3 rock	1108T	gas	IR	1
	22	1–CH OPLA	993T	gas	IR	1
	24	NH_2 wag	675m	gas	IR	1

References

[1]Y. Hamada, Y. Amatatsu, and M. Tsuboi, J. Mol. Spectrosc. **110**, 369 (1985).

$C_2H_3NHCH_3$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH stretch	3485	gas	IR	1
	2	CH_2 a–stretch	3120	gas	IR	1
	3	CH_2 s–stretch	3037	gas	IR	1
	4	CH stretch	2990	gas	IR	1
	5	CH_3 stretch	2928T	gas	IR	1
	6	CH_3 s–stretch	2868T	gas	IR	1
	7	C=C stretch	1655s	gas	IR	1
	8	CH_3 deform.	1495	gas	IR	1

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	9	NH bend	1465	gas	IR	1
	10	CH_2 scissors	1430T	gas	IR	1
	11	CH_3 s–deform.	1405	gas	IR	1
	12	CCH bend	1315	gas	IR	1
	13	CNC a–stretch	1230	gas	IR	1
			1223			
	14	CH_3 rock	1150	gas	IR	1
	15	CH_2 rock	1029	gas	IR	1
	16	CNC s–stretch	920	gas	IR	1
	17	CNC bend	527	gas	IR	1
a″	19	CH_3 stretch	2822T	gas	IR	1
	20	CH_3 deform.	1445T	gas	IR	1
	21	CH_3 rock	1063T	gas	IR	1
	22	CH OPLA	966	gas	IR	1
	23	CH_2 OPLA	795s	gas	IR	1
			788s			
	24	C=C torsion	661	gas	IR	1
	25	NH wag	408	gas	IR	1

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[1]Y. Amatatsu, Y. Hamada, M. Tsuboi, and M. Sugie, J. Mol. Spectrosc. **111**, 29 (1985).

$(CH_3)_3SiN$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_3 deform.	1248.0	N_2	IR	1
		Si–N stretch	871.4	N_2	IR	1
		Deformation	850T	N_2	IR	1
		CH_3 rock	746.6	N_2	IR	1
		SiC stretch	736.1	N_2	IR	1

References

[1]R. F. Ferrante, J. Phys. Chem. **94**, 3502 (1990).

$Mg(C_4H_4N)$

$\tilde{A}$ C_s
T_0 = 20222 gas LF[1] $\tilde{A}$–$\tilde{X}$ 464–512 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	8	Ring deform.	403	gas	LF	1
	11	Ring torsion	255	gas	LF	1
	12	Mg··ring stretch	343	gas	LF	1
	13	Mg··ring bend	136	gas	LF	1
a″	24	Mg··ring bend	136H	gas	LF	1

$\tilde{X}$ $^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	8	Ring deform.	363	gas	LF	1
	11	Ring torsion	224	gas	LF	1
	12	Mg··ring stretch	330	gas	LF	1
	13	Mg··ring bend	112	gas	LF	1

$Mg(C_4D_4N)$

$\tilde{A}$ C_s
T_0 = 20233 gas LF[1] $\tilde{A}$–$\tilde{X}$ 484–495 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	8	Ring deform.	363	gas	LF	1
	11	Ring torsion	232	gas	LF	1
	12	Mg··ring stretch	339	gas	LF	1
	13	Mg··ring bend	134	gas	LF	1

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[1]E. S. J. Robles, A. M. Ellis, and T. A. Miller, J. Phys. Chem. **96**, 8791 (1992).

$Ca(C_4H_4N)$

$\tilde{C}$ $^2A'$ C_s
T_0 = 14731 gas LF[1,2] $\tilde{C}$–$\tilde{X}$ 650–725 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	12	Ca··ring stretch	289	gas	LF	2
a″	24	Ca··ring bend	166H	gas	LF	2

$\tilde{B}$ C_s
T_0 = 14392 gas LF[1,2] $\tilde{B}$–$\tilde{X}$ 660–730 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	9	CH wag	753	gas	LF	2
	11	Ring torsion	595	gas	LF	2
	12	Ca··ring stretch	231	gas	LF	2
a″	24	Ca··ring bend	124H	gas	LF	2

$\tilde{A}$ C_s
T_0 = 14324 gas LF[1,2] $\tilde{A}$–$\tilde{X}$ 670–730 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	9	CH wag	797	gas	LF	2
	11	Ring torsion	598	gas	LF	2
	12	Ca··ring stretch	248	gas	LF	1,2
a″	24	Ca··ring bend	136H	gas	LF	2

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	12	Ca··ring stretch	316	gas	LF	1,2

$Ca(C_4D_4N)$

$\tilde{C}\ ^2A'$ C_s
T_0 = 14729 gas LF[2] $\tilde{C}-\tilde{X}$ 664–680 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	12	Ca··ring stretch	290	gas	LF	2
a''	24	Ca··ring bend	156H	gas	LF	2

$\tilde{B}$ C_s
T_0 = 14402 gas LF[2] $\tilde{B}-\tilde{X}$ 670–695 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	9	CD wag	524	gas	LF	2
	12	Ca··ring stretch	226	gas	LF	2
a''	24	Ca··ring bend	123H	gas	LF	2

$\tilde{A}$ C_s
T_0 = 14349 gas LF[2] $\tilde{A}-\tilde{X}$ 670–700 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	9	CD wag	566	gas	LF	2
	12	Ca··ring stretch	232	gas	LF	2
a''	24	Ca··ring bend	127H	gas	LF	2

References

[1]A. M. R. P. Bopegedera, W. T. M. L. Fernando, and P. F. Bernath, J. Phys. Chem. **94**, 4476 (1990).
[2]E. S. J. Robles, A. M. Ellis, and T. A. Miller, J. Am. Chem. Soc. **114**, 7171 (1992).

$Sr(C_4H_4N)$

$\tilde{B}\ ^2A_1$ *pseudo* C_{5v}
T_0 = 13620(10) gas LF[1] $\tilde{B}-\tilde{X}$ 710–795 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		Sr··ring stretch	225(10)	gas	LF	1

$\tilde{A}\ ^2E_1$ *pseudo* C_{5v}
T_0 = 13362(10) gas LF[1] $\tilde{A}-\tilde{X}$ 725–820 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		Sr··ring stretch	237(10)[a]	gas	LF	1

A = 300(10) gas LF[1]

$\tilde{X}\ ^2A_1$ *pseudo* C_{5v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		Sr··ring stretch	253(10)	gas	LF	1

[a] For $^2E_{1(1/2)}$ component.

References

[1]A. M. R. P. Bopegedera, W. T. M. L. Fernando, and P. F. Bernath, J. Phys. Chem. **94**, 4476 (1990).

$Zn(C_4H_4N)$

$\tilde{B}$ C_s
T_0 = 22253 gas LF[1] $\tilde{B}-\tilde{X}$ 420–466 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	8	Ring deform.	935	gas	LF	1
	10	CH wag	819	gas	LF	1
	11	Ring torsion	648	gas	LF	1
	12	Zn··ring stretch	278	gas	LF	1
	13	Zn··ring bend	159	gas	LF	1
a''	24	Zn··ring bend	127H	gas	LF	1

$\tilde{A}$ C_s
T_0 = 21733 gas LF[1] $\tilde{A}-\tilde{X}$ 437–460 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	12	Zn··ring stretch	280	gas	LF	1
a''	24	Zn··ring bend	131H	gas	LF	1

$\tilde{X}\ ^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	12	Zn··ring stretch	257	gas	LF	1
	13	Zn··ring bend	134	gas	LF	1
a''	24	Zn··ring bend	119H	gas	LF	1

References

[1]E. S. J. Robles, A. M. Ellis, and T. A. Miller, J. Phys. Chem. **96**, 3258 (1992).

$Cd(C_4H_4N)$

$\tilde{B}$ C_s

T_0 = 22065 gas LF[1] $\tilde{B}$–$\tilde{X}$ 430–471 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	8	Ring deform.	925	gas	LF	1
	10	CH wag	639T	gas	LF	1
	11	Ring torsion	564T	gas	LF	1
	12	Cd··ring stretch	222	gas	LF	1
	13	Cd··ring bend	151	gas	LF	1
a''	24	Cd··ring bend	121H	gas	LF	1

$\tilde{A}$ C_s

T_0 = 21675 gas LF[1] $\tilde{A}$–$\tilde{X}$ 438–462 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	12	Cd··ring stretch	225	gas	LF	1
a''	24	Cd··ring bend	127H	gas	LF	1

$\tilde{X}$ $^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	12	Cd··ring stretch	201	gas	LF	1
	13	Cd··ring bend	121	gas	LF	1
a''	24	Cd··ring bend	111H	gas	LF	1

References

[1]E. S. J. Robles, A. M. Ellis, and T. A. Miller, J. Phys. Chem. **96**, 3258 (1992).

$(CH_3)_2C{=}C{=}NH$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CCN a–stretch	2032vs	Ar	IR	1
			2026s	Xe	IR	1
			2018s			
			2008wm	Ar	IR	1
			1424wm	Ar	IR	1
			1350m	Ar	IR	1
			1352m	Xe	IR	1
			1315s	Xe	IR	1
			1309s			
		NH deform.	1075m	Ar	IR	1
			1050m	Ar	IR	1
			1050vs	Xe	IR	1
			1016ms	Xe	IR	1
			744w	Ar	IR	1
		Torsion	735m	Ar	IR	1
			734s	Xe	IR	1

References

[1]S. T. Collins and G. C. Pimentel, J. Phys. Chem. **88**, 4258 (1984).

$CH_3C{\equiv}C{-}NH(CH_3)$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C≡C stretch	2037wm	Xe	IR	1
			1429w	Xe	IR	1
		NH deform.	1329m	Xe	IR	1
			1114wm	Xe	IR	1
			1062wm	Xe	IR	1
			966vw	Xe	IR	1
		C–N stretch	860vs	Xe	IR	1
			851m	Xe	IR	1
		NH deform. + CH_3 rock	750w	Xe	IR	1
		NH deform. + CH_3 rock	707m	Xe	IR	1

References

[1]S. T. Collins and G. C. Pimentel, J. Phys. Chem. **88**, 4258 (1984).

cyc–C_5H_3N

3,4–Pyridyne

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2085	N_2	IR	1
			1558	N_2	IR	1
			1387	N_2	IR	1
			1355	N_2	IR	1
			1216	N_2	IR	1
			1055	N_2	IR	1
			996	N_2	IR	1
			853	N_2	IR	1
			848	N_2	IR	1
			802	N_2	IR	1
			489	N_2	IR	1

References

[1]H.–H. Nam and G. E. Leroi, J. Am. Chem. Soc. **110**, 4096 (1988).

cyc–$C_5H_3F_2N^+$

(2,6–Difluoropyridine Cation)

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4		1524	Ne	LF	1
	5		1499	Ne	LF	1
	6		1372	Ne	LF	1
	7		1039	Ne	LF	1
	8		967	Ne	LF	1
	9		728	Ne	LF	1
	10		535	Ne	LF	1
	11		365	Ne	LF	1

References

[1]V. E. Bondybey, J. H. English, and R. H. Shiley, J. Chem. Phys. **77**, 4826 (1982).

$CH_3(C\equiv C)_2CN^+$

$\tilde{C}\ ^2E$ C_{3v}
T_0 = 28720(160) gas PE[1]

$\tilde{B}\ ^2A_1$ C_{3v}
T_0 = 23960(160) gas PE[1]

$\tilde{A}\ ^2E$ C_{3v}
T_0 = 17694(2) gas EF[1,2]LF[2] $\tilde{A}$–$\tilde{X}$ 449–646 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C≡C stretch	2253(4)	gas	LF	2
	3	C≡C,C≡N str.	2080(4)	gas	LF	2
	4	C≡C,C≡N str.	1895(4)	gas	LF	2
	5	CH_3 deform.	1205(40)[a]	gas	LF	2
	8	C–C stretch	486(2)	gas	EF	2

τ_0 = 8(2) ns gas EF[1]

$\tilde{X}\ ^2E$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C≡C stretch	2207(2)	gas	EF	1,2
	3	C≡C,C≡N str.	2093(2)	gas	EF	1,2
	4	C≡C,C≡N str.	1980(2)	gas	EF	1,2
	5	CH_3 deform.	1340(2)[a]	gas	EF	1,2
	8	C–C stretch	513(2)	gas	EF	1,2

[a] Alternatively, may be assigned to ν_6, a C–C stretching mode.

References

[1]G. Bieri, E. Kloster-Jensen, S. Kvisle, J. P. Maier, and O. Marthaler, J. Chem. Soc., Faraday Trans. 2 **76**, 676 (1980).
[2]D. Klapstein, J. P. Maier, L. Misev, F. Thommen, and W. Zambach, J. Electron Spectrosc. Relat. Phenom. **31**, 283 (1983).

$(cyc\text{–}C_5H_4)CN$

$\tilde{B}\ ^2B_2$ C_{2v} Structure: LF[8]
T_0 = 27139.45(2) gas AB[1,2]LF[3–8] $\tilde{B}$–$\tilde{X}$ 350–405 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CN stretch	2056	gas	LF	6

τ_0 = 45(3) ns gas LF[3,4,7]
A_0 = 0.27; B_0 = 0.065; C_0 = 0.053 LF[5,8]

$\tilde{X}\ ^2B_2$ C_{2v}
A_0 = 0.27; B_0 = 0.066; C_0 = 0.054 LF[5,8]

References

[1]G. Porter and B. Ward, Proc. Roy. Soc. (London) **A303**, 139 (1968).
[2]P. A. Lehman and R. S. Berry, J. Am. Chem. Soc. **95**, 8614 (1973).
[3]G. Hancock and K. B. McKendrich, J. Chem. Soc., Faraday Trans. 2 **83**, 2011 (1987).
[4]K. Ozawa, T. Ishida, K. Fuke, and K. Kaya, Chem. Phys. Lett. **150**, 249 (1988).
[5]D. W. Cullin, L. Yu, J. M. Williamson, M. S. Platz, and T. A. Miller, J. Phys. Chem. **94**, 3387 (1990).
[6]T. Ishida, H. Abe, A. Nakajima, and K. Kaya, Chem. Phys. Lett. **170**, 425 (1990).
[7]H. S. Im and E. R. Bernstein, J. Chem. Phys. **95**, 6326 (1991).
[8]D. W. Cullin, L. Yu, J. M. Williamson, and T. A. Miller, J. Phys. Chem. **96**, 89 (1992).

$cyc\text{–}C_6H_5N$

(1–Aza–1,2,4,6–Cycloheptatetraene)

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			3025m	Ar	IR	1
			1895vs	Ar	IR	1
			1348s	Ar	IR	1
			1111ms	Ar	IR	1
			1105ms	Ar	IR	1
			980s	Ar	IR	1
			940m	Ar	IR	1
			748vs	Ar	IR	1
			683s	Ar	IR	1
			658s	Ar	IR	1
			650m	Ar	IR	1
			580ms	Ar	IR	1
			510ms	Ar	IR	1
			370m	Ar	IR	1

References

[1]O. L. Chapman and J.-P. Le Roux, J. Am. Chem. Soc. **100**, 282 (1978).

$3\text{–}CH(cyc\text{–}C_5H_4N)$

(3–Pyridylmethylene)

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1595s	Ar	IR	1
			1520s	Ar	IR	1
			1379ms	Ar	IR	1
			1325m	Ar	IR	1
			1233m	Ar	IR	1
			1221s	Ar	IR	1
			1110m	Ar	IR	1
			1015m	Ar	IR	1
			990ms	Ar	IR	1
			983ms	Ar	IR	1
			943m	Ar	IR	1
			788vs	Ar	IR	1
			688vs	Ar	IR	1

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			628ms	Ar	IR	1
			600wm	Ar	IR	1
			550m	Ar	IR	1
			505ms	Ar	IR	1
			441ms	Ar	IR	1
			430wm	Ar	IR	1

References

[1]O. L. Chapman and R. S. Sheridan, J. Am. Chem. Soc. **101**, 3690 (1979).

$NC(C\equiv C)_2CN^+$

$\tilde{E}\ ^2\Pi_u$ $D_{\infty h}$
T_0 = 30420(160) gas PE[1]

$\tilde{D}\ ^2\Pi_g$ $D_{\infty h}$
T_0 = 25580(160) gas PE[1]

$\tilde{B},\tilde{C}\ ^2\Sigma_g^+,^2\Sigma_u^+$ $D_{\infty h}$
T_0 = 22190(160) gas PE[1]

$\tilde{A}\ ^2\Pi_u$ $D_{\infty h}$
T_0 = 15260(10) gas EF[1] $\tilde{A}$–$\tilde{X}$ 630–770 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+			1940(80)	gas	PE	1

$\tilde{X}\ ^2\Pi_g$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡N stretch	2180(10)	gas	EF	1
	2	C≡C stretch	2100(10)	gas	EF	1
	3	C–C stretch	1360(10)	gas	EF	1
	4	C–C stretch	460(10)	gas	EF	1

References

[1]E. Kloster-Jensen, J. P. Maier, O. Marthaler, and M. Mohraz, J. Chem. Phys. **71**, 3125 (1979).

$C_2H_5(C\equiv C)_2CN^+$

$\tilde{C},\tilde{D}\ ^2A'',^2A'$ C_s
$T^a \cong$ 29530 gas PE[1]

$\tilde{B}\ ^2A'$ C_s
T_0 = 24450(160) gas PE[1]

$\tilde{A}\ ^2A'$ C_s
T_0 = 17530(10) gas EF[1] $\tilde{A}$–$\tilde{X}$ 570–720 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		C≡C stretch	2000(160)	gas	PE	1
			1050(160)	gas	PE	1

$\tau_0 \leq$ 6 ns gas EF[1]

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	C≡N,C≡C str.	2180(10)	gas	EF	1
	3	C≡N,C≡C str.	2080(10)	gas	EF	1
	5	C–C stretch	1320(10)	gas	EF	1
	6	C–C stretch	550(10)	gas	EF	1
			460(10)	gas	EF	1

[a] From vertical ionization potential.

References

[1]G. Bieri, E. Kloster-Jensen, S. Kvisle, J. P. Maier, and O. Marthaler, J. Chem. Soc., Faraday Trans. 2 **76**, 676 (1980).

$H_7O_3^+$

$\tilde{X}$ C_{2v} ?

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		H_2O a–stretch	3721.6	gas	PF	1
		H_3O^+ O–H str.	3667.0	gas	PF	1
		H_2O s–stretch	3637.4	gas	PF	1

References

[1]L. I. Yeh, M. Okumura, J. D. Myers, J. M. Price, and Y. T. Lee, J. Chem. Phys. **91**, 7319 (1989).

$H_9O_4^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		H_2O in–phase a–stretch	3730.4	gas	PF	1
		H_2O out–of–phase s–stretch	3644.9	gas	PF	1

References

[1]L. I. Yeh, M. Okumura, J. D. Myers, J. M. Price, and Y. T. Lee, J. Chem. Phys. **91**, 7319 (1989).

t–CH_3C–OCH_3

In a nitrogen matrix, a broad absorption with maximum near 390 nm behaves appropriately for assignment to CH_3C–OCH_3.[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1330	N_2	IR	1
			1288	N_2	IR	1
			1160	N_2	IR	1
			1100	N_2	IR	1
			550	N_2	IR	1

References

[1]R. S. Sheridan, R. A. Moss, B. K. Wilk, S. Shen, M. Wlostowski, M. A. Kesselmayer, R. Subramanian, G. Kmiecik-Lawrynowicz, and K. Krogh-Jesperson, J. Am. Chem. Soc. **110**, 7563 (1988).

c–CH_3C–OCH_3

In a nitrogen matrix, a broad absorption with maximum near 390 nm behaves appropriately for assignment to CH_3C–OCH_3.[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1320	N_2	IR	1
			1275	N_2	IR	1

References

[1]R. S. Sheridan, R. A. Moss, B. K. Wilk, S. Shen, M. Wlostowski, M. A. Kesselmayer, R. Subramanian, G. Kmiecik-Lawrynowicz, and K. Krogh-Jesperson, J. Am. Chem. Soc. **110**, 7563 (1988).

$(CH_3)_2CS$

$\tilde{E}\ ^1A_1$ C_{2v}
T_0 = 52329 gas AB[2,3] $\tilde{E}$–$\tilde{X}$ 189–191 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	8	C_3 deform.	259(5)	gas	AB	3

$\tilde{D}\ ^1B_2$ C_{2v}
T_0 = 51520 gas AB[2,3] $\tilde{D}$–$\tilde{X}$ 192–194 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	8	C_3 deform.	310(7)	gas	AB	3

$\tilde{C}\ ^1B_2$ C_{2v}
T_0 = 44256 gas AB[2,3] $\tilde{C}$–$\tilde{X}$ 212–228 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 stretch	2785	gas	AB	3
	3	C=S stretch	1308	gas	AB	3
	5	CH_3 deform.	1192	gas	AB	3
	6	C_3 deform.	323	gas	AB	2,3
		Torsion	117	gas	AB	3

$\tilde{B}\ ^1A_1$ C_{2v}
T^a = 45500(100) gas AB[2,3] $\tilde{B}$–$\tilde{X}$ 200–250 nm

$\tilde{A}\ ^1A_2$ C_{2v}
T_0 = 18800(100) gas AB[2,3] $\tilde{A}$–$\tilde{X}$ 410–510 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CS stretch	633	gas	AB	3
a_2	9	CH_3 stretch	2960T	gas	AB	3

$\tilde{a}\ ^3A''$ C_s
T_0 = 17327.8 gas AB[2,3]LF[4,5] $\tilde{a}$–$\tilde{X}$ 510–587 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	10	CS stretch	642.5	gas	AB,LF	2,3,5
	11	C_3 deform.	318.3	gas	LF	5
	12	S wag	195.0	gas	LF	5
	13	CH_3 torsion	127.0	gas	LF	5

τ_0 = 7.7 μs gas LF[4]

$\tilde{X}\ ^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	8	C_3 deform.	363	gas	AB	2,3
b_1	17	S wag	153.2	gas	LF	5

A = 0.291; B = 0.146; C = 0.109 MW[1]

$(CD_3)_2CS$

$\tilde{E}\ ^1A_1$ C_{2v}
T_0 = 52331 gas AB[3] $\tilde{E}$–$\tilde{X}$ 188–191 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	8	C_3 deform.	261(5)	gas	AB	3

$\tilde{D}\ ^1B_2$ C_{2v}
T_0 = 51510 gas AB[3] $\tilde{D}$–$\tilde{X}$ 192–194 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	8	C_3 deform.	284(7)	gas	AB	3

$\tilde{C}\ ^1B_2$ C_{2v}
T_0 = 44464 gas AB[3] $\tilde{C}$–$\tilde{X}$ 216–227 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	C=S stretch	1134	gas	AB	3
	5	CD_3 deform.	1058	gas	AB	3
	8	C_3 deform.	274	gas	AB	3

$\tilde{a}\ ^3A''$ C_s
T_0 = 17349.8 gas LF[5] $\tilde{a}$–$\tilde{X}$ 510–589 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	10	CS stretch	595.0	gas	LF	5
	11	C_3 deform.	273.0T	gas	LF	5
	12	S wag	173.8	gas	LF	5
	13	CD_3 torsion	101.4	gas	LF	5

τ_0 = 12.9 μs gas LF[4]

$\tilde{X}\ ^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	8	C_3 deform.	317	gas	AB	2,3
b_1	17	S wag	114.7	gas	LF	5

[a] Maximum of broad, unstructured absorption.

References

[1]H. W. Kroto, B. M. Landsberg, R. J. Suffolk, and A. Vodden, Chem. Phys. Lett. **29**, 265 (1974).
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[3]S. Paone, D. C. Moule, A. E. Bruno, and R. P. Steer, J. Mol. Spectrosc. **107**, 1 (1984).
[4]A. E. Bruno, D. C. Moule, and R. P. Steer, J. Photochem. Photobiol. A: Chem. **46**, 169 (1989).
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n-C_3H_7O

$\tilde{A}$
T_0 = 29000 gas LF[1] $\tilde{A}$–$\tilde{X}$ 340–450 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	450(50)	gas	LF	1

τ = 0.70(8) μs gas LF[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1065	gas	LF	1

References

[1]J. Bai, H. Okabe, and M. K. Emadi-Babaki, J. Photochem. Photobiol., A:Chem. **50**, 163 (1989).

$(CH_3)_2CHO$

$\tilde{A}$ C_s
$T_0 \cong$ 27167 gas EM[1,4]LF[2,3] $\tilde{A}$–$\tilde{X}$ 330–520 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		C–O stretch	560(10)	gas	LF	2,3

τ = 0.64(9) μs gas EM[4]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		C–O stretch	960(20)	gas	EM	4

References

[1]K. Ohbayashi, H. Akimoto, and I. Tanaka, J. Phys. Chem. **81**, 798 (1977).
[2]R. J. Balla, H. H. Nelson, and J. R. McDonald, Chem. Phys. **99**, 323 (1985).
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$(CH_3)_2SiO$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Si=O stretch	1209.6	Ar	IR	1–3

References

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[2]R. Withnall and L. Andrews, J. Am. Chem. Soc. **108**, 8118 (1986).
[3]R. Withnall and L. Andrews, J. Phys. Chem. **92**, 594 (1988).

CH_3SiH_2OH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3716.0m	Ar	IR	1
		SiH stretch	2138.0s	Ar	IR	1
		SiH stretch	2127.4s	Ar	IR	1
		SiH_2 bend	976.7ms	Ar	IR	1
		CH_3 rock	797.4m	Ar	IR	1
		SiOH bend	718.5s	Ar	IR	1
		SiH_2 rock	509.7w	Ar	IR	1

References

[1]R. Withnall and L. Andrews, J. Phys. Chem. **92**, 594 (1988).

SiH_3SiH_2OH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3708.5	Ar	IR	1
		SiH_3 deform.	961.6	Ar	IR	1
		SiH_2 bend	950.6	Ar	IR	1
		SiH_2 twist	855.0	Ar	IR	1
		SiOH bend	748br	Ar	IR	1
		SiH_2 rock	521.7	Ar	IR	1

SiD_3SiD_2OD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OD stretch	2733.5	Ar	IR	1
		SiO stretch	862.0	Ar	IR	1
		SiD_3 deform.	704.4	Ar	IR	1
		SiD_2 twist	637.4	Ar	IR	1
		SiOD bend	556.9	Ar	IR	1

References

[1]R. Withnall and L. Andrews, J. Phys. Chem. **92**, 594 (1988).

CH_3OSiCH_3

In an argon matrix, an absorption maximum has been observed[1] at 357 nm. Irradiation in that spectral region results in photoisomerization to $CH_3OSiH=CH_2$.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2842.2wm	Ar	IR	1
			1470.0wm	Ar	IR	1
			1218.8m	Ar	IR	1
			1106.5m	Ar	IR	1
			1086.7s	Ar	IR	1
			1084.3vs	Ar	IR	1
			844.2wm	Ar	IR	1
			791.7m	Ar	IR	1
			709.2wm	Ar	IR	1

References

[1]G. Maier, H. P. Reisenauer, K. Schöttler, and U. Wessolek-Kraus, J. Organomet. Chem. **366**, 25 (1989).

$CH_3OSiH=CH_2$

In an argon matrix, an absorption maximum has been observed[1] at 245 nm. Irradiation in that spectral region results in photoisomerization to CH_3OSiCH_3.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SiH stretch	2241.9m	Ar	IR	1
			1464.2w	Ar	IR	1
			1462.3wm	Ar	IR	1
			1318.1wm	Ar	IR	1
			1199.0w	Ar	IR	1
			1119.0m	Ar	IR	1
			1100.2vs	Ar	IR	1
			1002.5wm	Ar	IR	1
			862.5s	Ar	IR	1
			752.1w	Ar	IR	1
			671.1m	Ar	IR	1
			561.8wm	Ar	IR	1

References

[1]G. Maier, H. P. Reisenauer, K. Schöttler, and U. Wessolek-Kraus, J. Organomet. Chem. **366**, 25 (1989).

$CH_2=Si(OH)CH_3$ [a]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3737br 3715.4	Ar	IR	1
		Si=C stretch + CH_3 rock	899vs	Ar	IR	1
		SiO stretch	781.0 777.5	Ar	IR	1
		SiOH bend	729.7vs	Ar	IR	1
		Torsion	360.2	Ar	IR	1
		CSiC bend	285.1	Ar	IR	1

[a] Tentative assignment.

References

[1]R. Withnall and L. Andrews, J. Phys. Chem. **92**, 594 (1988).

$(CH_3)_2SiHOH$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3717.1	Ar	IR	1
		SiH stretch	2111.0	Ar	IR	1
			925vs	Ar	IR	1
			819.4 808.8	Ar	IR	1
		HSiO bend	764.5 757.2	Ar	IR	1

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SiOH bend	711.0	Ar	IR	1
			707.3			
			616.2	Ar	IR	1
		CSiC bend	283	Ar	IR	1

References

[1]R. Withnall and L. Andrews, J. Phys. Chem. **92**, 594 (1988).

$(CF_3)_2(cyc\text{–}CCO)$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1325m	Ar	IR	1
			1275s	Ar	IR	1
			1160m	Ar	IR	1
			875w	Ar	IR	1
			730w	Ar	IR	1
			660m	Ar	IR	1
			560w	Ar	IR	1

References

[1]M. Torres, J. L. Bourdelande, A. Clement, and O. P. Strausz, J. Am. Chem. Soc. **105**, 1698 (1983).

CF_3CCOCF_3 [a]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C=O stretch	1763m	Ar	IR	1
			1751w	Ar	IR	1
			1748w	Ar	IR	1
			1235m	Ar	IR	1
			1226s	Ar	IR	1
			1209s	Ar	IR	1
			1199s	Ar	IR	1
			1167m	Ar	IR	1
			1014w	Ar	IR	1
			1011w	Ar	IR	1
			905w	Ar	IR	1
			860m	Ar	IR	1
			720w	Ar	IR	1
			692m	Ar	IR	1
			545w	Ar	IR	1
			410w	Ar	IR	1

[a] Mixture of two geometric conformers.

References

[1]M. Torres, J. L. Bourdelande, A. Clement, and O. P. Strausz, J. Am. Chem. Soc. **105**, 1698 (1983).

CH_3SClCH_2

In an argon matrix, an absorption maximum at 35500 (282 nm) is contributed by CH_3SClCH_2.[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			3026.8w	Ar	IR	1
			1423.3m	Ar	IR	1
			1415.5m	Ar	IR	1
			1386.1s	Ar	IR	1
			1039.0s	Ar	IR	1
			993.7m	Ar	IR	1
			965.2m	Ar	IR	1
			747.8vs	Ar	IR	1

References

[1]G. Maier, U. Flögel, H. P. Reisenauer, B. A. Hess, Jr., and L. J. Schaad, Chem. Ber. **124**, 2603 (1991).

CH_3SBrCH_2

In an argon matrix, a prominent absorption at 32700 (406 nm) and a shoulder at 27800 (360 nm) are contributed by CH_3BrCH_2.[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			3019.1w	Ar	IR	1
			2940.5w	Ar	IR	1
			1421.8w	Ar	IR	1
			1414.6m	Ar	IR	1
			1379.9m	Ar	IR	1
			1312.4w	Ar	IR	1
			1138.8w	Ar	IR	1
			1033.7wm	Ar	IR	1
			980.2m	Ar	IR	1
			962.3wm	Ar	IR	1
			738.6vs	Ar	IR	1

References

[1]G. Maier, U. Flögel, H. P. Reisenauer, B. A. Hess, Jr., and L. J. Schaad, Chem. Ber. **124**, 2603 (1991).

CH_3SICH_2

In an argon matrix, a prominent absorption at 29900 (334 nm) and a weaker absorption at 22900 (436 nm) are contributed by CH_3SICH_2.[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			3019.6w	Ar	IR	1
			2935.2w	Ar	IR	1
			1420.4w	Ar	IR	1
			1412.2m	Ar	IR	1
			1371.7m	Ar	IR	1

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1310.4m	Ar	IR	1
			1028.4wm	Ar	IR	1
			971.5s	Ar	IR	1
			962.3s	Ar	IR	1
			719.3vs	Ar	IR	1
			529.4m	Ar	IR	1

References

[1]G. Maier, U. Flögel, H. P. Reisenauer, B. A. Hess, Jr., and L. J. Schaad, Chem. Ber. **124**, 2603 (1991).

$(CH_3)_2(cyc\text{–}CCS)$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	2970w	Ar	IR	1,2
		CH stretch	2921m	Ar	IR	1,2
		CH stretch	2865w	Ar	IR	1,2
			1923w	Ar	IR	1,2
			1440m	Ar	IR	1,2
			1427m	Ar	IR	1,2
			1041s	Ar	IR	1,2
			586w	Ar	IR	1,2
			471w	Ar	IR	1,2

References

[1]A. Krantz and J. Laureni, J. Am. Chem. Soc. **99**, 4842 (1977).
[2]A. Krantz and J. Laureni, J. Am. Chem. Soc. **103**, 486 (1981).

$(cyc\text{–}C_5H_4)O$

(Cyclopentadienone)

In an argon matrix, a very prominent absorption maximum at 195 nm and a weaker absorption maximum at 360 nm have been attributed[1] to cyclopentadienone.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1870wm	Ar	IR	1,2
			1789w	Ar	IR	1,2
			1727vs	Ar	IR	1,2
			1724vs			
			1678wm	Ar	IR	1,2
			1332s	Ar	IR	1,2
			1136s	Ar	IR	1,2
			1068wm	Ar	IR	1,2
			822vs	Ar	IR	1,2
			632s	Ar	IR	1,2
			458wm	Ar	IR	1,2

References

[1]G. Maier, L. H. Franz, H.-G. Hartan, K. Lanz, and H. P. Reisenauer, Chem. Ber. **118**, 3196 (1985).
[2]G. Maier, Pure Appl. Chem. **58**, 95 (1986).

$CF_3(cyc\text{–}CCO)C_2F_5$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1260	Ar	IR	1
			1225	Ar	IR	1
			1030	Ar	IR	1
			840	Ar	IR	1
			750	Ar	IR	1
			685	Ar	IR	1
			655	Ar	IR	1

References

[1]M. Torres, J. L. Bourdelande, A. Clement, and O. P. Strausz, J. Am. Chem. Soc. **105**, 1698 (1983).

$(CH_2)_3C{=}C{=}Se$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	2967s	Ar	IR	1
		CH stretch	2863s	Ar	IR	1
			1757m			
		CCSe a-stretch	1746vs	Ar	IR	1
			1432w	Ar	IR	1
			1232m	Ar	IR	1

References

[1]W. W. Sander and O. L. Chapman, J. Org. Chem. **50**, 543 (1985).

$(cyc\text{–}C_5H_4)CCO$

In an argon matrix, a prominent, structured absorption with maximum at 34600 has been assigned[4] to $(cyc\text{–}C_5H_4)CCO$.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2258w	Ar	IR	3
			2105s	Ar	IR	3
		CCO a-stretch	2085	Ne	IR	5
			2089vs[a]	Ar	IR	1,3,4
			2084[a]	N_2	IR	2
			2066m	Ar	IR	3
			2037w	Ar	IR	3
			1496w	Ar	IR	3
			1351w	Ar	IR	3
			1286w	Ar	IR	3

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1146w	Ar	IR	3
			1075wT	Ar	IR	3
			877w	Ar	IR	3
			778s	Ar	IR	3
			608m	Ar	IR	3
			392w	Ar	IR	3

(cyc–C_5D_4)CCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CCO a–stretch	2091	Ne	IR	5
			2093[a,b]	N_2	IR	2

[a] This absorption was previously assigned[1,2] to the C≡C stretching fundamental of o–benzyne.

[b] Nitrogen–matrix absorptions at 1483, 1029, 822, 730, and 616, previously attributed[2] to C_6D_4, may instead be contributed by (*cyc*–C_5D_4)CCO.[5]

References

[1]O. L. Chapman, C.–C. Chang, J. Kolc, N. R. Rosenquist, and H. Tomioka, J. Am. Chem. Soc. **97**, 6586 (1975).

[2]I. R. Dunkin and J. G. MacDonald, J. Chem. Soc., Chem. Commun. 772 (1979).

[3]R. F. C. Brown, N. R. Browne, K. J. Coulston, F. W. Eastwood, M. J. Irvine, A. D. E. Pullin, and U. E. Wiersum, Aust. J. Chem. **42**, 1321 (1989).

[4]J. G. G. Simon, N. Münzel, and A. Schweig, Chem. Phys. Lett. **170**, 187 (1990).

[5]J. G. Radziszewski, B. A. Hess, Jr., and R. Zahradnik, J. Am. Chem. Soc. **114**, 52 (1992).

cyc–$C_6H_4C{=}O$

In an argon matrix, absorption maxima at 36500 and 44600 and a prominent absorption maximum at 51700 are attributed[2] to transitions of this species.

In an argon matrix, irradiation at 29000 (ca. 334 nm) results in the formation of (*cyc*–C_5H_4)CCO and *o*–benzyne.[1]

$\tilde{X}\ ^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		C=O stretch	1869vs	Ar	IR	2
		Ring stretch	1591wm	Ar	IR	2
		Ring stretch	1059w	Ar	IR	2
b_1		CH OPLA	749wm	Ar	IR	2
		C=O OPLA	591wm	Ar	IR	2
b_2		Mixed	1451wm	Ar	IR	2
		C=O bend	721wm	Ar	IR	2
		Ring deform.	620w	Ar	IR	2

References

[1]J. G. G. Simon, N. Münzel, and A. Schweig, Chem. Phys. Lett. **170**, 187 (1990).

[2]J. G. G. Simon, A. Schweig, Y. Xie, and H. F. Schaefer III, Chem. Phys. Lett. **200**, 631 (1992).

$C_2H_5O_2$

An unstructured gas–phase absorption between 200 and 290 nm, with maximum at 240 nm, has been assigned[1,3–5,7,8] to $C_2H_5O_2$.

$\tilde{A}$

T_0 = 7593(6) gas AB^2 $\tilde{A}$–$\tilde{X}$ 1175–1317 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	918(9)	gas	AB	2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_2 a–stretch	3016wm	Ar	IR	6
		CH_2 scissors	1474m	Ar	IR	6
		CH_3 deform.	1451sh	Ar	IR	6
		CH_3 deform.	1389vs	Ar	IR	6
		CH_3 deform.	1380sh	Ar	IR	6
		CH_2 wag	1351m	Ar	IR	6
		CH_2 twist	1242w	Ar	IR	6
		CH_3 rock	1136m,br	Ar	IR	6
		OO stretch	1112ms	Ar	IR	6
		CC stretch	1009s	Ar	IR	6
		CO stretch	838m	Ar	IR	6
		CH_2 rock	800m	Ar	IR	6
		Skel. bend	499vs	Ar	IR	6

References

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[2]H. E. Hunziker and H. R. Wendt, J. Chem. Phys. **64**, 3488 (1976).

[3]H. Adachi, N. Basco, and D. G. L. James, Int. J. Chem. Kinet. **11**, 1211 (1979).

[4]C. Anastasi, D. J. Waddington, and A. Woolley, J. Chem. Soc., Faraday Trans. 1 **79**, 505 (1983).

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[6]G. Chettur and A. Snelson, J. Phys. Chem. **91**, 3483 (1987).

[7]M. M. Maricq and T. J. Wallington, J. Phys. Chem. **96**, 986 (1992).

[8]D. Bauer, J. N. Crowley, and G. K. Moortgat, J. Photochem. Photobiol. A: Chem. **65**, 329 (1992).

$(CH_3)_2CHO_2$

A gas–phase absorption between 220 and 290 nm, with maximum near 240 nm, has been attributed[2,3] to $(CH_3)_2CHO_2$.

$\tilde{A}$

T_0 = 7564(11) gas AB[1] $\tilde{A}$–$\tilde{X}$ 1178–1322 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	924(9)	gas	AB	1

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH bend	1372	Ar	IR	4
		CH bend	1310	Ar	IR	4
			1178	Ar	IR	4
			1153	Ar	IR	4
			1130	Ar	IR	4
		OO stretch	1101vs	Ar	IR	4
		CC stretch	884ms	Ar	IR	4
		CO stretch	789m	Ar	IR	4
		Skel. bend	515s	Ar	IR	4
		Skel. bend	450wm	Ar	IR	4
		Skel. bend	348m	Ar	IR	4
		Skel. bend	305m	Ar	IR	4

References

[1]H. E. Hunziker and H. R. Wendt, J. Chem. Phys. **64**, 3488 (1976).
[2]L. J. Kirsch, D. A. Parkes, D. J. Waddington, and A. Woolley, J. Chem. Soc., Faraday Trans. 1 **74**, 2293 (1978).
[3]H. Adachi and N. Basco, Int. J. Chem. Kinet. **14**, 1125 (1982).
[4].G. Chettur and A. Snelson, J. Phys. Chem. **91**, 913 (1987).

$(CH_3O)_2Si$

In an argon matrix, an absorption maximum has been observed[1] at 243 nm. Irradiation in that spectral region results in photoisomerization to $CH_3SiOOCH_3$.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2948.2w	Ar	IR	1
			2828.0w	Ar	IR	1
			1460.9w	Ar	IR	1
			1191.6wm	Ar	IR	1
			1178.1w	Ar	IR	1
			1074.7vs	Ar	IR	1
			752.4wm	Ar	IR	1
			737.9wm	Ar	IR	1

References

[1]G. Maier, H. P. Reisenauer, K. Schöttler, and U. Wessolek-Kraus, J. Organomet. Chem. **366**, 25 (1989).

$CH_3SiOOCH_3$ [a]

In an argon matrix, an absorption maximum has been observed[1] at 232 nm.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2981.0wm	Ar	IR	1
			2851.1wm	Ar	IR	1
			1453.9wm	Ar	IR	1
			1237.6wm	Ar	IR	1
			1182.5m	Ar	IR	1
			1174.0m	Ar	IR	1
			1121.2s	Ar	IR	1
			1104.8m	Ar	IR	1
			1094.4vs	Ar	IR	1

[a] Tentative assignment.

References

[1]G. Maier, H. P. Reisenauer, K. Schöttler, and U. Wessolek-Kraus, J. Organomet. Chem. **366**, 25 (1989).

t–$C_4H_9O_2$

A gas–phase absorption between 210 and 300 nm, with maximum near 240 nm, has been attributed[2] to t– $C_4H_9O_2$.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_3 rock	1187vs	Ar	IR	3
		CH_3 rock	1139m	Ar	IR	3
		OO stretch	1124s	Ar	IR	3
		CC stretch	808ms	Ar	IR	3
			760(2)	gas	IR	1
		CO stretch	730m	Ar	IR	3
			693.7(5)	gas	IR	1
		Skel. bend	539ms	Ar	IR	3
		Skel. bend	403wm	Ar	IR	3
		Skel. bend	361m	Ar	IR	3
		Skel. bend	337m	Ar	IR	3

References

[1]D. A. Parkes and R. J. Donovan, Chem. Phys. Lett. **36**, 211 (1975).
[2]C. Anastasi, I. W. M. Smith, and D. A. Parkes, J. Chem. Soc., Faraday Trans. 1 **74**, 1693 (1978).
[3]G. Chettur and A. Snelson, J. Phys. Chem. **91**, 5873 (1987).

cyc–C_5H_4O–1–O

(Cyclopentadienone O–Oxide)

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	1395s	Ar	IR	1,2
			1385vs			
			1184m	Ar	IR	1,2
			1179w			
			1142m	Ar	IR	1,2
			1023w	Ar	IR	1,2
			983w	Ar	IR	1,2
			938vw	Ar	IR	1,2
		Ring CH deform.	895vs	Ar	IR	1,2
		Ring CH deform.	741s	Ar	IR	1,2

References

[1]G. A. Bell and I. R. Dunkin, J. Chem. Soc., Chem. Commun. 1213 (1983).
[2]O. L. Chapman and T. C. Hess, J. Am. Chem. Soc. **106**, 1842 (1984).

C_7O_2

In an argon matrix, absorption maxima at 34720 and 36230 (288 and 276 nm) behave appropriately for assignment to C_7O_2.[1]

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		2279T	Ar	IR	1
	4		445T	Ar	IR	1
Σ_u^+	5		2187.4wm	Ar	IR	1
	6		2118.5vs	Ar	IR	1
	7		1696.1w	Ar	IR	1
	8		856.3vw	Ar	IR	1

References

[1]G. Maier, H. P. Reisenauer, and A. Ulrich, Tetrahed. Lett. **32**, 4469 (1991).

p–$C_6H_4S_2$

(Dithio–p–Benzoquinone)

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1549	Ar	IR	1
			1521	Ar	IR	1
			1418	Ar	IR	1
			1164	Ar	IR	1
			844	Ar	IR	1
			478	Ar	IR	1

References

[1]H. Bock, S. Mohmand, T. Hirabayashi, G. Maier, and H. P. Reisenauer, Chem. Ber. **116**, 273 (1983).

1,2,3–cyc–$C_2H_4O_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_2 deform.	1214m	Xe	IR	2
		CO stretch +	983s	Xe	IR	2
		CH_2 deform.	982	CO_2	IR	1,2
		CO stretch	927s	Xe	IR	2
			926	CO_2	IR	1,2
		O_3 s–stretch	846wm	Xe	IR	2
		COO bend +	727vs	Xe	IR	2
		CO stretch	726	CO_2	IR	1,2
		O_3 a–stretch	647vs	Xe	IR	2
			648	CO_2	IR	1,2
		O_3 bend	409m	Xe	IR	2
			406	CO_2	IR	1,2

1,2,3–$C_2D_4O_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD_2 deform.	1089wm	Xe	IR	2
		CO stretch	892s	Xe	IR	2
		O_3 a–stretch	636vs	Xe	IR	2
		O_3 bend	387m	Xe	IR	2

References

[1]B. Nelander and L. Nord, Tetrahedron Lett. 2821 (1977).
[2]C. K. Kohlmiller and L. Andrews, J. Am. Chem. Soc. **103**, 2578 (1981).

1,2,4–cyc–$C_2H_4O_3$

$\tilde{X}$ C_2 Structure: MW[1,2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	CH stretch	2973m	Ar	IR	3,7
	2	CH stretch	2894vs	Ar	IR	3,7
	4	CH_2 wag	1387m	Ar	IR	3,7
	5	CH_2 twist	1196m	Ar	IR	3,7
	6	CH_2 rock	1129s	Ar	IR	3,6,7
			1130	Xe	IR	6
	7	C–O_e stretch	955wm	gas	IR	5
			952vs	Ar	IR	3,6,7
			945	Xe	IR	6
	8	C–O_p stretch	926w	Ar	IR	3,7
	9	O–O stretch	810w	gas	IR	5
			808s	Ar	IR	3,6,7
			802	Xe	IR	6

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	10	Skeletal	737vw	Ar	IR	3,7
	11	Ring pucker	352vw	Ar	IR	3
	12	CH stretch	2967s	Ar	IR	3,7
	13	CH stretch	2900m	Ar	IR	3,7
	14	CH_2 bend	1483vw	Ar	IR	3
	15	CH_2 wag	1346m	Ar	IR	3,7
	16	CH_2 twist	1202m	Ar	IR	3,7
	17	CH_2 rock	1143vw	Ar	IR	3
	18	C–O_e stretch	1081.8s	gas	IR	5
			1078vs	Ar	IR	3,6,7
			1072	Xe	IR	6
	19	C–O_p stretch	1029s	Ar	IR	3,6,7
			1021	Xe	IR	6
	20	Skeletal	698m	Ar	IR	3,7
	21	Ring bend	193m	Ar	IR	3

1,2,4-*cyc*-$C_2D_4O_3$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	CD stretch	2249m	Ar	IR	3,7
	2	CD stretch	2118w	Ar	IR	3,7
	3	CD_2 wag + skel.	1160s	Ar	IR	3,7
	4	CD_2 def. + skel.	1135s	Ar	IR	3,7
	5	Skeletal	1021s	Ar	IR	3,7
	6	Skeletal	972m	Ar	IR	3,7
	7	CD_2 rock + skel.	911w	Ar	IR	3,7
	8	CD_2 twist	851m	Ar	IR	3,7
	9	OO stretch	759s	Ar	IR	3,7
	10	Skeletal	672m	Ar	IR	3,7
	11	Ring pucker	338vw	Ar	IR	3
b	12	CD stretch	2246w	Ar	IR	3,7
	13	CD stretch	2092w	Ar	IR	3,7
	14	CD_2 wag	1143s	Ar	IR	3,7
	15	CD_2 bend	1059vs	Ar	IR	3,7
	16	Skeletal	980w	Ar	IR	3,7
	17	CD_2 twist	930m	Ar	IR	3,7
	18	CD_2 rock	904m	Ar	IR	3,7
	19	CD_2 rock	830w	Ar	IR	3,7
	20	Skeletal	707w	Ar	IR	3,7

[a] Assignments of Ref. 3 adopted, except for C–O and O–O stretching modes of *sec*-$C_2H_4O_3$, for which assignments of Ref. 7, suggested by data for ^{18}O-substituted species, are used.
O_p – peroxy O-atom; O_e – ether O-atom.

References

[1]C. W. Gillies and R. L. Kuczkowski, J. Am. Chem. Soc. **94**, 6337, 7609 (1972).
[2]R. L. Kuczkowski, C. W. Gillies, and K. L. Gallaher, J. Mol. Spectrosc. **60**, 361 (1976).
[3]H. Kuhne and H. H. Gunthard, J. Phys. Chem. **80**, 1238 (1976).
[4]U. Mazur and R. L. Kuczkowski, J. Mol. Spectrosc. **65**, 84 (1977).
[5]H. Niki, P. D. Maker, C. M. Savage, and L. P. Breitenbach, J. Phys. Chem. **85**, 1024 (1981).
[6]C. K. Kohlmiller and L. Andrews, J. Am. Chem. Soc. **103**, 2578 (1981).
[7]M. Hawkins, C. K. Kohlmiller, and L. Andrews, J. Phys. Chem. **86**, 3154 (1982).

c-$HCOOCH_2OH$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3471m	Ar	IR	4
		C=O stretch	1760s	gas	IR	2,3
			1746vs	Ar	IR	1,4
		COH deform.	1288br[a]	Ar	IR	4
		COH deform.	1278ms[a]	Ar	IR	4
		C–O stretch	1167s	gas	IR	2,3
			1164s	Ar	IR	1,4
		C–O(H) stretch	1068sh[a]	Ar	IR	4
		Skel. stretch	1047s	gas	IR	2,3
			1042vs[a]	Ar	IR	4
			1035sh[a]	Ar	IR	4
		O=C–O deform.	536m[a]	Ar	IR	4
		C–O–C deform.	325m[a]	Ar	IR	4

[a] Specific assignment to *cis*- or *trans*-structure uncertain.

References

[1]H. Kuhne, S. Vaccani, A. Bauder, and H. H. Gunthard, Chem. Phys. **28**, 11 (1978).
[2]F. Su, J. G. Calvert, and J. H. Shaw, J. Phys. Chem. **84**, 239 (1980).
[3]H. Niki, P. D. Maker, C. M. Savage, and L. P. Breitenbach, J. Phys. Chem. **85**, 1024 (1981).
[4]M. Hawkins, C. K. Kohlmiller, and L. Andrews, J. Phys. Chem. **86**, 3154 (1982).

t-$HCOOCH_2OH$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C=O stretch	1786vs	Ar	IR	1,4
		COH deform.	1288br[a]	Ar	IR	4
		COH deform.	1278ms[a]	Ar	IR	4
		C–O stretch	1139m	Ar	IR	4
		C–O(H) stretch	1068sh[a]	Ar	IR	4
		Skel. stretch	1047s	gas	IR	2,3
			1042vs[a]	Ar	IR	4
			1035sh[a]	Ar	IR	4
		O=C–O deform.	536m[a]	Ar	IR	4
		C–O–C deform.	325m[a]	Ar	IR	4

[a] Specific assignment to *cis*- or *trans*- structure uncertain.

References

[1]H. Kuhne, S. Vaccani, A. Bauder, and H. H. Gunthard, Chem. Phys. **28**, 11 (1978).
[2]F. Su, J. G. Calvert, and J. H. Shaw, J. Phys. Chem. **84**, 239 (1980).
[3]H. Niki, P. D. Maker, C. M. Savage, and L. P. Breitenbach, J. Phys. Chem. **85**, 1024 (1981).
[4]M. Hawkins, C. K. Kohlmiller, and L. Andrews, J. Phys. Chem. **86**, 3154 (1982).

$HOCH_2CH_2O_2$

In the gas phase, continuous absorption beginning near 33300 (300 nm) with a maximum near 40800 (245 nm) has been attributed[1,2] to $HOCH_2CH_2O_2$.

References

[1]M. E. Jenkin and R. A. Cox, J. Phys. Chem. **95**, 3229 (1991).
[2]T. P. Murrels, M. E. Jenkin, S. J. Shalliker, and G. D. Hayman, J. Chem. Soc., Faraday Trans. **87**, 2351 (1991).

$HOCH_2CH_2OOH$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3635m	gas	IR	1
		OH stretch	3600m	gas	IR	1
		CH stretch	2955s	gas	IR	1
		Deformation	1465w	gas	IR	1
		Deformation	1390m	gas	IR	1
		Deformation	1355m	gas	IR	1
		Deformation	1225m	gas	IR	1
		CO stretch	1080s	gas	IR	1
		CO stretch	1025s	gas	IR	1
		Mixed	870m	gas	IR	1
		OO stretch	800w	gas	IR	1

References

[1]I. Barnes, K. H. Becker, and L. Ruppert, Chem. Phys. Lett. **203**, 295 (1993).

$CH_3O_4CH_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	978(2)	Ar	IR	1
		CO stretch	960(2)	Ar	IR	1
		OO stretch	775(2)	Ar	IR	1
		OOO bend	580(2)	Ar	IR	1
		COO bend	457(2)	Ar	IR	1
		OOO bend	296(2)	Ar	IR	1

$CD_3O_4CD_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	902(2)	Ar	IR	1
		CO stretch	893(2)	Ar	IR	1
		OOO bend	570(2)	Ar	IR	1
		COO bend	416(2)	Ar	IR	1

References

[1]P. Ase, W. Bock, and A. Snelson, J. Phys. Chem. **90**, 2099 (1986).

c–$CH_3CH(NO)OH$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3458.5m	Ar	IR	1
		NO stretch	1552s	Ar	IR	1
		CO stretch	1176vs	Ar	IR	1
		CH_3 rock	1080ms	Ar	IR	1
		CH_3 rock	999m	Ar	IR	1
		CNO bend + CN stretch	793.5m	Ar	IR	1
		OH torsion	326m	Ar	IR	1
		OCN scissors	303.5w	Ar	IR	1

References

[1]R. P. Muller, S. Murata, M. Nonella, and J. R. Huber, Helv. Chim. Acta **67**, 953 (1984).

CH_3NHCH_2NO (A)

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NH stretch	3399w[a]	Ar	IR	1
		NO stretch	1552vs	Ar	IR	1
		CH_3 deform.	1483wm	Ar	IR	1
		CH_3 deform.	1455wm	Ar	IR	1
		CH_3 deform.	1428vw	Ar	IR	1
		CH_3 rock	1105wm	Ar	IR	1
		CNO bend + CN stretch	821w	Ar	IR	1
		NH deform.	662vs[b]	Ar	IR	1
		NCN scissors	318wm	Ar	IR	1

[a] ND stretch of CD_3NDCD_2NO at 2537 cm^{-1}.
[b] ND deform. of CD_3NDCD_2NO at 540 cm^{-1}.

References

[1]R. P. Muller, S. Murata, M. Nonella, and J. R. Huber, Helv. Chim. Acta **67**, 953 (1984).

CH_3NHCH_2NO (B)

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NH stretch	3393w	Ar	IR	1
		NO stretch	1568vs	Ar	IR	1
		CH_3 deform.	1486wm	Ar	IR	1
		CH_3 deform.	1465wm	Ar	IR	1
		CH_3 deform.	1428vw	Ar	IR	1
		CH_3 rock	1102wm	Ar	IR	1

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CNO bend + CN stretch	761w	Ar	IR	1
		NH deform.	657vs	Ar	IR	1
		NCN scissors	308wm	Ar	IR	1

References

[1]R. P. Muller, S. Murata, M. Nonella, and J. R. Huber, Helv. Chim. Acta **67**, 953 (1984).

CH_3OONO_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO_2 a–stretch	1723.8s	gas	IR	1
		NO_2 s–stretch	1299.2m	gas	IR	1
			988w	gas	IR	1
		NO_2 scissors	791.4wm	gas	IR	1

References

[1]H. Niki, P. D. Maker, C. M. Savage, and L. P. Breitenbach, Chem. Phys. Lett. **55**, 289 (1978).

$C_2H_5OONO_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO_2 a–stretch	1718.9s	gas	IR	1
		NO_2 s–stretch	1297.4m	gas	IR	1
		NO_2 scissors	793.6wm	gas	IR	1

References

[1]H. Niki, P. D. Maker, C. M. Savage, and L. P. Breitenbach, Chem. Phys. Lett. **55**, 289 (1978).

$HOCH_2OONO_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3645wm	gas	IR	2
			3006w	gas	IR	2
			2951w	gas	IR	2
			2899w	gas	IR	2
		NO_2 a–stretch	1725vs	gas	IR	1,2
			1404wm	gas	IR	1,2

$\tilde{X}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO_2 s–stretch	1299s	gas	IR	1,2
			1106m	gas	IR	1,2
			1054m	gas	IR	1,2
			943m	gas	IR	1,2
			796ms	gas	IR	1,2
			721w	gas	IR	2
			610wm	gas	IR	2

References

[1]H. Niki, P. D. Maker, C. M. Savage, and L. P. Breitenbach, Chem. Phys. Lett. **72**, 71 (1980).
[2]I. Barnes, K. H. Becker, E. H. Fink, A. Reimer, F. Zabel, and H. Niki, Chem. Phys. Lett. **115**, 1 (1985).

$CH_2ClOONO_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO_2 a–stretch	1734.3	gas	IR	1

References

[1]H. Niki, P. D. Maker, C. M. Savage, and L. P. Breitenbach, Chem. Phys. Lett. **61**, 100 (1979).

$CHCl_2OONO_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO_2 a–stretch	1743	gas	IR	1

References

[1]H. Niki, P. D. Maker, C. M. Savage, and L. P. Breitenbach, Chem. Phys. Lett. **61**, 100 (1979).

$CF_2ClOONO_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO_2 a–stretch	1761	gas	IR	1
			1227	gas	IR	1
			1176	gas	IR	1
			1046	gas	IR	1
			902w	gas	IR	1

References

[1]H. Niki, P. D. Maker, C. M. Savage, and L. P. Breitenbach, Chem. Phys. Lett. **61**, 100 (1979).

$CFCl_2OONO_2$

χ

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO_2 a–stretch	1757	gas	IR	1
		NO_2 s–stretch	1300	gas	IR	1
			1118	gas	IR	1
			1009	gas	IR	1
			943	gas	IR	1
		NO_2 scissors	780T	gas	IR	1

References

[1]H. Niki, P. D. Maker, C. M. Savage, and L. P. Breitenbach, Chem. Phys. Lett. **61**, 100 (1979).

CCl_3OONO_2

χ

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO_2 a–stretch	1754	gas	IR	1
		NO_2 s–stretch	1301	gas	IR	1
			986	gas	IR	1
			893	gas	IR	1
		NO_2 scissors	785	gas	IR	1

References

[1]H. Niki, P. D. Maker, C. M. Savage, and L. P. Breitenbach, Chem. Phys. Lett. **61**, 100 (1979).

$SiCl_3OONO_2$

χ

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO_2 a–stretch	1748	gas	IR	1
		NO_2 s–stretch	1297.2	gas	IR	1
		SiO stretch	924	gas	IR	1
		NO_2 scissors	786	gas	IR	1
		SiCl stretch	634	gas	IR	1

References

[1]H. Niki, P. D. Maker, C. M. Savage, L. P. Breitenbach, and M. D. Hurley, J. Phys. Chem. **89**, 3725 (1985).

6.17. Molecules Related to Benzene

$2,4–C_6H_3OH$

In an argon matrix, an absorption maximum at 29100 (344 nm), with a shoulder at 28100 (356 nm), behaves appropriately for assignment to $2,4–C_6H_3OH$.[1]

χ

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3612.0s	Ar	IR	1
			1516.3s	Ar	IR	1
			1429.0w	Ar	IR	1
			1368.2m	Ar	IR	1
			1290.1w	Ar	IR	1
			1254.9m	Ar	IR	1
			1209.1m	Ar	IR	1
		OH deform.	1157.6m	Ar	IR	1
			1128.6vw	Ar	IR	1
			971.0w	Ar	IR	1
			877.0w	Ar	IR	1
			694.7m	Ar	IR	1
			641.2s	Ar	IR	1
			518.8s	Ar	IR	1

References

[1]G. Bucher, W. Sander, E. Kraka, and D. Cremer, Angew. Chem. **104**, 1225 (1992); Angew. Chem. Int. Ed. Engl. **31**, 1230 (1992).

$C_6S_4O_2$

χ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C=O stretch	1678.8s	Ar	IR	1
			1512.9s	Ar	IR	1
			1295.5w	Ar	IR	1
			1276.2w	Ar	IR	1
			1252.1w	Ar	IR	1
			1239.6w	Ar	IR	1
			1174.0m	Ar	IR	1
			752.1s	Ar	IR	1
			707.3w	Ar	IR	1

References

[1]G. Maier, J. Schrot, H. P. Reisenauer, G. Frenking, and V. Jonas, Chem. Ber. **125**, 265 (1992).

C_6S_6 (A)

In an argon matrix, there is a prominent absorption maximum at 21650 (462 nm).[1] Irradiation of the sample with light of wavelength longer than 400 nm leads to isomerization to Conformer B.

$\tilde{X}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1454.1	Ar	IR	1
			1440.6	Ar	IR	1
			1314.3	Ar	IR	1
			1276.7	Ar	IR	1
			713.1	Ar	IR	1

References

[1]G. Maier, J. Schrot, H. P. Reisenauer, G. Frenking, and V. Jonas, Chem. Ber. **125**, 265 (1992).

C_6S_6 (B)

Argon-matrix deposits of this conformer are colorless, but irradiation with the unfiltered output of a mercury-arc lamp leads to isomerization to Conformer A.[1]

$\tilde{X}$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1330.2	Ar	IR	1
			896.3	Ar	IR	1

References

[1]G. Maier, J. Schrot, H. P. Reisenauer, G. Frenking, and V. Jonas, Chem. Ber. **125**, 265 (1992).

o-C_6H_4F

$\tilde{B}$

In an argon matrix, an absorption maximum at 35840 (279 nm) and other absorptions out to 272 nm have been assigned[2] to the $\tilde{B}$–$\tilde{X}$ transition of o-C_6H_4F.

$\tilde{A}$

T_0 = 16060 gas AB[1] $\tilde{A}$–$\tilde{X}$ 539–623 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			501	gas	AB	1

References

[1]G. Porter and B. Ward, Proc. Roy. Soc. (London) **A287**, 457 (1965).
[2]P. Hassanzadeh and J. H. Miller, J. Phys. Chem. **96**, 2096 (1992).

m-C_6H_4F

$\tilde{B}$

In an argon matrix, an absorption maximum at 34720 (288 nm) has been assigned[2] to the $\tilde{B}$–$\tilde{X}$ transition of m-C_6H_4F.

$\tilde{A}$

T_0 = 18375 gas AB[1] $\tilde{A}$–$\tilde{X}$ 470–545 nm

References

[1]G. Porter and B. Ward, Proc. Roy. Soc. (London) **A287**, 457 (1965).
[2]P. Hassanzadeh and J. H. Miller, J. Phys. Chem. **96**, 2096 (1992).

p-C_6H_4F

$\tilde{B}$ $^2B_1$ C_{2v}

In an argon matrix, an absorption maximum at 35140 (285 nm) has been assigned[2] to the $\tilde{B}$–$\tilde{X}$ transition of p-C_6H_4F.

$\tilde{A}$ $^2B_1$ C_{2v}

T_0 = 17436 gas AB[1] $\tilde{A}$–$\tilde{X}$ 435–575 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			895	gas	AB	1
			739	gas	AB	1
			504	gas	AB	1

References

[1]G. Porter and B. Ward, Proc. Roy. Soc. (London) **A287**, 457 (1965).
[2]P. Hassanzadeh and J. H. Miller, J. Phys. Chem. **96**, 2096 (1992).

o-C_6H_4Cl

$\tilde{B}$

In an argon matrix, an absorption maximum at 36470 (274 nm) has been assigned[1] to the $\tilde{B}$–$\tilde{X}$ transition of o-C_6H_4Cl.

References

[1]P. Hassanzadeh and J. H. Miller, J. Phys. Chem. **96**, 2096 (1992).

m-C_6H_4Cl

$\tilde{B}$

In an argon matrix, an absorption maximum at 33990 (294 nm) has been assigned[1] to the $\tilde{B}$–$\tilde{X}$ transition of m-C_6H_4Cl.

References

[1]P. Hassanzadeh and J. H. Miller, J. Phys. Chem. **96**, 2096 (1992).

p-C_6H_4Cl

$\tilde{B}$ $^2B_1$ C_{2v}

In an argon matrix, an absorption maximum at 34920 (286 nm) has been assigned[2] to the $\tilde{B}$–$\tilde{X}$ transition of p-C_6H_4Cl.

$\tilde{A}$ $^2B_1$ C_{2v}

T_0 = 18425 gas AB[1] $\tilde{A}$–$\tilde{X}$ 475–545 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			900	gas	AB	1
			175	gas	AB	1

References

[1]G. Porter and B. Ward, Proc. Roy. Soc. (London) **A287**, 457 (1965).
[2]P. Hassanzadeh and J. H. Miller, J. Phys. Chem. **96**, 2096 (1992).

o–C_6H_4Br

$\tilde{B}$

In an argon matrix, an absorption maximum at 35970 (278 nm) has been assigned[1] to the $\tilde{B}$–$\tilde{X}$ transition of o–C_6H_4Br.

References

[1]P. Hassanzadeh and J. H. Miller, J. Phys. Chem. **96**, 2096 (1992).

m–C_6H_4Br

$\tilde{B}$

In an argon matrix, an absorption maximum at 33900 (295 nm) has been assigned[2] to the $\tilde{B}$–$\tilde{X}$ transition of m–C_6H_4Br.

$\tilde{A}$

T_0 = 18534 gas AB[1] $\tilde{A}$–$\tilde{X}$ 500–540 nm

References

[1]G. Porter and B. Ward, Proc. Roy. Soc. (London) **A287**, 457 (1965).
[2]P. Hassanzadeh and J. H. Miller, J. Phys. Chem. **96**, 2096 (1992).

p–C_6H_4Br

$\tilde{B}\ ^2B_1$ C_{2v}

In an argon matrix, an absorption maximum at 35090 (285 nm) has been assigned[2] to the $\tilde{B}$–$\tilde{X}$ transition of p–C_6H_4Br.

$\tilde{A}\ ^2B_1$ C_{2v}

T_0 = 18551 gas AB[1]

References

[1]G. Porter and B. Ward, Proc. Roy. Soc. (London) **A287**, 457 (1965).
[2]P. Hassanzadeh and J. H. Miller, J. Phys. Chem. **96**, 2096 (1992).

o–C_6H_4I

$\tilde{B}$

In an argon matrix, an absorption maximum at 33360 (300 nm) has been assigned[1] to the $\tilde{B}$–$\tilde{X}$ transition of o–C_6H_4I.

References

[1]P. Hassanzadeh and J. H. Miller, J. Phys. Chem. **96**, 2096 (1992).

$C_6H_5F^+$

$\tilde{H}, \tilde{I}\ ^2B_2, ^2B_1$ C_{2v}

T^a = 57900(1000) gas PE[2]

$\tilde{G}\ ^2A_1$ C_{2v}

T^a = 48250(1000) gas PE[2]

$\tilde{F}\ ^2B_2$ C_{2v}

T^a = 43400(1000) gas PE[2]

$\tilde{E}\ ^2B_2$ C_{2v}

T_0 = 37680(160) gas PE[2]

$\tilde{D}\ ^2A_1$ C_{2v}

T^a = 30500(1000) gas PE[2]

$\tilde{C}\ ^2B_1$ C_{2v}

T^a = 24800(1000) gas PE[2]
T_0 = 23220 Ar AB[1,3] $\tilde{C}$–$\tilde{X}$ 410–435 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			510	Ar	AB	3

$\tilde{B}\ ^2B_2$ C_{2v}

T_0 = 20740(160) gas PE[2]PF[4] $\tilde{B}$–$\tilde{X}$ 440–490 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1118	gas	PF	4
			890	gas	PF	4
			460	gas	PF	4
a_2			632T	gas	PF	4
			267T	gas	PF	4

$\tilde{A}\ ^2A_2$ C_{2v}

T^a = 4680(1000) gas PE[2]

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1370(40)	gas	PE	2
			815T	gas	PE	4
			508T	gas	PE	2,4

[a] From vertical ionization potential.

References

[1]B. W. Keelan and L. Andrews, J. Am. Chem. Soc. **103**, 829 (1981).
[2]G. Bieri, L. Åsbrink, and W. von Niessen, J. Electron Spectrosc. Relat. Phenom. **23**, 281 (1981).
[3]J. T. Lurito and L. Andrews, Chem. Phys. **97**, 121 (1985).
[4]K. Walter, U. Boesl, and E. W. Schlag, Chem. Phys. Lett. **162**, 261 (1989).

$C_6H_5Cl^+$

$\tilde{F}\ ^2B_1$ C_{2v}

T^a = 33430(160) gas PE[3]
T_0 = 33410(10) Ar AB[6] $\tilde{F}$–$\tilde{X}$ 287–300 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			710(10)	Ar	AB	6

$\tilde{E}\ ^2B_2$ C_{2v}
T^a = 31570(160) gas PE[3]

$\tilde{D}\ ^2A_1$ C_{2v}
T^a = 25920(160) gas PE[1,3]

$\tilde{C}\ ^2B_1$ C_{2v}
T_0 = 21250(80) gas PE[1,3] $\tilde{C}-\tilde{X}$ 434–482 nm
20750(10) Ar AB[4,6]
Photodissociation into $C_6H_5^+$ + Cl occurs.[2,7–9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1370(10)	Ar	AB	6
			900(80)	gas	PE	3
			900(10)	Ar	AB	6
			370(10)	Ar	AB	6

$\tilde{B}\ ^2B_2$ C_{2v}
T_0 = 18300(80) gas PE[1,3]PF[7–9] $\tilde{B}-\tilde{X}$ 485–580 nm
Ar AB[6] $\tilde{B}-\tilde{X}$ 498–534 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			940T	gas	PE,PF	3,7
			930(10)	Ar	AB	6
			385T	gas	PE,PF	3,7
a_2			627T	gas	PF	7
			179T	gas	PF	7
b_2			430T	Ar	AB	6

$\tilde{A}\ ^2A_2$ C_{2v}
T^a = 5160(160) gas PE[1,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1020(80)	gas	PE	3

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1460(40)	gas	PE	3
			1145(15)	gas	PE	3,5
			661(10)	gas	PE	5
			419(10)	gas	PE,PF	3,5,7
a_2			203T	gas	PF	7
b_2			451(10)	gas	PE	5
			266(15)	gas	PE	5

[a] From vertical ionization potential.

References

[1]A. D. Baker, D. P. May, and D. W. Turner, J. Chem. Soc. B 22 (1968).
[2]R. C. Dunbar, H. H.-I. Teng, and E. W. Fu, J. Am. Chem. Soc. **101**, 6506 (1979).
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[5]S. L. Anderson, D. M. Rider, and R. N. Zare, Chem. Phys. Lett. **93**, 11 (1982).
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$1,2\text{–}C_6H_4F_2^+$

$\tilde{E}\ ^2A_1$ C_{2v}
T_0 = 38480(160) gas PE[1]

$\tilde{D}\ ^2B_2$ C_{2v}
T^a = 33080(1000) gas PE[1]

$\tilde{C}\ ^2A_1$ C_{2v}
T^a = 25820(1000) gas PE[1]

$\tilde{B}\ ^2B_1$ C_{2v}
T_0 = 23157 gas PF[3] $\tilde{B}-\tilde{X}$ 420–442 nm
Ar AB[2] $\tilde{B}-\tilde{X}$ 420–445 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			480	Ar	AB	2
b_1			135H	gas	PF	3
b_2			513	gas	PF	3
			344	gas	PF	3

$\tilde{A}\ ^2A_2$ C_{2v}
T^a = 4840(1000) gas PE[1]

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			831	gas	PF	3
b_1			253	gas	PF	3
b_2			540	gas	PF	3
			396	gas	PF	3

[a] From vertical ionization potential.

References

[1]G. Bieri, L. Åsbrink, and W. von Niessen, J. Electron Spectrosc. Relat. Phenom. **23**, 281 (1981).
[2]J. T. Lurito and L. Andrews, Chem. Phys. **97**, 121 (1985).
[3]Y. Tsuchiya, K. Takazawa, M. Fujii, and M. Ito, J. Phys. Chem. **96**, 99 (1992).

$1,3\text{–}C_6H_4F_2^+$

$\tilde{D},\tilde{E}\ ^2B_2,^2B_2$ C_{2v}
$T^a \cong$ 34500 gas PE[3]

$\tilde{C}\ ^2A_1$ C_{2v}
$T^a \cong$ 28900 gas PE[3]

$\tilde{B}\ ^2B_1$ C_{2v}

T_0 = 23169 gas PE[1,3]EF[1]PF[5,6] $\tilde{B}$–$\tilde{A}$,$\tilde{X}$ 400–600 nm
22998 Ne LF[2] $\tilde{B}$–$\tilde{A}$,$\tilde{X}$ 400–485 nm
22680 Ar AB[4] $\tilde{B}$–$\tilde{A}$,$\tilde{X}$ 410–445 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1290(40)	gas	PE	3
			970(40)	gas	PE	3
			506	Ne	LF	2
			500	Ar	AB	4
			320	gas	PF	6
b_1			100H	gas	PF	5,6
b_2			467	gas	PF	6

$\tilde{A}\ ^2B_1$ C_{2v}

T_0 = 2900(160) gas PE[3]

$\tilde{X}\ ^2A_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4		1560	Ne	LF	2
	5		1476	Ne	LF	2
	6		1274	Ne	LF	2
	7		1092	Ne	LF	2
	10		485(40)	gas	PE	3
			504	Ne	LF	2
	11		335	gas	PF	6
			344	Ne	LF	2
b_1			184	gas	PF	6
b_2			411	gas	PF	6

[a] From vertical ionization potential.

References

[1]M. Allan, J. P. Maier, and O. Marthaler, Chem. Phys. **26**, 131 (1977).
[2]V. E. Bondybey, J. H. English, and T. A. Miller, Chem. Phys. Lett. **66**, 165 (1979).
[3]G. Bieri, L. Åsbrink, and W. von Niessen, J. Electron Spectrosc. Relat. Phenom. **23**, 281 (1981).
[4]J. T. Lurito and L. Andrews, Chem. Phys. **97**, 121 (1985).
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[6]Y. Tsuchiya, K. Takazawa, M. Fujii, and M. Ito, J. Phys. Chem. **96**, 99 (1992).

1,4–$C_6H_4F_2^+$

$\tilde{E}\ ^2A_g$ D_{2h}

T^a = 41600(1000) gas PE[2]

$\tilde{D}\ ^2B_{2u}$ D_{2h}

T^a = 36800(1000) gas PE[2]

$\tilde{C}\ ^2B_{3g}$ D_{2h}

T^a = 27100(1000) gas PE[2]

$\tilde{B}\ ^2B_{3u}$ D_{2h}

T_0 = 23754 gas PE[2]ID[5,6] $\tilde{B}$–$\tilde{X}$ 390–425 nm
23200 Ne AB[1]
Ar AB[3] $\tilde{B}$–$\tilde{X}$ 395–425 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g			1450(40)	gas	PE	2
			404(10)	gas	ID	6
			400T	Ne	AB	1
			400	Ar	AB	3
a_u	8		200H	gas	ID	6
b_{3u}	30		144H	gas	ID	5,6

$\tilde{A}\ ^2B_{1g}$ D_{2h}

T_0 = 7180(160) gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g			1355(40)	gas	PE	2

$\tilde{X}\ ^2B_{2g}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2		1640	gas	TPE	7
	3		1375	gas	TPE	7
	4		1149	gas	TPE	7
	5		836	gas	TPE	7
	6		440	gas	ID,TPE	6,7
a_u	8		358	gas	ID,TPE	6,7
b_{2g}	17		302	gas	TPE	7
b_{3u}	29		508(10)H	gas	PE	4
	30		126	gas	ID,TPE	5,7

1,4–$C_6D_4F_2^+$

$\tilde{B}\ ^2B_{3g}$ D_{2h}

T_0 = 23340 Ne AB[1]

[a] From vertical ionization potential.

References

[1]V. E. Bondybey, T. A. Miller, and J. H. English, J. Chem. Phys. **72**, 2193 (1980).
[2]G. Bieri, L. Åsbrink and W. von Niessen, J. Electron Spectrosc. Relat. Phenom. **23**, 281 (1981).
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$1,3\text{–}C_6H_4Cl_2^+$

$\tilde{E}$

T_0 = 28880(800) gas PE[1]

$\tilde{C},\tilde{D}$ $^2A_1,^2B_2$ D_{2h}

T_0 = 19930(160) gas PE[1]

$\tilde{B}$ $^2B_1$ D_{2h}

T_0 = 18770(10) gas PE,EF[1] $\tilde{B}$–$\tilde{X}$ 525–625 nm
18610 Ne LF[2]

τ_0 < 6 ns gas EF[1]

$\tilde{A}$ $^2B_1$ D_{2h}

T_0 = 4280(400) gas PE[1]

$\tilde{X}$ $^2A_2$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1100(80)	gas	PE	1
			400(80)	gas	PE	1

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[1]J. P. Maier and O. Marthaler, Chem. Phys. **32**, 419 (1978).

[2]V. E. Bondybey and T. A. Miller, *Molecular Ions: Spectroscopy, Structure, and Chemistry*, V. E. Bondybey and T. A. Miller, Eds., pp. 125–173 (North-Holland, Amsterdam, 1983).

$1,4\text{–}C_6H_4Cl_2^+$

$\tilde{E}$

T_0 = 31060(800) gas PE[1]
31017 Ar AB[3,4] $\tilde{E}$–$\tilde{X}$ 283–323 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4		1085	Ar	AB	3,4
	5		729	Ar	AB	3,4

$\tilde{C},\tilde{D}$ $^2B_{2u},^2B_{3g}$ D_{2h}

T_0 = 20500(160) gas PE[1]
20383 Ar AB[3,4] $\tilde{C},\tilde{D}$–$\tilde{X}$ 449–491 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		1547	Ar	AB	4
	6		338	Ar	AB	3,4

$\tilde{B}$ $^2B_{3u}$ D_{2h}

T_0 = 19620(10) gas PE,EF[1] $\tilde{B}$–$\tilde{X}$ 500–590 nm
19452 Ne LF[2]
19130[a] Ar AB[3,4]LF[4] $\tilde{B}$–$\tilde{X}$ 498–612 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1000T	gas	PE	1
			780T	gas	PE	1
	6		320(10)	gas	EF	1
			331	Ar	AB	3,4

τ_0 < 6 ns gas EF[1]

$\tilde{A}$ $^2B_{1g}$ D_{2h}

T_0 = 7420(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1080(80)	gas	PE	1
			520(80)	gas	PE	1

$\tilde{X}$ $^2B_{2g}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		1590(10)	gas	EF	1
			1598	Ar	Ra,LF	4
	3		1189	Ar	Ra	4
	4		1113	Ar	Ra,LF	4
	6		330(10)	gas	EF	1
			330	Ar	Ra,LF	4
b_{1u}	11		1429	Ar	IR	4
	13		1110	Ar	IR	4
b_{2u}	21		986	Ar	IR	4
b_{3u}	28		843	Ar	IR	4

$1,4\text{–}C_6D_4Cl_2^+$

$\tilde{B}$ $^2B_{3u}$ D_{2h}

T_0 = 19680(10) gas EF[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			310(10)	gas	EF	1

$\tilde{X}$ $^2B_{2g}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1570(10)	gas	EF	1
			330(10)	gas	EF	1

[a] Mean of absorption and emission values.

References

[1]J. P. Maier and O. Marthaler, Chem. Phys. **32**, 419 (1978).

[2]V. E. Bondybey and T. A. Miller, *Molecular Ions: Spectroscopy, Structure, and Chemistry*, V. E. Bondybey and T. A. Miller, Eds., pp. 125–173 (North-Holland, Amsterdam, 1983).

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1,2,3-$C_6H_3F_3^+$

$\tilde{B}\ ^2B_1$ C_{2v}

T_0 = 22463.8 gas LF[1,2]EM[4] $\tilde{B}-\tilde{X}$ 445–459 nm
22289 Ne LF[1,2] $\tilde{B}-\tilde{X}$ 419–467 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1567T	Ne	LF	1
			1501T	Ne	LF	1
			1264T	Ne	LF	1
			931	Ne	LF	1
			735	Ne	LF	1
			664	Ne	LF	1
			482	Ne	LF	1
			460	Ne	LF	1
			302	Ne	LF	1

τ_0 = 48(4) ns gas LF[1]PEFCO[3]
51(5) ns Ne LF[1]
A_0 = 0.076; B_0 = 0.057; C_0 = 0.033 EM[4]

$\tilde{A}\ ^2A_2$ C_{2v}

T_0 = 191.8 gas EM[4] $\tilde{B}-\tilde{A}$ 448–463 nm
197 Ne LF[1,2] $\tilde{B}-\tilde{A}$ 419–467 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			677.6	gas	EM	4
			680	Ne	LF	1
			603.7	gas	EM	4
			608	Ne	LF	1
			470.3	gas	EM	4
			213.5	gas	EM	4
			218	Ne	LF	1
			145.4	gas	EM	4
			119.9	gas	EM	4
			120	Ne	LF	1

A_0 = 0.078; B_0 = 0.057; C_0 = 0.033 EM[4]

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			695.6	gas	EM	4
			698	Ne	LF	1
			595.0	gas	EM	4
			601	Ne	LF	1
			518.5	gas	EM	4
			526	Ne	LF	1
			458.2	gas	EM	4
			466	Ne	LF	1
			389[a]	Ne	LF	1
			289.3	gas	EM	4
			294	Ne	LF	1

A_0 = 0.079; B_0 = 0.057; C_0 = 0.033 EM[4]

1,2,3-$C_6D_3F_3^+$

$\tilde{B}\ ^2B_1$ C_{2v}

T_0 = 22405 Ne LF[1] $\tilde{B}-\tilde{X},\tilde{A}$ 417–465 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1558T	Ne	LF	1
			1523T	Ne	LF	1
			1503T	Ne	LF	1
			1480T	Ne	LF	1
			1200T	Ne	LF	1
			661	Ne	LF	1
			540	Ne	LF	1
			462	Ne	LF	1
			303	Ne	LF	1

$\tilde{X},\tilde{A}\ ^2B_1,^2A_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			867[a]	Ne	LF	1
			781[a]	Ne	LF	1
			680[a]	Ne	LF	1
			595[a]	Ne	LF	1
			464[a]	Ne	LF	1
			415[a]	Ne	LF	1
			317[a]	Ne	LF	1
			292[a]	Ne	LF	1

[a] May arise from $\tilde{B}-\tilde{A}$ transition, necessitating correction by approximately 97 cm^{-1}.

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1,2,4-$C_6H_3F_3^+$

$\tilde{B}\ ^2A''$ C_s

T_0 = 24274.4 gas EF[1,7]EM[3] $\tilde{B}-\tilde{X}$ 400–470 nm
24177 Ne AB,LF[5] $\tilde{B}-\tilde{X}$ 390–445 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1330	Ne	LF	5
			1086	Ne	LF	5
			485	Ne	LF	5
			422	Ne	LF	5
			339	Ne	LF	5
			287	Ne	LF	5

τ_0 = 16(5) ns gas EF[2]PIFCO[4]PEFCO[6]
10T ns Ne LF[8]

$\tilde{A}\ ^2A'$ C_s
T_0 = 5089 Ne LF[5] $\tilde{B}-\tilde{A}$ 485–585 nm

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1623	gas	EM	3
			1623	Ne	LF	5
	5		1615	gas	EM,EF	3,7
			1616	Ne	LF	5
			1608	Ne	LF	5
			1595	Ne	LF	5
			1407	Ne	LF	5
			1119	Ne	LF	5
	17		675	gas	EF	7
	18		485	gas	EM,EF	3,7
			484	Ne	LF	5
	19		405	gas	EM,EF	3,7
			403	Ne	LF	5
	20		360	gas	EM	3
			357	Ne	LF	5
	21		293	gas	EM	3
			293	Ne	LF	5

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$1,3,5\text{–}C_6H_3F_3^+$

$\tilde{B}\ ^2A_2''$ D_{3h}
T_0 = 21867.479 gas EF[1,12]EM[5]LF[3,9,15,17]ID[16] $\tilde{B}-\tilde{X}$ 425–571 nm
21776 Ne LF[7] $\tilde{B}-\tilde{X}$ 364–460 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	3		995	gas	EM,LF	5,9
			1005	Ne	LF	7
	4		569	gas	LF,EM	3,5,9
			571	Ne	LF	7
e'	9		1499	gas	LF	3,9
			1505	Ne	LF	7
	12		954	gas	LF	9
			959	Ne	LF	7
	13		489.99	gas	LF	3,8,9,17
			484	Ne	LF	7,14
	14		323.81	gas	LF	8,9,17
			327	Ne	LF	7
	17		198H	gas	LF	9
			209H	Ne	LF	7
e''			80H	gas	ID	16

τ_0 = 59(3) ns gas EF[2]PIFCO[10]PEFCO[11]
53(2) ns Ne LF[13]
B_0 = 1.748(4); C_0 = 0.874(2) LF[17]

$\tilde{X}\ ^2E''$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1		2911	gas	EM	5
	2		1465	gas	EM	5
	3		1039.1	gas	EM,EF	5,12,15
			1043	Ne	LF	7
	4		592.1	gas	EM,LF	5,7
					EF	12,15
			596	Ne	LF	7
e'	9		1665	gas	EM	5
			1664	Ne	LF	7
	10		1533	gas	EM	5
	12		945	Ne	LF	7
	13		550.0	gas	EM,LF	5,7
					EF	12,15
			557	Ne	LF	7,14
	14		334	Ne	LF	7,14

B_0 = 1.769(3); C_0 = 0.885(2) LF[17]

$1,3,5\text{–}C_6D_3F_3^+$

$\tilde{B}\ ^2A_2''$ D_{3h}
T_0 = 21923.8 gas EM[6]LF[4,15] $\tilde{B}-\tilde{X}$ 437–544 nm
21831 Ne LF[7] $\tilde{B}-\tilde{X}$ 400–458 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	3		923	gas	EM	6
			932	Ne	LF	7
	4		560	gas	LF,EM	4,6
			569	Ne	LF	7
e'	9		1470	gas	LF	4
			1475	Ne	LF	7
	12		777	Ne	LF	7
	13		458	gas	LF,EM	4,6
			469	Ne	LF	7,14
	14		320	Ne	LF	7
	17		198H	Ne	LF	7

$\tilde{X}\ ^2E''$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1		2247	gas	EM	6
	3		976.1	gas	EM,EF	6,15
	4		586.5	gas	EM,EF	6,15
			592	Ne	LF	7
e'	9		1625	gas	EM	6
			1612	Ne	LF	7
	10		1484	gas	EM	6
	11		1053.0	gas	EF	15
	12		780	Ne	LF	7
	13		532.3	gas	EM,EF	6,15
			541	Ne	LF	7,14
	14		334	Ne	LF	7,14

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1,3,5-$C_6H_3ClF_2^+$

$\tilde{B}$ C_{2v}
T_0 = 19220(10) gas EF[1] $\tilde{B}-\tilde{X}$ 510–620 nm
19095 Ne AB[2] $\tilde{B}-\tilde{X}$ 480–530 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1530(10)	Ne	AB	2
			1055(10)	Ne	AB	2
			415(10)	Ne	AB	2

$\tau_0 \leq$ 6 ns gas EF[1]

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1,3,5-$C_6H_3Cl_2F^+$

$\tilde{B}$ C_{2v}
T_0 = 17205(10) gas EF[1] $\tilde{B}-\tilde{X}$ 555–710 nm
17073 Ne AB,LF[2] $\tilde{B}-\tilde{X}$ 540–650 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1561	Ne	LF	2
			1548	Ne	LF	2
			1064	Ne	LF	2
			992	Ne	LF	2
			973	Ne	LF	2
			843	Ne	LF	2
			680	Ne	LF	2

$\tilde{B}$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			513	Ne	LF	2
			421	Ne	LF	2
			402	Ne	LF	2
			373	Ne	LF	2
			192	Ne	LF	2

τ_0 = 8(2) ns gas EF[1]

$\tilde{A}$ C_{2v}
T_0 = 159 Ne LF[2] $\tilde{B}-\tilde{A}$ 540–650 nm

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1747T	Ne	LF	2
			1680T	Ne	LF	2
			1306	Ne	LF	2
			1289	Ne	LF	2
			1107	Ne	LF	2
			1101	Ne	LF	2
			1062	Ne	LF	2
			999	Ne	LF	2
			973	Ne	LF	2
			961	Ne	LF	2
			783	Ne	LF	2
			543	Ne	LF	2
			529	Ne	LF	2
			450	Ne	LF	2
			437	Ne	LF	2
			422	Ne	LF	2
			333	Ne	LF	2
			201	Ne	LF	2

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1,3,5-$C_6H_3Cl_3^+$

$\tilde{F}$ $^2E''$ D_{3h}
T_0 = 29530(800) gas PE[1]

$\tilde{D}$ $^2E'$ D_{3h}
T_0 = 20900(160) gas PE[1]

$\tilde{C}$ $^2A_2'$ D_{3h}
T_0 = 17510(160) gas PE[1]

$\tilde{B}\ ^2A_2''$ D_{3h}

T_0				$\tilde{B}$–$\tilde{X}$
= 15410(5)	gas	$PE^1EF^1LF^2EM^3$		575–770 nm
15266	Ne	LF^2		580–710 nm
14886	Ar	LF^2		580–730 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	2		1096	gas	LF,EM	2,3
			1096	Ne	LF	2,4
			1091	Ar	LF	2
	3		978	gas	LF	2
			974	Ne	LF	2,4
			970	Ar	LF	2
	4		358	gas	LF	2
			368	Ar	LF	2
e'	9		1510	gas	LF	2
			1510	Ne	LF	2,4
			1508	Ar	LF	2
	10		1417	gas	LF	2
			1412	Ne	LF	2,4
			1411	Ar	LF	2
	11		995	Ne	LF	2,4
	12		809	Ar	LF	2
	13		428	gas	LF,EM	2,3
			427	Ne	LF	4
			426	Ar	LF	2
	14		181	gas	LF,EM	2,3
			195	Ne	LF	2,4
			190	Ar	LF	2

τ_0 = 22(2) ns gas EF^1

$\tilde{X}\ ^2E''$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1		2925	gas	EM	3
	2		1189	gas	PE,EM	1,3
			1190	Ne	LF	2,4
			1183	Ar	LF	2
	3		1068	gas	EM	3
			982	Ne	LF	4
	4		438	gas	LF	2
			442	Ne	LF	2,4
e'	9		1584	gas	EM	3
			1588	Ne	LF	4
	10		1519	gas	EM	3
	11		1074	Ne	LF	4
	13		498	gas	EF,EM	1,3
			501	Ne	LF	2,4
	14		191	gas	LF	2
			195	Ne	LF	2,4

1,3,5–$C_6D_3Cl_3^+$

$\tilde{B}\ ^2A_2''$ D_{3h}

T_0				$\tilde{B}$–$\tilde{X}$
= 15270	Ne	LF^4		520–765 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	2		1099	Ne	LF	4
	3		943	Ne	LF	4
	4		628	Ne	LF	4

$\tilde{B}\ ^2A_2''$—Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	9		1494	Ne	LF	4
	10		1332	Ne	LF	4
	11		811T	Ne	LF	4
	12		800T	Ne	LF	4
	13		418	Ne	LF	4
	14		193	Ne	LF	4

$\tilde{X}\ ^2E''$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	2		1200	Ne	LF	4
	3		940	Ne	LF	4
	4		442	Ne	LF	4
e'	9		1527	Ne	LF	4
	11		853	Ne	LF	4
	13		491	Ne	LF	4
	14		197	Ne	LF	4

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1,2,3,4–$C_6H_2F_4^+$

$\tilde{B}\ ^2B_1$ C_{2v}

T_0				$\tilde{B}$–$\tilde{X}$
= 23291.7	gas	$EF^1EM^2LF^{3,7}$		415–465 nm
23192	Ne	LF^4		387–480 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		1539	Ne	LF	4
	4		1355	Ne	LF	4
	6		1172	Ne	LF	4
	7		1060	Ne	LF	4
	8		654	gas	LF	3
			668	Ne	LF	4
	9		433	gas	EM,LF	2,3
			442	Ne	LF	4
	10		324	gas	LF	7
			324	Ne	LF	4
	11		271	gas	EM,LF	2,3
			277	Ne	LF	4

τ_0 = 50(3) ns gas $EF^1PIFCO^5PEFCO^6$
44(2) ns Ne LF^9

$\tilde{A}\ ^2A_2$ C_{2v}

			$\tilde{B}$–$\tilde{A}$
	gas	EF^1	520–600 nm
T_0 = 2767T	Ne	LF^8	

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		1665	gas	EM,EF	2,7
			1665	Ne	LF	4
			1228	gas	EM	2
	6		1198	Ne	LF	4
	7		1083	gas	EF	7
			1082	Ne	LF	4
	8		678	gas	EF	7
			680	Ne	LF	4
			593	gas	EM	2
	9		441	gas	EM,LF	2,3
					EF	7
			443	Ne	LF	4
	10		339	gas	EF	7
			340	Ne	LF	4
	11		271	gas	EM,LF	2,3
					EF	7
			273	Ne	LF	4

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$1,2,3,5\text{-}C_6H_2F_4^+$

$\tilde{B}\ ^2B_1$ C_{2v}

T_0 = 23323.7 gas $EF^1EM^2LF^{3,8}$ $\tilde{B}\text{-}\tilde{X}$ 400–470 nm
23232 Ne LF^5 $\tilde{B}\text{-}\tilde{X}$ 400–502 nm
22903 Ar LF^4

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		1580	Ne	LF	5
			1582	Ar	LF	4
	3		1445T	Ne	LF	5
			1536T	Ar	LF	4
	5		1264	gas	LF	3
			1259	Ne	LF	5
			1263	Ar	LF	4
	6		1140	Ne	LF	5
	8		783	Ne	LF	5
			783	Ar	LF	4
	9		569	gas	LF	3
			573	Ne	LF	5
			576	Ar	LF	4
	10		424	gas	EM,LF	2,3
			428	Ne	LF	5
			431	Ar	LF	4

$\tilde{B}\ ^2B_1$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	11		307	gas	EM,LF	2,3
			305	Ne	LF	5
			307	Ar	LF	4

τ_0 = 50(3) ns gas $EF^1PIFCO^6PEFCO^7$
43(2) ns Ne LF^{10}

$\tilde{A}\ ^2A_2$ C_{2v}
gas EF^1 $\tilde{B}\text{-}\tilde{A}$ 520–600 nm
T_0 = 2442 Ne LF^9

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		1650	gas	EM,EF	2,8
			1647	Ne	LF	5
	3		1458	gas	EF	8
			1449	Ne	LF	5
	5		1318	gas	EM,EF	2,8
			1305	Ne	LF	5
	8		785	Ne	LF	5
	9		584	gas	EF	8
			581	Ne	LF	5
			586	Ar	LF	4
	10		427	gas	EM,EF	2,8
			426	Ne	LF	5
			429	Ar	LF	4
	11		305	gas	EM,EF	2,8
			303	Ne	LF	5
			307	Ar	LF	4

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1,2,4,5-$C_6H_2F_4^+$

$\tilde{B}\ ^2B_{1u}$ D_{2h}

T_0 = 24443.5 gas EF[1]EM[2]LF[3,8]PI[11] $\tilde{B}$–$\tilde{X}$ 385–500 nm
24352 Ne LF[5] $\tilde{B}$–$\tilde{X}$ 385–510 nm
24072 Ar LF[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2		1536	Ne	LF	5
			1536	Ar	LF	4
	3		1392	Ar	LF	4
	4		725	Ne	LF	5
			722	Ar	LF	4
	5		460	gas	LF	3
			465	Ne	LF	5
			470	Ar	LF	4
	6		270	gas	LF	3
			276	Ne	LF	5
			279	Ar	LF	4

τ_0 = 32(2) ns gas EF[1]PIFCO[6]PEFCO[7]
30(2) ns Ne LF[10]

$\tilde{A}\ ^2B_{3g}$ D_{2h}

gas EF[1] $\tilde{B}$–$\tilde{A}$ 550–650 nm
T_0 = 6115 Ne LF[9] $\tilde{B}$–$\tilde{A}$ 545–625 nm

$\tilde{X}\ ^2B_{2g}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2		1558	gas	EF	8
			1558	Ne	LF	5
	3		1477	gas	EF	8
			1476	Ne	LF	5
	4		726	Ne	LF	5
	5		482	gas	EM,EF	2,8
					PI	11
			485	Ne	LF	5
			480	Ar	LF	4
	6		287	gas	EF	8
			287	Ne	LF	5
			289	Ar	LF	4
b_{1u}			183H	gas	PI	11

1,2,4,5-$C_6D_2F_4^+$

$\tilde{B}\ ^2B_{1u}$ D_{2h}

T_0 = 24400 Ne LF[5] $\tilde{B}$–$\tilde{X}$ 370–465 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2		1531	Ne	LF	5
	3		1383T	Ne	LF	5
	4		722	Ne	LF	5
	5		466	Ne	LF	5
	6		276	Ne	LF	5

τ_0 = 38(3) ns gas PEFCO[7]

$\tilde{X}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2		1542	Ne	LF	5
	3		1472	Ne	LF	5
	4		706	Ne	LF	5
	5		480	Ne	LF	5
	6		286	Ne	LF	5

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$C_6HF_5^+$

$\tilde{B}\ ^2B_1$ C_{2v}

T_0 = 23097.3 gas EF[1]EM[2]LF[3,8] $\tilde{B}$–$\tilde{X}$ 400–475 nm
23014 Ne LF[5] $\tilde{B}$–$\tilde{X}$ 410–465 nm
22810 Ar LF[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		1534	gas	LF	3
			1547	Ne	LF	5
			1545	Ar	LF	4
	3		1452	gas	LF	3
			1459	Ne	LF	5
			1450	Ar	LF	4
	5		1335	Ne	LF	5
	7		676T	Ne	LF	5
			678	Ar	LF	4
	8		572	gas	LF	3
			566	Ne	LF	5
			567	Ar	LF	4
	9		450	gas	LF	3
			456	Ne	LF	5
			455	Ar	LF	4
	10		438T	gas	EM	2
			429	Ne	LF	5
	11		265	gas	LF	3
			268	Ne	LF	5
			273	Ar	LF	4

τ_0 = 48(3) ns gas EF[1]PIFCO[6]PEFCO[7]
40(2) ns Ne LF[9]

$\tilde{X}\ ^2A_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		1598	gas	EF	8
			1595	Ne	LF	5
	3		1546	gas	EM,EF	2,8
			1533	Ne	LF	5
	5		1356	Ne	LF	5
	6		902T	Ne	LF	5
	8		582	gas	EM,EF	2,8
			575	Ne	LF	5
	9		457	gas	EM,LF	2,3
					EF	8
			460	Ne	LF	5
			462	Ar	LF	4
	10		423	gas	EF	8
			438T	Ne	LF	5
	11		277	gas	EM,LF	2,3
					EF	8
			278	Ne	LF	5
			284	Ar	LF	4

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$C_6F_6^+$

$\tilde{C}\ ^2B_{2u}$ D_{6h}
$T_0 \cong 32300$ gas PE[10]
$\tau < 15$ ns gas PEPCO[10]

$\tilde{B}\ ^2A_u$ D_{6h}
$T_0 = 21616.16$ gas EF[1,11]EM[4]LF[5,9,14,16] $\tilde{B}-\tilde{X}$ 426–510 nm
21553.7 Ne LF[7,8,15] $\tilde{B}-\tilde{X}$ 405–523 nm
21372 Ar LF[3,6] $\tilde{B}-\tilde{X}$ 418–468 nm
21027 Kr LF[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1		1520.0	Ne	LF	8,15
			1561	Ar	LF	3,6
	2		535.5	gas	EM,LF	4,9,14
			538.3	Ne	LF	8,15
			547	Ar	LF	3,6
a_{2g}	3		603.6	gas	LF	14
			629.1	Ne	LF	15
a_{2u}	4		203.7	gas	LF	14
b_{1u}	6		611.0	gas	LF	14
b_{2g}	7		706.2	gas	LF	14
	8		166.8	gas	LF	14
b_{2u}	10		274.0	gas	LF	14
e_{1g}	11		299.0	gas	LF	14

$\tilde{B}\ ^2A_u$ —Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e_{1u}	14		308.4	gas	LF	14
e_{2g}	15		1554.0	gas	LF	9
			1552	Ne	LF	8
			1603	Ar	LF	6
	16		1187.0	gas	LF	9,15
			1185.7	Ne	LF	8,15
			1196	Ar	LF	6
	17		421.86	gas	EM,LF	4,5,9,14
						16
			424.4	Ne	LF	8,15
			428	Ar	LF	3,6
	18		262.02	gas	EM,LF	4,5,9,14
						16
			264.4	Ne	LF	8,15
			270	Ar	LF	3,6
e_{2u}	19		573.8	gas	LF	14
	20		114.1	gas	LF	14

τ_0 = 48(2) ns gas EF[2]PEFCO[10,13]
42(2) ns Ne LF[12]
$B_0 = 1.01$; $C_0 = 0.50$ LF[16]

$\tilde{X}\ ^2E_{1g}$ D_{6h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	2		556	gas	UV,LF	4,9
					EF	11
			554	Ne	LF	8
			557	Ar	LF	3,6
e_{2g}	15		1698	Ne	LF	8
	16		1226	Ne	LF	8
	17		406	gas	UV,EF	9,11
			417	Ne	LF	8
			444	Ar	LF	3,6
	18		284	gas	UV,LF	4,9
					EF	11
			289	Ne	LF	8
			300	Ar	LF	3,6

$B_0 = 1.02$; $C_0 = 0.51$ LF[16]

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$C_6F_5Cl^+$

$\tilde{B}\ ^2B_1$ C_{2v}
T_0 = 19990(10) gas EF[2] $\tilde{B}-\tilde{X}$ 485–625 nm
19914 Ne LF[1] $\tilde{B}-\tilde{X}$ 450–525 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	7		583	Ne	LF	1
	8		507	Ne	LF	1
	9		387	Ne	LF	1
	11		268	Ne	LF	1

τ_0 = 43(3) ns gas EF[2]
36 ns Ne LF[1]

$\tilde{A}\ ^2B_1$ C_{2v}
T_0 = 185 Ne LF[1,3]

$\tilde{X}\ ^2A_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			590	Ne	LF	1
			512	Ne	LF	1
			385	Ne	LF	1
			252	Ne	LF	1

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sym-$C_6F_3Cl_3^+$

$\tilde{B}\ ^2A_2'$ D_{3h}
T_0 = 16948 gas EF[2]LF[3] $\tilde{B}-\tilde{X}$ 540–710 nm
16785 Ne LF[1] $\tilde{B}-\tilde{X}$ 490–660 nm
16636 Ar LF[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		1146	gas	LF	3
			1148	Ne	LF	1
	3		576	gas	LF	3
			581	Ne	LF	1
e'	8		1529	gas	LF	3
			1538	Ne	LF	1
	9		1475	gas	LF	3
			1483	Ne	LF	1
	10		1109	gas	LF	3
			1111	Ne	LF	1

$\tilde{B}\ ^2A_2'$—Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	12		393	gas	LF	3
			398	Ne	LF	1
	13		294	gas	LF	3
			298	Ne	LF	1
	14		180	gas	LF	3
			186	Ne	LF	1

τ_0 = 34(3) ns gas EF[2]
29(5) ns Ne LF[1]

$\tilde{X}\ ^2E''$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	3		584	gas	LF	3
			585	Ne	LF	1
e'	8		1629[a]	Ne	LF	1
	9		1428[a]	Ne	LF	1
	10		1128[a]	Ne	LF	1
	12		409[a]	gas	LF	3
			429[a]	Ne	LF	1
	13		318[a]	gas	LF	3
			324[a]	Ne	LF	1
	14		192[a]	Ne	LF	1

[a] Transition to $v = 1, j = \frac{1}{2}$ level.

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sym-$C_6F_3Br_3^+$

$\tilde{B}\ ^2A_2''$ D_{3h}
T_0 = 13510(10) gas EF[1] $\tilde{B}-\tilde{X}$ 725–830 nm
13255 Ne LF[2] $\tilde{B}-\tilde{X}$ 600–870 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	2		1073T	Ne	AB,LF	2
	3		578	Ne	AB,LF	2
e'	8		1555	Ne	AB,LF	2
	9		1398T	Ne	AB,LF	2
	10		1045	Ne	AB,LF	2
	11		685T	Ne	AB,LF	2
	12		381	Ne	AB,LF	2
	13		253	Ne	AB,LF	2

$\tau_0 \leq 6$ ns gas EF[1]

$\tilde{X}\ ^2E''$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	3		583	Ne	LF	2
e'	8		1727	Ne	LF	2
	10		1147	Ne	LF	2
	12		387	Ne	LF	2
	13		292	Ne	LF	2

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LiC_6H_6

$\tilde{X}$ C_{6v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3055w	Ar	IR	1
			1458w,br	Ar	IR	1
		C_6 a–stretch	1325m	Ar	IR	1
			990vw	Ar	IR	1
		C_6 s–stretch	924s	Ar	IR	1
			701w,sh	Ar	IR	1
		CH deform.	607s	Ar	IR	1
		Ax. LiC stretch	451s	Ar	IR	1

LiC_6D_6

$\tilde{X}$ C_{6v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD stretch	2234vw	Ar	IR	1
			1425w,br	Ar	IR	1
			1217w	Ar	IR	1
		C_6 a–stretch	1134w	Ar	IR	1
			883s	Ar	IR	1
			757m	Ar	IR	1
		Ax. LiC stretch	478s	Ar	IR	1
		CD deform.	401vw	Ar	IR	1
			281w	Ar	IR	1

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C_6H_6F

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1428s	Ar	IR	1
			1287ms	Ar	IR	1
			1094wm	Ar	IR	1
			1000ms	Ar	IR	1
			924vs	Ar	IR	1
			912wm	Ar	IR	1
			883s	Ar	IR	1
			823wm	Ar	IR	1
			693vs	Ar	IR	1
			599vs	Ar	IR	1

C_6D_6F

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1247s	Ar	IR	1
			1013vs	Ar	IR	1
			919s	Ar	IR	1
			904wm	Ar	IR	1
			863s	Ar	IR	1
			841m	Ar	IR	1
			783m	Ar	IR	1
			672m	Ar	IR	1
			613s	Ar	IR	1
			455vs	Ar	IR	1

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C_6H_5CF

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1595s	Ar	IR	1
			1450m	Ar	IR	1
			1311m	Ar	IR	1
			1222s	Ar	IR	1
			1164s	Ar	IR	1
			1107s	Ar	IR	1
			1082s	Ar	IR	1
			1061s	Ar	IR	1
			1020m	Ar	IR	1
			834m	Ar	IR	1
			758s	Ar	IR	1
			690m	Ar	IR	1
			678m	Ar	IR	1
			623m	Ar	IR	1

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C_6H_5CCl

In an argon matrix, C_6H_5CCl has a prominent absorption maximum at 300 nm[2,3] and a weaker absorption maximum at 276 nm.[3]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1600m	Ar	IR	2–4
			1582s	Ar	IR	2–4
			1477w	Ar	IR	1–4
			1440m	Ar	IR	1–4
			1318w	Ar	IR	1–4
			1301m	Ar	IR	1–4
			1244m	Ar	IR	1–4
			1222vs	Ar	IR	1–4
			1205w	Ar	IR	2
			1168s	Ar	IR	1–4
			995w	Ar	IR	2,4
			840vs	Ar	IR	1–4
			761m	Ar	IR	1–4
			744vs	Ar	IR	1–4
			671s	Ar	IR	1–4
			563w	Ar	IR	1–4

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$(2\text{-}ClC_6H_4)CH$

In an argon matrix, this species contributes prominent absorptions with maxima at 239.5 and 245.5 nm, a less intense absorption at 308 nm, and a relatively weak absorption at 456 nm.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1058s	Ar	IR	1
			739s	Ar	IR	1
			680m	Ar	IR	1

The positions of weaker absorptions are not given in Ref. 1.

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sym-$C_6H_2F_3CH_3^+$

$\tilde{B}$ C_{2v}
T_0 = 22636 Ne LF[1] $\tilde{B}$–$\tilde{X}$ 410–485 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	5		1240	Ne	LF	1
	6		1161	Ne	LF	1
	9		569	Ne	LF	1
	10		433	Ne	LF	1
	11		333	Ne	LF	1

τ_0 = 41 ns Ne LF[1]

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		1648	Ne	LF	1
	3		1401	Ne	LF	1
	5		1300	Ne	LF	1
	9		580	Ne	LF	1
	10		427	Ne	LF	1
	11		333	Ne	LF	1

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$C_6F_5CH_3^+$

$\tilde{B}$ C_s
T_0 = 21900 gas LF[3]
21751 Ne LF[1] $\tilde{B}$–$\tilde{X}$ 410–475 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1546	Ne	LF	1
			1463	Ne	LF	1
			537	Ne	LF	1
			426	Ne	LF	1
			274	Ne	LF	1

τ_0 = 43 ns gas LF[3]
40 ns Ne LF[1,3]

$\tilde{A}$ C_s
T_0 = 220 Ne LF[2]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			277[a]	Ne	LF	1

[a] Complicated pattern of unassigned emission peaks results from overlap of $\tilde{B}$–$\tilde{X}$ and $\tilde{B}$–$\tilde{A}$ band systems.

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$C_6F_5CF_3^+$

$\tilde{B}$ C_s
T_0 = 23030 Ne LF[1] $\tilde{B}$–$\tilde{X}$ 395–470 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1547	Ne	LF	1
			1386	Ne	LF	1
			577	Ne	LF	1
			479	Ne	LF	1
			281	Ne	LF	1
			255	Ne	LF	1

τ_0 = 45 ns gas LF[2]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1617	Ne	LF	1
			586	Ne	LF	1
			492	Ne	LF	1
			292	Ne	LF	1
			258	Ne	LF	1

References

[1]V. E. Bondybey, T. A. Miller, and J. H. English, J. Chim. Phys. **77**, 667 (1980).
[2]V. E. Bondybey and T. A. Miller, *Molecular Ions: Spectroscopy, Structure, and Chemistry*, V. E. Bondybey and T. A. Miller, Eds., pp. 125–173 (North-Holland, Amsterdam, 1983).

C_6H_5N

In an argon or a nitrogen matrix, irradiation at wavelengths longer than 450 nm leads to isomerization to *cyc*-C_6H_5N.[1]

$\tilde{a}$ $^1A_2$ C_{2v}
T_0 = 6300(700) gas PE[2]

$\tilde{X}$ $^3A_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1552s	Ar	IR	1
			1524m	Ar	IR	1
			1497w	Ar	IR	1
			1426wm	Ar	IR	1
			1408w	Ar	IR	1
			1309w	Ar	IR	1
			1300T	gas	PE	2
			1299w	Ar	IR	1

$\tilde{X}$ $^3A_2$ – Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1286ms	Ar	IR	1
			1250w	Ar	IR	1
			1148m	Ar	IR	1
			1079wm	Ar	IR	1
			1008wm	Ar	IR	1
			964w	Ar	IR	1
			885w	Ar	IR	1
			820wm	Ar	IR	1
		OPLA CH-bend	746vs	Ar	IR	1
		Ring torsion	654s	Ar	IR	1
		Ring breathing	515T	gas	PE	2

References

[1]J. C. Hayes and R. S. Sheridan, J. Am. Chem. Soc. **112**, 5879 (1990).
[2]M. J. Travers, D. C. Cowles, E. P. Clifford, and G. B. Ellison, J. Am. Chem. Soc. **114**, 8699 (1992).

C_6F_5N

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1575m	N_2	IR	1
			1565m	N_2	IR	1
			1502vs	N_2	IR	1
			1462vs	N_2	IR	1
			1454vs	N_2	IR	1
			1359s	N_2	IR	1
			1284m	N_2	IR	1
			1204w	N_2	IR	1
			1149w	N_2	IR	1
			1029vs	N_2	IR	1
			1007s	N_2	IR	1
			990m	N_2	IR	1
			981vs	N_2	IR	1

References

[1]I. R. Dunkin and P. C. P. Thomson, J. Chem. Soc., Chem. Commun. 1192 (1982).

$C_6H_5N^-$

Threshold for electron detachment from ground-state $C_6H_5N^-$ = 11700(160) gas PE[1]

$\tilde{X}$ $^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1350T	gas	PE	1
		Ring breathing	500T	gas	PE	1

$C_6D_5N^-$

Threshold for electron detachment from ground-state $C_6D_5N^-$ = 11620(160) gas PE[1]

References

[1]M. J. Travers, D. C. Cowles, E. P. Clifford, and G. B. Ellison, J. Am. Chem. Soc. **114**, 8699 (1992).

C_6H_5NH

$\tilde{A}$
T_0 = 33250 gas AB[1]

References

[1]G. Porter and F. J. Wright, Trans. Faraday Soc. **51**, 1469 (1955).

$C_6H_5NH_2^+$

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	8a[a]		1593(4)	gas	TPE	2,4
	19a		1436(10)T	gas	PE	2
	13a		1388(4)	gas	TPE	2,4
	9a		1187(4)	gas	TPE	2,4
	18a		993(4)	gas	TPE	4
	12	Ring s–stretch	983(4)	gas	PI,TPE	1,2,4
	1		837(15)	gas	PI,PE	1,2
	6a	N–ring s–str.	521(4)	gas	PI,TPE	1–4
a_2	16a		356H	gas	PI,TPE	2–4
b_1		Inversion	656(4)	gas	PI,TPE	2–4
	10b		177(4)	gas	PI,TPE	3,4
b_2	15		551HT[b]	gas	TPE	4

$C_6D_5ND_2^+$

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_1		Inversion	465(10)	gas	PI	3

[a] Vibrational numbering and assignments parallel those given by Chernoff and Rice (J. Chem. Phys. **70**, 2511 (1979)) for aniline.
[b] Ref. 3 gives 724(15).

References

[1]M. A. Smith, J. W. Hager, and S. C. Wallace, J. Chem. Phys. **80**, 3097 (1984).
[2]J. T. Meek, E. Sekreta, W. Wilson, K. S. Viswanathan, and J. P. Reilly, J. Chem. Phys. **82**, 1741 (1985).
[3]J. Hager, M. A. Smith, and S. C. Wallace, J. Chem. Phys. **84**, 6771 (1986).
[4]X. Zhang, J. M. Smith, and J. L. Knee, J. Chem. Phys. **97**, 2843 (1992).

C_6H_5O

$\tilde{C}$ C_{2v}
gas AB[1,2] $\tilde{C}$–$\tilde{X}$ 380–395 nm
T_0 = 25175(10) Ar AB[4] $\tilde{C}$–$\tilde{X}$ 351–397 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1462(20)	Ar	AB	4
			1140(20)	Ar	AB	4
			920(20)	Ar	AB	4

$\tilde{B}$ C_{2v}
$T_0 \cong$ 16360 gas AB[2,3] $\tilde{B}$–$\tilde{X}$ 559–612 nm
Ar AB[4] $\tilde{B}$–$\tilde{X}$ 573–629 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			500T	gas	AB	3
			504(10)	Ar	AB	4

$\tilde{A}$ C_{2v}
T_0 = 8550(40) gas PE[5]

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1490(25)T	gas	PE	5
			515(15)	gas	PE	5

C_6D_5O

$\tilde{C}$ C_{2v}
T_0 = 25240(10) Ar AB[4] $\tilde{C}$–$\tilde{X}$ 349–397 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1349(20)	Ar	AB	4
			809(20)	Ar	AB	4

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[1]G. Porter and F. J. Wright, Trans. Faraday Soc. **51**, 1469 (1955).
[2]G. Porter and B. Ward, J. Chim. Phys. **61**, 1517 (1964).
[3]B. Ward, Spectrochim. Acta **24a**, 813 (1968).
[4]D. Pullin and L. Andrews, J. Mol. Struct. **95**, 181 (1982).
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C_6H_5S

$\tilde{C}$
$T_0 \cong$ 32260 gas AB[1]

$\tilde{B}$ C_{2v}
T_0 = 19328(4) gas LF[2] $\tilde{B}$–$\tilde{X}$ 490–600 nm

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	Ring deform.	483(5)	gas	LF	2
	CS stretch	410(5)	gas	LF	2
	CH deform.	275(5)	gas	LF	2

τ_0 < 20 ns gas LF[2]

$\tilde{X}$ C_{2v}

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CH deform.	1165(20)	gas	LF	2
	Ring deform.	610(20)	gas	LF	2
	CS stretch	430(20)	gas	LF	2

References

[1]G. Porter and F. J. Wright, Trans. Faraday Soc. **51**, 1469 (1955).
[2]K. Shibuya, M. Nemoto, A. Yanagibori, M. Fukushima, and K. Obi, Chem. Phys. **121**, 237 (1988).

$C_6H_5OH^+$

$\tilde{X}$ C_{2v}

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		1669(33)	gas	PE	1
		1500(30)	gas	PE	1
		1395(28)	gas	PE	1
		1210(24)	gas	PE	1
		1040(21)	gas	PE	1
		1027(21)	gas	PE	1
		976(20)	gas	PE	1
		815(16)	gas	PE	1
		556(12)	gas	PE	1
		516(12)	gas	PE	1
	Ring torsion ?	169(12)	gas	PE	1

References

[1]S. L. Anderson, L. Goodman, K. Krogh-Jesperson, A. G. Ozkabak, R. N. Zare, and C.-F. Zheng, J. Chem. Phys. **82**, 5329 (1985).

$2,5\text{–}F_2C_6H_3OH^+$

$\tilde{B}$ $^2A''$ C_s
T_0 = 23784(6) gas EF^1LF^2 $\tilde{B}$–$\tilde{X}$ 410–500 nm

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		485(10)	gas	LF	2
		425(10)	gas	LF	2
		290(10)	gas	LF	2

τ_0 = 13(3) ns gas EF^1

$\tilde{X}$ $^2A''$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		1560(10)	gas	LF	2
		1530(10)	gas	LF	2
		940(10)	gas	LF	2
		500(10)	gas	LF	2
		360(10)	gas	LF	2
		310(10)	gas	LF	2

References

[1]J. P. Maier, O. Marthaler, M. Mohraz, and R. H. Shiley, J. Electron Spectrosc. Relat. Phenom. **19**, 11 (1980).
[2]J. P. Maier, L. Misev, and R. H. Shiley, Helv. Chim. Acta **63**, 1920 (1980).

$3,5\text{–}F_2C_6H_3OH^+$

$\tilde{B}$ $^2A''$ C_s
T_0 = 21994(6) gas EF^1LF^2 $\tilde{B}$–$\tilde{X}$ 410–525 nm

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		1557	Ne	LF	3
		996	Ne	LF	3
		964	Ne	LF	3
		580(10)	gas	LF	2
		579	Ne	LF	3
		490(10)	gas	LF	2
		491	Ne	LF	3
		325	gas	LF	2
		326	Ne	LF	3

τ_0 = 36(4) ns gas EF^1
32 ns Ne LF^4

$\tilde{A}$ $^2A''$ C_s
T_0 = 1334 Ne LF^3 $\tilde{B}$–$\tilde{A}$ 485–500 nm

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		598	Ne	LF	3
		477	Ne	LF	3

$\tilde{X}$ $^2A''$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		1620(10)	gas	LF	2
		1608	Ne	LF	3
		1205	Ne	LF	3
		992	Ne	LF	3
		600(10)	gas	LF	2
		590	Ne	LF	3
		480(10)	gas	LF	2
		486	Ne	LF	3
		340(10)	gas	LF	2
		325	Ne	LF	3
		230(10)	gas	LF	2

References

[1]J. P. Maier, O. Marthaler, M. Mohraz, and R. H. Shiley, J. Electron Spectrosc. Relat. Phenom. **19**, 11 (1980).
[2]J. P. Maier, L. Misev, and R. H. Shiley, Helv. Chim. Acta **63**, 1920 (1980).
[3]V. E. Bondybey, J. H. English, T. A. Miller, and R. H. Shiley, J. Chem. Phys. **78**, 2227 (1983).
[4]V. E. Bondybey and T. A. Miller, *Molecular Ions: Spectroscopy, Structure, and Chemistry*, V. E. Bondybey and T. A. Miller, Eds., pp. 125–173 (North-Holland, Amsterdam, 1983).

2,3,4–$F_3C_6H_2OH^+$

$\tilde{B}\ ^2A''$ C_s
T_0 = 23795(6) gas EF^1LF^2 $\tilde{B}-\tilde{X}$ 400–500 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			680(10)	gas	LF	2
			450(10)	gas	LF	2
			270(10)	gas	LF	2

τ_0 = 26(3) ns gas EF^1

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1660(10)	gas	LF	2
			460(10)	gas	LF	2
			260(10)	gas	LF	2

References

[1]J. P. Maier, O. Marthaler, M. Mohraz, and R. H. Shiley, J. Electron Spectrosc. Relat. Phenom. **19**, 11 (1980).
[2]J. P. Maier, L. Misev, and R. H. Shiley, Helv. Chim. Acta **63**, 1920 (1980).

2,4,5–$F_3C_6H_2OH^+$

$\tilde{B}\ ^2A''$ C_s
T_0 = 24245(6) gas EF^1LF^2 $\tilde{B}-\tilde{X}$ 405–500 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			250(10)	gas	LF	2

$\tau_0 \leq$ 6 ns gas EF^1

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1620(10)	gas	LF	2
			480(10)	gas	LF	2
			290(10)	gas	LF	2

References

[1]J. P. Maier, O. Marthaler, M. Mohraz, and R. H. Shiley, J. Electron Spectrosc. Relat. Phenom. **19**, 11 (1980).
[2]J. P. Maier, L. Misev, and R. H. Shiley, Helv. Chim. Acta **63**, 1920 (1980).

2,3,5,6–$F_4C_6HOH^+$

$\tilde{B}\ ^2A''$ C_s
T_0 = 21860(10) gas EF^1 $\tilde{B}-\tilde{X}$ 445–625 nm
21798 Ne AB^2LF^2 $\tilde{B}-\tilde{X}$ 420–475 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1557	Ne	AB	2
			1503	Ne	AB	2
			1334	Ne	AB	2
			1221	Ne	AB	2
			1098T	Ne	AB	2
			708T	Ne	AB	2
			572	Ne	AB	2
			421	Ne	AB	2
			270	Ne	AB	2

τ_0 = 41(4) ns gas EF^1
40 ns Ne LF^2

$\tilde{A}\ ^2A''$ C_s
T_0 = 207 Ne LF^2 $\tilde{B}-\tilde{A}$ 455–475 nm

$\tilde{X}\ ^2A''$ C_s

References

[1]J. P. Maier, O. Marthaler, M. Mohraz, and R. H. Shiley, J. Electron Spectrosc. Relat. Phenom. **19**, 11 (1980).
[2]V. E. Bondybey, J. H. English, T. A. Miller, and R. H. Shiley, J. Chem. Phys. **78**, 2227 (1983).

$C_6F_5OH^+$

$\tilde{B}\ ^2A''$ C_s
T_0 = 22406(6) gas EF^1LF^2 $\tilde{B}-\tilde{X}$ 425–500 nm
22403 Ne AB^3LF^3 $\tilde{B}-\tilde{X}$ 410–500 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1548	Ne	LF	3
			1186	Ne	LF	3
			700(10)	gas	LF	2
			540(10)	gas	LF	2
			543	Ne	LF	3
			435(10)	gas	LF	2
			430	Ne	LF	3
			270(10)	gas	LF	2
			268	Ne	LF	3

τ_0 = 33(3) ns gas EF^1
32(2) ns Ne LF^3

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2		1680(10)	gas	LF	2
			1688	Ne	LF	3
	3		1656	Ne	LF	3
	5		1489	Ne	LF	3
	6		1472	Ne	LF	3
	7		1350	Ne	LF	3
	10		1182	Ne	LF	3
	11		1147	Ne	LF	3
	16		560(10)	gas	LF	2
			558	Ne	LF	3
	17		420(10)	gas	LF	2
			431	Ne	LF	3
	19		383	Ne	LF	3
	21		260(10)	gas	LF	2
			266	Ne	LF	3

References

[1]J. P. Maier, O. Marthaler, M. Mohraz, and R. H. Shiley, J. Electron Spectrosc. Relat. Phenom. **19**, 11 (1980).
[2]J. P. Maier, L. Misev, and R. H. Shiley, Helv. Chim. Acta **63**, 1920 (1980).
[3]V. E. Bondybey, J. H. English, T. A. Miller, and C. B. Vaughn, J. Phys. Chem. **85**, 1667 (1981).

$C_6H_5O^-$

Threshold for electron detachment from ground-state $C_6H_5O^-$ = 18180(50) gas PE[1]

References

[1]R. F. Gunion, M. K. Gilles, M. L. Polak, and W. C. Lineberger, Int. J. Mass Spectrom. Ion Proc. **117**, 601 (1992).

1,2-$C_6H_4(NO)_2$

In an argon matrix, a structured absorption between 300 and 350 nm has been assigned[1] to 1,2-$C_6H_4(NO)_2$. When the sample is exposed to 320 nm radiation, isomerization to benzofurazan-1-oxide occurs.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO stretch	1516s	Ar	IR	1
			1423w	Ar	IR	1
			1257w	Ar	IR	1
			1162w	Ar	IR	1
			1108m	Ar	IR	1
			1077w	Ar	IR	1
			805w	Ar	IR	1
			772w	Ar	IR	1
			622vw	Ar	IR	1

References

[1]I. R. Dunkin, M. A. Lynch, A. J. Boulton, and N. Henderson, J. Chem. Soc., Chem. Commun. 1178 (1991).

C_6H_5OCCl

In a nitrogen matrix, an absorption maximum at 320 nm has been assigned[1] to C_6H_5OCCl.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1285B	N_2	IR	1
			1275B	N_2	IR	1
			1251A	N_2	IR	1
			850A	N_2	IR	1
			800B	N_2	IR	1

The infrared spectrum between 400 and 2000 cm^{-1} is shown in Ref. 1, but the positions of only a few very prominent absorptions are given. There is evidence for the stabilization of two rotational isomers, labelled A and B.

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[1]M. A. Kesselmayer and R. S. Sheridan, J. Am. Chem. Soc. **108**, 844 (1986).

7. Molecule Index

Formula	*Structure/Name*	*Page*	*Formula*	*Structure/Name*	*Page*
$BrGeH_3^+$	GeH_3Br^+	241	CBrCl	CClBr	99
$BrHI^-$	$BrHI^-$	55	$CBrCl_2^+$	CCl_2Br^+	211
BrHO	HOBr	52	$CBrCl_2$	CCl_2Br	218
BrHSi	HSiBr	44	$CBrClF_2^-$	CF_2ClBr^-	303
BrH_2N^+	H_2NBr^+	152	CBrF	CFBr	98
BrH_3Si^+	SiH_3Br^+	241	$CBrF_2^+$	CF_2Br^+	210
BrKrXe	KrXeBr	123	$CBrF_2$	CF_2Br	216
$BrKr_2$	Kr_2Br	123	$CBrF_2^-$	CF_2Br^-	225
$BrNO^+$	$BrNO^+$	94	$CBrF_3^+$	CF_3Br^+	291
$BrNO_2$	$BrNO_2$	213	$CBrF_3^-$	CF_3Br^-	303
$BrNO_2$	BrONO	213	$CBrF_4$	CF_3BrF	356
$BrNO_3$	$BrONO_2$	289	$CBrN^+$	$BrCN^+$	80
$BrNS^+$	$NSBr^+$	95	CBrN	BrNC	88
BrNS	NSBr	104	$CBrNO^+$	$BrNCO^+$	193
BrN_3^+	BrN_3^+	197	CBrNO	BrCNO	199
BrNeXe	NeXeBr	123	CBrNO	BrNCO	198
BrOP	BrPO	103	$CBrNS^+$	$BrSCN^+$	194
BrOPS	BrP(O)S	214	CBrNS	BrSCN	199
BrO_2	BrOO	110	$CBrNSe^+$	$BrSeCN^+$	195
BrO_2	OBrO	114	CBr_2^+	CBr_2^+	91
BrO_2P	PO_2Br	214	CBr_2	CBr_2	100
BrPS	BrPS	104	CBr_2Cl^+	$CClBr_2^+$	211
BrS_2	SSBr	111	CBr_2Cl	$CClBr_2$	218
$BrXe_2$	Xe_2Br	123	CBr_2F^+	$CFBr_2^+$	210
Br_2Cl^-	$BrClBr^-$	119	CBr_2F	$CFBr_2$	216
Br_2Cl^-	$ClBrBr^-$	119	$CBr_2F_2^+$	$CF_2Br_2^+$	292
Br_2F	BrBrF	117	$CBr_2F_2^-$	$CF_2Br_2^-$	303
Br_2F_2	Br_2F_2	227	CBr_3^+	CBr_3^+	211
Br_2Ge^+	$GeBr_2^+$	92	CBr_3	CBr_3	218
$Br_2GeH_2^+$	$GeH_2Br_2^+$	263	CBr_3F^+	$CFBr_3^+$	293
Br_2H^-	$BrHBr^-$	55	CBr_3F^-	$CFBr_3^-$	303
Br_2HN^+	$HNBr_2^+$	179	CBr_4^+	CBr_4^+	294
$Br_2H_2Si^+$	$SiH_2Br_2^+$	262	CCaN	CaNC	62
Br_2N	NBr_2	108	CCaNO	CaNCO	182
Br_2O	BrOBr	114	CClF	CFCl	98
Br_2O	BrBrO	116	CClFOS	ClFCSO(I)	288
Br_2OP	$OPBr_2$	221	CClFOS	ClFCSO(II)	288
Br_2P	PBr_2	109	$CClFS^+$	$FClCS^+$	205
Br_2S^+	SBr_2^+	112	$CClF_2^+$	CF_2Cl^+	210
Br_2S	SBr_2	115	$CClF_2$	CF_2Cl	216
$Br_2S_2^+$	$S_2Br_2^+$	224	$CClF_2NO^+$	CF_2ClNO^+	353
Br_2S_2	$SSBr_2$	226	$CClF_2NO_4$	$CF_2ClOONO_2$	425
Br_2Se^+	$SeBr_2^+$	113	$CClF_3^+$	CF_3Cl^+	290
Br_2Si	$SiBr_2$	101	$CClF_3^-$	CF_3Cl^-	303
Br_3^-	Br_3^-	119	$CClF_4$	CF_3ClF	356
Br_3P^+	PBr_3^+	221	$CClN^+$	$ClCN^+$	79
Br_3PO^+	Br_3PO^+	299	CClN	ClNC	88
Br_3PS^+	Br_3PS^+	299	$CClNO^+$	$ClNCO^+$	193
Br_3Sb^+	$SbBr_3^+$	222	CClNO	ClCNO	199
Br_4Ge^+	$GeBr_4^+$	297	CClNO	ClNCO	198
Br_4Si^+	$SiBr_4^+$	296	$CClNS^+$	$ClSCN^+$	194
CAsN	AsCN	71	CClNS	ClSCN	198
CAlO	AlCO	68	$CClNSe^+$	$ClSeCN^+$	195
CBO	BCO	68	CClO	ClCO	90
CBO_2	OBCO	186	$CClP^+$	$ClCP^+$	81
CBaN	BaCN	62	CClS	ClCS	105
$CBrCl^+$	$CClBr^+$	91	CCl_2^+	CCl_2^+	91

Formula	*Structure/Name*	*Page*	*Formula*	*Structure/Name*	*Page*
CH_3NO	CH_2NOH	320	CNO^-	NCO^-	85
CH_3NO_2	c–$CH_2(NO)OH$	367	$CNOSr$	$SrNCO$	182
CH_3NO_2	t–$CH_2(NO)OH$	367	CNP	PCN	70
CH_3NO_4	CH_3OONO_2	425	CNS	NCS	77
CH_3NO_5	$HOCH_2OONO_2$	425	CNS^-	NCS^-	86
CH_3NS^+	$HCSNH_2^+$	319	$CNSr$	$SrNC$	62
CH_3Na	$NaCH_3$	229	CN_2	NCN	70
CH_3O^+	CH_2OH^+	235	CN_2	CNN	71
CH_3O	CH_3O	236	CN_2O^+	$ONCN^+$	186
CH_3O	CH_2OH	237	CN_2O	$NCNO$	188
CH_3O^-	CH_3O^-	242	CN_4^+	N_3CN^+	278
CH_3OSr	$SrOCH_3$	315	COP	PCO	77
CH_3O_2	CH_3O_2	321	COS^+	OCS^+	78
CH_3O_3	$HOCH_2O_2$	368	$COSi$	$SiCO$	70
CH_3P^+	CH_2PH^+	233	CO_2^+	CO_2^+	77
CH_3S^+	CH_3S^+	235	CO_2^-	CO_2^-	90
CH_3S^+	CH_2SH^+	235	CO_3	CO_3	199
CH_3S	CH_3S	237	CO_3^-	CO_3^-	203
CH_3S	CH_2SH	238	CO_4^-	CO_4^-	287
CH_3S^-	CH_3S^-	242	CS_2^+	CS_2^+	79
CH_3SSr	$SrSCH_3$	315	CSi_2	Si_2C	67
CH_3S_2	CH_3S_2	322	CSi_3	Si_3C	181
$CH_3S_2^-$	$CH_3S_2^-$	322	C_2B	cyc–BCC	62
CH_3Si	CH_2SiH	232	C_2BrCl^+	$ClCCBr^+$	191
CH_3Si	CH_3Si	232	C_2BrF_3	CF_3CBr	354
CH_3Si^-	CH_2SiH^-	233	C_2BrN	$BrCCN$	189
CH_3Si^-	CH_3Si^-	233	$C_2Br_2^+$	$C_2Br_2^+$	191
CH_3Sr	$SrCH_3$	230	$C_2ClF_3^+$	$CF_2=CFCl^+$	352
CH_3Te	CH_3Te	238	C_2ClF_3	CF_3CCl	354
CH_3Zn	$ZnCH_3$	230	C_2ClN	$ClCCN$	189
CH_4^+	CH_4^+	227	$C_2Cl_2^+$	$C_2Cl_2^+$	190
CH_4Fe	$HFeCH_3$	306	$C_2Cl_2F_2^+$	$CF_2=CCl_2^+$	352
CH_4Ga	CH_3GaH	307	$C_2Cl_2O^+$	Cl_2CCO^+	285
CH_4N^+	$CH_2NH_2^+$	310	C_2Cl_2O	Cl_2CCO	285
CH_4Ni	$HNiCH_3$	306	$C_2Cl_2O_2^+$	t–$(ClCO)_2^+$	348
CH_4NiO	$HNiOCH_3$	362	$C_2Cl_4^+$	$C_2Cl_4^+$	353
CH_4NiO	CH_3NiOH	362	$C_2F_2^+$	$C_2F_2^+$	190
CH_4O^+	CH_3OH^+	310	C_2F_2	$FCCF$	197
CH_4OSi	HCH_3SiO	363	C_2F_2	$F_2C=C:$	197
CH_4O_3	HO_2CH_2OH	379	$C_2F_2^-$	$F_2C=C:^-$	203
CH_4S^+	CH_3SH^+	310	$C_2F_2N_2$	$F_2C=C=N=N$	347
CH_4Si^+	$CH_2=SiH_2^+$	308	$C_2F_2O_2^+$	t–$(FCO)_2^+$	348
CH_4Si	$CH_2=SiH_2$	309	C_2F_3	C_2F_3	287
CH_4Si	CH_3SiH	309	$C_2F_4^+$	$C_2F_4^+$	351
CH_5BO	$H_2B=OCH_3$	374	C_2F_4	CF_3CF	354
CH_6BN	$H_2B=NHCH_3$	398	C_2F_5	C_2F_5	371
CH_6OSi	CH_3SiH_2OH	416	C_2F_5P	$CF_2=PCF_3$	382
CIN^+	ICN^+	81	C_2H	HCC	32
$CINO^+$	$INCO^+$	193	C_2H^-	HCC^-	37
$CINO$	$INCO$	198	C_2HBr^+	$HCCBr^+$	158
$CINS^+$	$ISCN^+$	195	C_2HCa	$CaCCH$	155
$CINS$	$ISCN$	199	C_2HCl^+	$HCCCl^+$	158
CI_3	CI_3	218	$C_2HClF_2^+$	$CHCl=CF_2^+$	340
$CMgN$	$MgNC$	62	C_2HClO	$HClCCO$	269
CNO^+	NCO^+	71	$C_2HCl_3^+$	$CHCl=CCl_2^+$	341
CNO	CNO	82	$C_2HF_3^+$	$CHF=CF_2^+$	340
CNO	NCO	76	C_2HF^+	$HCCF^+$	158

Formula	*Structure/Name*	*Page*	*Formula*	*Structure/Name*	*Page*
C_2HF	$HFC=C:$	162	C_2H_3ClO	CH_3OCCl	366
C_2HF^-	$HFC=C:^-$	168	$C_2H_3F^+$	$CH_2=CHF^+$	319
C_2HFO	HFCCO	269	$C_2H_3N^+$	CH_3CN^+	312
C_2HI^+	$HCCI^+$	159	$C_2H_3N^+$	CH_3NC^+	313
C_2HN	HCCN	156	$C_2H_3N^+$	$CH_2=C=NH^+$	313
C_2HNO	HCOCN	269	C_2H_3N	$CH_2=C=NH$	316
$C_2HN_2^+$	$HNCCN^+$	268	C_2H_3N	$HCCNH_2$	316
C_2HO	HCCO	156	C_2H_3NO	CH_3CNO	366
C_2HS	HCCS	157	C_2H_3NO	$HOCH_2CN$	366
C_2HS	HSCC	157	$C_2H_3NO_2$	CH_3ONCO	380
C_2HSr	SrCCH	155	C_2H_3O	CH_3CO	317
$C_2H_2^+$	$HCCH^+$	133	C_2H_3O	CH_2CHO	317
C_2H_2	$H_2C=C:$	137	$C_2H_3O^-$	CH_2CHO^-	320
$C_2H_2^-$	$H_2C=C:^-$	139	$C_2H_3O_2Sr$	CH_3COOSr	380
C_2H_2Br	$CHBr=CH$	257	$C_2H_3O_3$	CH_3COO_2	380
$C_2H_2ClF^+$	$CH_2=CFCl^+$	334	$C_2H_3P^+$	CH_3CP^+	314
$C_2H_2ClF^+$	c–$CHF=CHCl^+$	334	C_2H_3P	CH_3CP	316
$C_2H_2ClF^+$	t–$CHF=CHCl^+$	334	$C_2H_4^+$	$C_2H_4^+$	307
$C_2H_2ClN^+$	CH_2ClCN^+	331	C_2H_4Al	AlC_2H_4	361
$C_2H_2Cl_2^+$	$CH_2=CCl_2^+$	335	C_2H_4F	FCH_2CH_2	364
$C_2H_2Cl_2^+$	c–$CHCl=CHCl^+$	335	C_2H_4Fe	$HFeC_2H_3$	360
$C_2H_2Cl_2^+$	t–$CHCl=CHCl^+$	336	C_2H_4FeO	$CH_2=CHFeOH$	378
C_2H_2F	t–$CHF=CH$	257	C_2H_4FeO	cyc–C_2H_4OFe	378
$C_2H_2FN^+$	CH_2FCN^+	330	C_2H_4In	InC_2H_4	361
$C_2H_2FO^-$	CH_2COF^-	337	C_2H_4Li	C_2H_4Li	360
$C_2H_2F_2^+$	$CH_2=CF_2^+$	332	$C_2H_4Li_2$	1,2–$C_2H_4Li_2$	377
$C_2H_2F_2^+$	c–$CHF=CHF^+$	333	$C_2H_4N^+$	CH_3CNH^+	362
$C_2H_2F_2^+$	t–$CHF=CHF^+$	333	$C_2H_4O^+$	$CH_2=CHOH^+$	362
C_2H_2Fe	HFeCCH	245	C_2H_4O	$CH_2=CHOH$	363
C_2H_2Li	LiC_2H_2	244	$C_2H_4O_3$	1,2,3–cyc–$C_2H_4O_3$	422
C_2H_2N	H_2CCN	250	$C_2H_4O_3$	1,2,4–cyc–$C_2H_4O_3$	422
C_2H_2N	H_2CNC	250	$C_2H_4O_3$	c–$HCOOCH_2OH$	423
$C_2H_2N^-$	H_2CCN^-	252	$C_2H_4O_3$	t–$HCOOCH_2OH$	423
$C_2H_2N^-$	H_2CNC^-	252	$C_2H_4S^+$	CH_3CHS^+	363
$C_2H_2N_2^+$	$HN=CHCN^+$	327	C_2H_4S	CH_3CHS	363
$C_2H_2N_2^+$	$H_2C=NCN^+$	327	$C_2H_5^+$	$C_2H_5^+$	359
$C_2H_2N_2$	c–$HN=CHCN$	327	C_2H_5	C_2H_5	359
$C_2H_2N_2$	t–$HN=CHCN$	328	C_2H_5BrS	CH_3SBrCH_2	418
$C_2H_2N_2$	$H_2C=NCN$	328	C_2H_5ClS	CH_3SClCH_2	418
$C_2H_2N_2O_2$	$HON=CHCNO$	381	C_2H_5IS	CH_3SICH_2	418
$C_2H_2N_2O_2$	$HON=CHNCO$	381	C_2H_5N	c–$CH_3CH=NH$	374
C_2H_2Ni	$(C_2H_2)Ni$	245	C_2H_5N	t–$CH_3CH=NH$	374
C_2H_2Ni	$NiC=CH_2$	245	C_2H_5N	$C_2H_3NH_2$	375
$C_2H_2O^+$	H_2CCO^+	250	C_2H_5N	$H_2C=NCH_3$	375
C_2H_2O	HCCOH	255	$C_2H_5NO_2$	c–$CH_3CH(NO)OH$	424
C_2H_2OS	CHOCHS	330	$C_2H_5NO_4$	$C_2H_5OONO_2$	425
$C_2H_2O_2^+$	$(HCO)_2^+$	329	C_2H_5O	C_2H_5O	376
$C_2H_2O_3$	$(HCO)_2O$	368	C_2H_5O	CH_3CHOH	376
$C_2H_2S^+$	H_2CCS^+	253	C_2H_5O	$HOCH_2CH_2$	376
C_2H_2S	H_2CCS	255	$C_2H_5O_2$	$C_2H_5O_2$	420
C_2H_2S	HCCSH	256	$C_2H_5O_3$	$HOCH_2CH_2O_2$	424
C_2H_2S	cyc–C_2H_2S	256	C_2H_5S	C_2H_5S	376
$C_2H_2S_2$	$HS–CH=C=S$	331	C_2H_6Ge	$(CH_3)_2Ge$	400
$C_2H_3^+$	$C_2H_3^+$	232	$C_2H_6N_2O$	CH_3NHCH_2NO (A)	424
C_2H_3	C_2H_3	232	$C_2H_6N_2O$	CH_3NHCH_2NO (B)	424
$C_2H_3CaO_2$	CH_3COOCa	379	C_2H_6OSi	$(CH_3)_2SiO$	416
$C_2H_3Cl^+$	$CH_2=CHCl^+$	319	C_2H_6OSi	$CH_2=Si(OH)CH_3$	417

Formula	*Structure/Name*	*Page*
C_4F_6O	CF_3CCOCF_3	418
C_4F_6O	$(CF_3)_2(cyc\text{-}CCO)$	418
C_4H	C_4H	266
C_4HBr^+	$H(CC)_2Br^+$	339
C_4HCl^+	$H(CC)_2Cl^+$	339
C_4HF^+	$H(CC)_2F^+$	339
C_4HI^+	$H(CC)_2I^+$	340
$C_4H_2^+$	$C_4H_2^+$	325
C_4H_2	H_2CCCC:	326
$C_4H_4^+$	$cyc\text{-}C_4H_4^+$	377
$C_4H_4^+$	$H_2C=(cyc\text{-}C_3H_2)^+$	377
C_4H_4	$cyc\text{-}C_4H_4$	378
C_4H_4	$H_2C=(cyc\text{-}C_3H_2)$	377
C_4H_4CaN	$Ca(C_4H_4N)$	410
C_4H_4CdN	$Cd(C_4H_4N)$	412
C_4H_4MgN	$Mg(C_4H_4N)$	410
C_4H_4NSr	$Sr(C_4H_4N)$	411
C_4H_4NZn	$Zn(C_4H_4N)$	411
C_4H_6S	$(CH_3)_2(cyc\text{-}CCS)$	419
C_4H_7N	$(CH_3)_2C=C=NH$	412
C_4H_7N	$CH_3CC\text{-}NHCH_3$	412
$C_4H_9^+$	$t\text{-}C_4H_9^+$	384
C_4H_9	$n\text{-}C_4H_9$	384
C_4H_9	$i\text{-}C_4H_9$	384
C_4H_9	$t\text{-}C_4H_9$	384
$C_4H_9O_2$	$t\text{-}C_4H_9O_2$	421
$C_4H_{10}Si$	$(CH_3)_2Si=CHCH_3$	401
$C_4I_2^+$	$I(CC)_2I^+$	345
$C_4N_2^+$	$NCCCCN^+$	343
C_4N_2	NCCCNC	343
C_4N_2	CNCCNC	343
C_4O	C_4O	278
C_4OS	C_4OS	344
C_4O_2	C_4O_2	344
C_4S	C_4S	278
C_4S_2	C_4S_2	344
C_4Si	C_4Si	277
C_5^+	$cyc\text{-}C_5^+$	277
C_5	C_5	277
C_5^-	C_5^-	278
$C_5F_4^+$	$CF_3(CC)_2F^+$	407
C_5F_6O	$(CF_3)_2(cyc\text{-}CCO)$	418
C_5F_8O	$CF_3(cyc\text{-}CCO)C_2F_5$	419
C_5HN^+	$H(CC)_2CN^+$	369
$C_5H_3Br^+$	$CH_3(CC)_2Br^+$	406
$C_5H_3Cl^+$	$CH_3(CC)_2Cl^+$	406
$C_5H_3F_2N^+$	$cyc\text{-}C_5H_3F_2N^+$	412
C_5H_3N	$cyc\text{-}C_5H_3N$	412
$C_5H_4^+$	$CH_3(CC)_2H^+$	385
C_5H_4	$cyc\text{-}C_5H_4$	385
C_5H_4Cl	$cyc\text{-}C_5H_4Cl$	407
C_5H_4F	$cyc\text{-}C_5H_4F$	407
C_5H_4O	$(cyc\text{-}C_5H_4)O$	419
$C_5H_4O_2$	$cyc\text{-}C_5H_4O\text{-}1\text{-}O$	422
C_5H_5	$cyc\text{-}C_5H_5$	385
C_5H_5Ca	CaC_5H_5	402
C_5H_5Cd	CdC_5H_5	403
C_5H_5Mg	MgC_5H_5	401
C_5H_5Sr	SrC_5H_5	402
C_5H_5Zn	ZnC_5H_5	402
C_5H_6Se	$(CH_2)_3C=C=Se$	419
$C_5H_6Si^+$	$C_5SiH_6^+$	404
C_5H_6Si	C_5SiH_6	404
C_5H_6Si	C_5SiH_6 (Dewar)	405
C_5H_{11}	$n\text{-}C_5H_{11}$	386
C_5H_{11}	$(CH_3)_3CCH_2$	386
C_5OS	C_5OS	370
C_5O_2	C_5O_2	370
C_5S	C_5S	343
C_5S_2	C_5S_2	370
C_6	C_6	342
C_6^-	C_6^-	342
$C_6Br_3F_3^+$	$sym\text{-}C_6F_3Br_3^+$	439
$C_6ClF_5^+$	$C_6F_5Cl^+$	439
$C_6Cl_3F_3^+$	$sym\text{-}C_6F_3Cl_3^+$	439
C_6F_5N	C_6F_5N	442
$C_6F_6^+$	$CF_3(CC)_2CF_3^+$	307
$C_6F_6^+$	$C_6F_6^+$	438
C_6H	C_6H	369
$C_6HF_5^+$	$C_6HF_5^+$	437
$C_6HF_5O^+$	$C_6F_5OH^+$	445
$C_6H_2^+$	$C_6H_2^+$	380
$C_6H_2F_4^+$	$1,2,3,4\text{-}C_6H_2F_4^+$	435
$C_6H_2F_4^+$	$1,2,3,5\text{-}C_6H_2F_4^+$	436
$C_6H_2F_4^+$	$1,2,4,5\text{-}C_6H_2F_4^+$	437
$C_6H_2F_4O^+$	$2,3,5,6\text{-}F_4C_6HOH^+$	445
$C_6H_3ClF_2^+$	$1,3,5\text{-}C_6H_3ClF_2^+$	434
$C_6H_3Cl_2F^+$	$1,3,5\text{-}C_6H_3Cl_2F^+$	434
$C_6H_3Cl_3^+$	$1,3,5\text{-}C_6H_3Cl_3^+$	434
$C_6H_3F_3^+$	$1,2,3\text{-}C_6H_3F_3^+$	432
$C_6H_3F_3^+$	$1,2,4\text{-}C_6H_3F_3^+$	432
$C_6H_3F_3^+$	$1,3,5\text{-}C_6H_3F_3^+$	433
$C_6H_3F_3O^+$	$2,3,4\text{-}F_3C_6H_2OH^+$	445
$C_6H_3F_3O^+$	$2,4,5\text{-}F_3C_6H_2OH^+$	445
$C_6H_3N^+$	$CH_3(CC)_2CN^+$	413
$C_6H_4^+$	$C_6H_4^+$	386
C_6H_4	C_6H_4	386
$C_6H_4^-$	$C_6H_4^-$	387
C_6H_4Br	$o\text{-}C_6H_4Br$	428
C_6H_4Br	$m\text{-}C_6H_4Br$	428
C_6H_4Br	$p\text{-}C_6H_4Br$	428
C_6H_4Cl	$o\text{-}C_6H_4Cl$	427
C_6H_4Cl	$m\text{-}C_6H_4Cl$	427
C_6H_4Cl	$p\text{-}C_6H_4Cl$	427
$C_6H_4Cl_2^+$	$1,3\text{-}C_6H_4Cl_2^+$	431
$C_6H_4Cl_2^+$	$1,4\text{-}C_6H_4Cl_2^+$	431
C_6H_4F	$o\text{-}C_6H_4F$	427
C_6H_4F	$m\text{-}C_6H_4F$	427
C_6H_4F	$p\text{-}C_6H_4F$	427
$C_6H_4F_2^+$	$1,2\text{-}C_6H_4F_2^+$	429
$C_6H_4F_2^+$	$1,3\text{-}C_6H_4F_2^+$	429
$C_6H_4F_2^+$	$1,4\text{-}C_6H_4F_2^+$	430
$C_6H_4F_2O^+$	$2,5\text{-}F_2C_6H_3OH^+$	444
$C_6H_4F_2O^+$	$3,5\text{-}F_2C_6H_3OH^+$	444

Formula	*Structure/Name*	*Page*	*Formula*	*Structure/Name*	*Page*
ClH_3Si^+	SiH_3Cl^+	240	Cl_2SSi	Cl_2SiS	211
ClIO	OICl	116	$Cl_2S_2^+$	$S_2Cl_2^+$	224
$ClIO_2$	O_2ICl	226	Cl_2S_2	$SSCl_2$	226
ClKrNe	NeKrCl	122	Cl_2Se^+	$SeCl_2^+$	112
ClKrXe	KrXeCl	122	$Cl_2Se_2^+$	$Se_2Cl_2^+$	224
$ClKr_2$	Kr_2Cl	122	Cl_2Si^+	$SiCl_2^+$	92
$ClNO^+$	$ClNO^+$	93	Cl_2Si	$SiCl_2$	101
$ClNO_2^+$	$ClNO_2^+$	208	Cl_2Xe	$XeCl_2$	121
$ClNO_2$	$ClNO_2$	212	Cl_2Zn^+	$ZnCl_2^+$	72
$ClNO_2$	ClONO	213	Cl_3^-	Cl_3^-	119
$ClNO_2$	OClNO	213	Cl_3FS	SCl_3F	304
$ClNO_3$	$ClONO_2$	288	Cl_3FSi^+	$SiFCl_3^+$	296
$ClNO_5$	O_2ClONO_2	371	$Cl_3F_2Si^-$	$SiF_2Cl_3^-$	357
$ClNS^+$	$NSCl^+$	95	Cl_3Ge	$GeCl_3$	219
ClN_3^+	ClN_3^+	196	Cl_3HOSi	$SiCl_3OH$	342
ClOP	ClPO	103	Cl_3HSi^+	$HSiCl_3^+$	276
ClO_2^+	$OClO^+$	106	Cl_3N^+	NCl_3^+	219
ClO_2	OClO	113	Cl_3NO_3Si	$SiCl_3ONO_2$	382
ClO_2	ClOO	110	Cl_3NO_4Si	$SiCl_3OONO_2$	426
ClO_2^-	$OClO^-$	115	Cl_3OP^+	Cl_3PO^+	298
ClO_2P	PO_2Cl	213	Cl_3O_2P	$OPCl_2OCl$	355
ClPS	ClPS	104	Cl_3P^+	PCl_3^+	220
ClS_2	SSCl	111	Cl_3PS^+	Cl_3PS^+	299
$ClXe_2$	Xe_2Cl	122	Cl_3Sb^+	$SbCl_3^+$	222
Cl_2F	ClClF	116	Cl_3Si^+	$SiCl_3^+$	211
Cl_2F^-	$ClFCl^-$	118	Cl_3Si	$SiCl_3$	218
Cl_2F^-	$FClCl^-$	118	Cl_4FSi^-	$SiFCl_4^-$	358
Cl_2F_2	Cl_2F_2	227	Cl_4Ge^+	$GeCl_4^+$	297
Cl_2F_2S	SCl_2F_2	304	Cl_4Si^+	$SiCl_4^+$	296
$Cl_2F_2Si^+$	$SiF_2Cl_2^+$	295	Cl_4SiO	$SiCl_3OCl$	356
$Cl_2F_3Si^-$	$SiF_3Cl_2^-$	357	Cl_5P^+	PCl_5^+	357
Cl_2Ga	$GaCl_2$	90	CoH_2	CoH_2	15
Cl_2GaH	$HGaCl_2$	169	CoH_2^-	CoH_2^-	17
Cl_2Ge^+	$GeCl_2^+$	92	CoH_2O	HCoOH	136
Cl_2Ge	$GeCl_2$	102	CrH_2	CrH_2	15
$Cl_2GeH_2^+$	$GeH_2Cl_2^+$	263	CrH_2O	HCrOH	136
Cl_2GeS	Cl_2GeS	211	CrH_3	CrH_3	123
Cl_2H^-	$ClHCl^-$	54	CrH_3O_2	$HCr(OH)_2$	316
Cl_2HN^+	$HNCl_2^+$	179	Cr_2H	CrCrH	26
$Cl_2H_2Si^+$	$SiH_2Cl_2^+$	262	Cr_2H^-	$CrCrH^-$	26
Cl_2Mn^+	$MnCl_2^+$	73	CuHO	CuOH	31
Cl_2N	NCl_2	108	CuH_2N	$CuNH_2$	133
Cl_2Ni^+	$NiCl_2^+$	73	CuH_2O	HCuOH	137
Cl_2O^+	Cl_2O^+	111	CuH_3N	$HCuNH_2$	232
Cl_2O	ClClO	116	Cu_2H_2	Cu_2H_2	131
Cl_2OP	$OPCl_2$	220	Cu_3	Cu_3	59
Cl_2OS^+	Cl_2SO^+	223	Cu_3H_2	Cu_3H_2	244
Cl_2OSi	Cl_2SiO	211	DOSc	ScOD	30
Cl_2O_2	ClOOCl	225	FFeH	HFeF	35
Cl_2O_2	$ClClO_2$	225	FFe_2H	HFe_2F	155
$Cl_2O_2S^+$	$Cl_2SO_2^+$	301	FGaO	OGaF	85
Cl_2O_2Si	*cyc*–Cl_2SiO_2	287	$FGeH_3^+$	GeH_3F^+	241
Cl_2O_3	Cl_2O_3	302	FHI^-	FHI^-	54
Cl_2O_4	$ClOClO_3$	355	FHN	HNF	48
Cl_2O_6	$O_3ClOClO_2$	382	FHO^+	HOF^+	51
Cl_2P	PCl_2	108	FHO	HOF	51
Cl_2S^+	SCl_2^+	112	FHSi	HSiF	43

Formula	*Structure/Name*	*Page*	*Formula*	*Structure/Name*	*Page*
GeH_2O_3	H_2GeO_3	338	HO_3P	$HOPO_2$	273
GeH_3^+	GeH_3^+	125	HO_3P	HOOPO	273
GeH_3	GeH_3	128	HO_3P	$HP(O_2)O$	273
GeH_3I^+	GeH_3I^+	242	HO_3S	$HOSO_2$	277
GeH_4^+	GeH_4^+	228	HO_3Sb	$HSbO_3$	274
GeH_4O	GeH_3OH	311	HO_3Sb	$HOSbO_2$	274
GeH_4S^+	GeH_3SH^+	311	HSSr	SrSH	29
GeI_2^+	GeI_2^+	92	HS_2	HS_2	50
GeOS	OGeS	86	HS_2^-	HS_2^-	53
GeO_2	GeO_2	86	HXe_2^+	HXe_2^+	56
GeS_2	GeS_2	86	HXe_2	Xe_2H	57
Ge_2H_2O	HGe_2OH	256	H_2Hg	HgH_2	16
Ge_2O_2	Ge_2O_2	188	$H_2I_2Si^+$	$SiH_2I_2^+$	263
Ge_3O_3	$(GeO)_3$	346	H_2InO	HInOH	139
HIO	HOI	52	H_2Mg	MgH_2	14
HISi	HSiI	44	H_2MgO	HMgOH	134
HI_2^-	IHI^-	55	H_2Mg_2O	HMgOMgH	246
HInO	InOH	37	H_2Mg_2O	HMg_2OH	246
HKO^+	KOH^+	27	H_2Mn	MnH_2	15
HKrXe	KrXeH	57	H_2Mn^-	MnH_2^-	17
HKr_2^+	HKr_2^+	56	H_2MnO	HMnOH	136
HKr_2	Kr_2H	57	H_2Mn_2O	HMn_2OH	247
HLi_2	Li_2H	26	H_2Mn_2O	HMnOMnH	247
HMgO	MgOH	27	H_2Mo	MoH_2	16
HNO^+	HNO^+	41	H_2N^+	NH_2^+	20
HNO	HNO	45	H_2N	NH_2	21
HNO^-	HNO^-	48	H_2N^-	NH_2^-	26
$HNOS^+$	$HNSO^+$	169	H_2NO^+	H_2NO^+	148
HNOS	*t*–HONS	174	H_2NO	H_2NO	151
HNOS	*t*–HSNO	174	H_2NSr	$SrNH_2$	133
HNOS	*c*–HSNO	174	$H_2N_2^+$	t–$N_2H_2^+$	142
HNOS	*c*–HNSO	175	H_2N_2	t–N_2H_2	147
HNOS	*t*–HNSO	175	H_2N_2	H_2NN	148
HNOS	*c*–HOSN	176	H_2N_2O	NH_2NO	260
HNO_2	*t*–HONO	172	$H_2N_2O_2$	NH_2NO_2	337
HNO_2	*c*–HONO	173	H_2Ni	NiH_2	16
HNO_3^+	HNO_3^+	270	H_2Ni^-	NiH_2^-	17
HNO_3	$HONO_2$	271	H_2NiO	HNiOH	136
HNO_3	HOONO	272	H_2NiO_2	$Ni(OH)_2$	252
HNO_4	$HOONO_2$	341	H_2Ni_2O	HNi_2OH	248
HNSi	HNSi	38	H_2O^+	H_2O^+	24
HNY	YNH	27	H_2OS	HSOH	154
HN_2^+	HN_2^+	39	H_2OSc	HScOH	135
HN_2O^+	$HONN^+$	165	H_2OSi	HSiOH	146
HN_3^+	HN_3^+	161	H_2OSi	H_2SiO	145
$HNaO^+$	$NaOH^+$	27	H_2OSn	HSnOH	146
HNiO	NiOH	30	H_2OSn_2	HSn_2OH	257
HOP	HPO	46	H_2OSr	HSrOH	134
HOS	HSO	50	H_2OTi	HTiOH	135
$HOSi^+$	$HOSi^+$	39	H_2OV	HVOH	135
HOSr	SrOH	29	$H_2O_2^+$	$HOOH^+$	152
HOXe	XeOH	53	H_2O_2	HOOH	153
HOZn	ZnOH	31	H_2O_2S	HSO_2H	265
HO_2^+	HO_2^+	47	H_2O_2Si	HSiOOH	260
HO_2	HO_2	49	H_2O_3Si	H_2SiO_3	338
HO_2^-	HO_2^-	51	H_2OP	H_2PO	151
HO_2P	*c*–HOPO	174	H_2OP	HPOH	151

8. Acknowledgment

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