Vibrational and Electronic Energy Levels of Polyatomic Transient Molecules. Supplement 1

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New information on the experimentally determined vibrational and electronic energy levels of approximately 500 neutral and ionic transient molecules possessing from 3 to 16 atoms has been evaluated and added to the previously established database for these species. There has been selective extension of the compilation to somewhat less reactive species such as HNCO, HCNO, H_2O_2, and *cis*- and *trans*-HONO, as well as to many transient molecules which include atoms beyond the third row of the Periodic Table. Electronic spectral data are also given for a number of transient molecules which possess more than six atoms. 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 spectra; 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.

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1. Introduction

Most chemical processes—including those which occur in flames, propellant systems, the initiation of energetic materials, atmospheric pollution, chemical vapor deposition, and microcircuit etching—consist of a complicated sequence of interrelated reactions in which neutral and charged molecular fragments play essential roles. Because of their high chemical reactivity, the detection of these reaction intermediates and the determination of their molecular properties has provided a major scientific challenge, to which molecular spectroscopy has risen. In recent years, the application of sophisticated sampling and observation techniques has yielded a wealth of vibrational and electronic spectral data for these species.

For some years, the compilation of spectroscopic data for small polyatomic molecules (3–12 atoms) given by Herzberg[1] stood alone as an information source on the vibrational and electronic energy levels of these species. 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 3 to 16 atoms, appeared in 1984. A second compilation,[3] concerned with the electronic energy levels of approximately 500 transient molecules possessing from 3 to 6 atoms, was published in 1988. Vibrational fundamentals of 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 molecules common to these two sets of tables, there were significant revisions to the ground-state vibrational energy levels in the four-year period between the two compilations. These two sets of tables have provided the basis for a recently released software database for personal computers,[4] designed to supplement the published compilations by providing a capability for rapid searches by molecule or wavenumber.

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 compilation revises and extends the evaluated spectral database for transient molecules, in order to support further research.

2. Scope of Review

New and revised data for approximately 500 molecules are included in this compilation. There has been selective inclusion of data for somewhat less reactive molecules, including HNCO, HCNO, H_2O_2, and *cis*- and *trans*-HONO. These species are important in many chemical reaction mechanisms but are difficult to study in conventional systems because of the ease with which they decompose, rearrange, or polymerize. Reaction intermediates containing the heavier elements are also included. The subject matter of the two published databases has been merged; in this and future supplements all of the properties given in the published electronic spectral tables plus the approximate relative infrared absorption intensities given in the first vibrational data compilation will appear together. The evaluation of electronic energy levels has also been selectively extended to transient species which possess from 7 to 16 atoms.

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. However, tunable infrared laser absorption studies of individual vibrational bands have been far more frequent.

As in the two 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 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 these predominate—over a range of a few cm^{-1}. 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%. A similar comparison is shown in Fig. 1 for the ground-state vibrational fundamentals of both neutral and charged transient molecules in the gas phase and in neon and argon matrices. Many of the available neon-matrix data are for molecular cations, with a heavy representation of halogen-substituted benzene cations. For these species, as well as for uncharged molecules, 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%. Many more data are available for the argon-matrix comparison. Again, there is almost an equal probability of a negative or positive shift from the gas-phase band origin, and matrix shifts greater than 1% occur for only about 10% of the frequencies available for the comparison.

Many other matrix materials have 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 solution 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 reaction intermediates has a relatively 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 found 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 development of probes for chemical reaction intermediates in the environment, the laboratory, and industrial processes. 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.

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.[7] As for 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.[3,5,7]

Contrary to earlier expectation, it has been found that 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.[8] In a neon matrix, such a correction typically decreases the radiative lifetime by about 15%. For relatively large 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 two 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.

The earlier electronic spectral data compilation[3] contained spectral data for many molecular cations derived from observations of the photoelectron spectrum of the corresponding neutral molecule. Most of these studies were conducted at low to moderate resolution, and uncertainties amounting to more than 100 cm^{-1} are common. There have been comparatively few more recent ultraviolet photoelectron studies of small molecules; most of the photoelectron data given in this supplement have been carried over from the earlier compilation, in which a more detailed discussion is given.

4. Guide to the Compilation

The goals of this compilation are to bring up to date the earlier evaluations of spectroscopic data for small polyatomic transient molecules and to provide a selective extension of these evaluations to other important, comparatively unstable simple molecules and to transient species which contain heavier atoms. The literature has been surveyed through February 1990; only limited addition of more recent data has been possible. Unfortunately, it is not possible to include data for stable molecules. However, the spectra of many of these species are relatively well established, and sources of data such as the tables of Herzberg[1] remain extremely useful. In using the present compilation and its two earlier companions[2,3] for spectral identifications, it is crucial that the literature on the spectra of stable molecules also be consulted.

Considerable effort has been given to providing a critical evaluation of the data. However, for many species the number of reports is meager. The identity of some species has been proposed on the basis of chemical evidence. While this 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.

This compilation is designed as a supplement to the earlier vibrational and electronic spectral data compilations[2,3]; it is not feasible to repeat all of the data previously given. The convention has been adopted that all of the data for an electronic state *for which new information is available* are shown. Therefore, the earlier compilations may give data for electronic states which are not shown in this supplement. Only the new references are

given. If the list of references starts with a number greater than 1, data for the molecule are also included in an earlier compilation, which should be consulted. A Master Index is included in this compilation in order to aid in finding these earlier data. The first electronic spectral compilation,[3] designated in the following discussion and in the Master Index by *E*, provided a revision of the ground-state vibrational data given in the initial vibrational energy level compilation,[2] hereafter designated by *V*, for the subset of species with from 3 to 6 atoms for which excited electronic energy levels have been identified. Therefore, if data for a molecule are present in both *V* and *E*, only *E* need be consulted. For some molecules, the reference number starts with 1 in this supplement even though data are present in *V* and/or *E*. This may occur if an early reference was inadvertently omitted from the earlier tables, necessitating renumbering of later references, if data have been removed by revision of an assignment, or if so few data are available for the species that it is decided that the record for it should not be fragmented. Whenever the reference number for a molecule starts with 1 in this compilation, the spectral data given for that molecule are complete.

While every effort has been made to make these compilations as complete as possible, for various reasons omissions do occur. The extension of the evaluation to heavier-atom species and the addition of electronic spectral data for larger molecules has necessitated selection of the species to be included. It is planned to support this database, with further selective extension, by periodic supplements. Data from the earlier tables may have been omitted from this supplement because later 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 date 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 heavy 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. As in *V* and *E*, 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., N before O) are used. Halogen-substituted species are placed immediately after related hydrides. Data for substituted acetylene and benzene cations, which were placed in special groupings in the earlier vibrational tables, are merged with data for other species of similar size (e.g., eight-atom molecules, large molecules) in this compilation. As before, data are given for both the normal and the fully deuterium-substituted molecule. However, only the hydrogen-containing species is listed in the Master 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 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,[9] has been adopted. Often this has required the interchange of published assignments of energy levels with B_1 and B_2 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 either from the photoelectron studies or from other photoionization measurements, 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. Because of inherent uncertainties in the determination of higher ionization potentials in many photoelectron measurements, photoelectron data 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 vibrational frequency (e.g., 1234.56(78) ≡ 1234.56 ± 0.78). Where the error includes a decimal point, the decimal point has been included. 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 of studies using cooled molecular beams. Often these latter studies give T_0 values 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 measurements. 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 two 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[10] 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 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 $\Delta G(\frac{1}{2})$, the separation between the $v = 0$ and $v = 1$ levels for the vibration of interest, have been used. For some systems, vibrational frequencies have been determined with a precision greater than two decimal places, and 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. It is not feasible to give these intensities for various techniques. However, the relative intensities *of ground-state infrared absorptions*, omitted from the electronic data tables, have been restored in this supplement. Abbreviations used for these 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 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 electronic band systems observed with moderately 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. The references to the experimental literature should facilitate the location of such data.

5. Abbreviations

Many sophisticated laser techniques—frequently employing two or more laser beams—have been used for studies of transient molecules. Often the developers of these 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 symbols 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 ob-

servation. The type of laser used for the absorption measurement in a detection scheme employing velocity modulation is instead specified in these tables.)

AB	—	near infrared-visible-ultraviolet absorption
CC	—	color-center laser absorption
CL	—	chemiluminescence
DL	—	diode laser absorption
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
IR	—	infrared absorption (conventional or Fourier transform)
LD	—	laser difference frequency absorption
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 absorption
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 scattering
SEP	—	stimulated emission pumping
TPE	—	threshold photoelectron spectroscopy
UV	—	near infrared-visible-ultraviolet absorption and emission

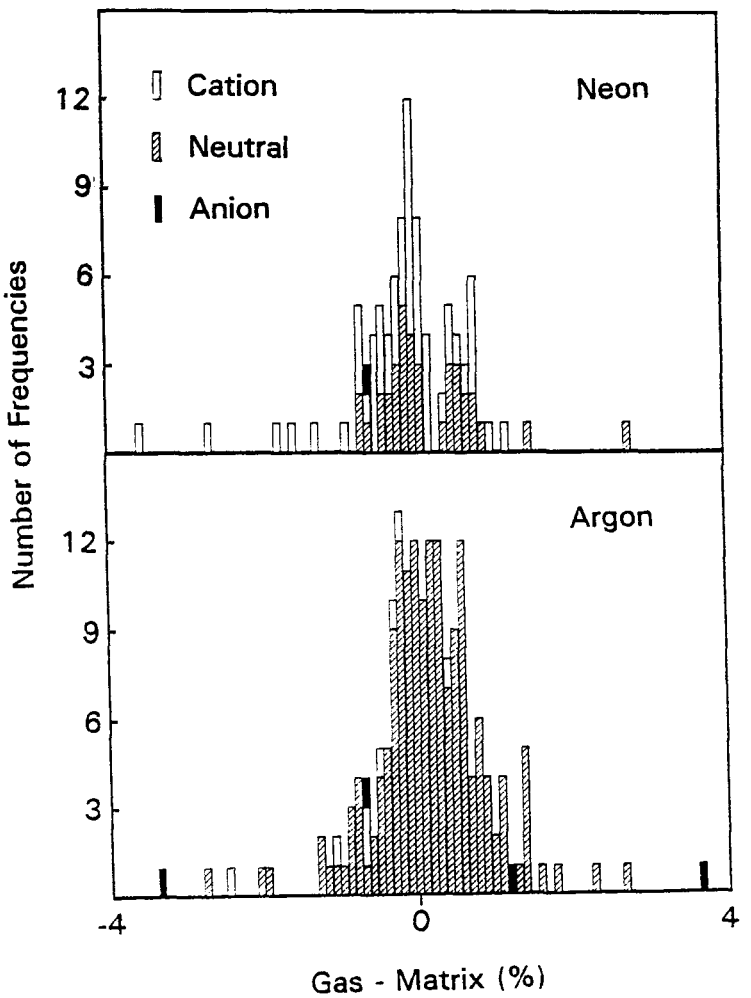

FIG. 1. Comparison of ground-state vibrational frequencies reported for transient molecules (2–16 atoms) in neon and argon matrices with corresponding values obtained from gas-phase measurements.
Beyond scale of neon-matric plot: XeF −7.8%
Beyond scale of argon-matrix plot: $C_6H_6^+(\nu_{17})$ −9.4%; (ν_{18}) −5.6%

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	gas	IR,PI	11,13,14
e'	2	Deformation	2521.31	gas	LD,IR	1,4,16

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

H_2D^+

$\tilde{X}$

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^+

$\tilde{X}$

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^+

$\tilde{X}$

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

B_0 = 21.824; C_0 = 10.510 DL[10]

[a] *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]

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

T_0[a] = 18511	gas	EM[8]	$3d\text{-}2p^2A_2''$	568–615 nm
		EM[8]	$3d\text{-}3p^2E'$	3891–4456 cm^{-1}
B_0 = 42.99;	C_0 = 22.735	EM[8]		

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

T_0[a] = 18409	gas	EM[8]PF[14]	$3d\text{-}2p^2A_2''$	568–615 nm
		EM[8]	$3d\text{-}3p^2E'$	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]	$3d\text{-}2p^2A_2''$	568–615 nm
		EM[8]	$3d\text{-}3p^2E'$	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]	$3p^2A_2''\text{-}2s^2A_1'$	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]	$3s^2A_1'\text{-}2p^2A_2''$	592–615 nm
		EM[6]	$3s^2A_1'\text{-}3p^2E'$	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]	$3s^2A_1'$-$3^2E'$	3178–3847 cm^{-1}
		EM[8]	$3d$-$3^2E'$	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]

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

	gas	EM[2,3]	$3p^2A_2''$-$2s^2A_1'$	556–574 nm
		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}

$\tau \sim 4$ ns gas EM[20]

3p $^2B_1$ C_{2v}

τ = 29(3) ns gas EM[20]

3p $^2A_1$,$^2B_2$

τ = 2.5(+0.3, −0.7) ns gas EM[21]

D_2H

3s $^2A_1$ C_{2v}

$\tau \sim 5$ 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; $\tau_2 \sim$ 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.	Type meas.	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 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[a] = 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}
$\tau \sim 10$ 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	$\sim$2145[d]	gas	EM	21
e'	2	Deformation	$\sim$1750[d]	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.	Type meas.	Refs.
a_1'	1	Ring breathing	2457(10)	gas	EM	4,20,21
e'	2	Deformation	$\sim$1890	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+ 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]

[d]Tentative assignment.

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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^+	Asym. stretch		1153	Kr	IR	1
			1160	Xe	IR	1
			1144			

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CrH_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	CrH a-stretch	1591	Ar	IR	1

CrD_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	CrD a-stretch	1145	Ar	IR	1

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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

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CH_2

$\tilde{b}\ ^1B_1$ [b] C_{2v} Structure: $AB^{3,29}$

$T_0 = 10255(20)$ gas $AB^{1,3,27}LMR^{21}LF^{33}$ $\tilde{b}$–$\tilde{a}$ 490–920 nm

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

$\tau = 1.90(15)$ μs LF^8
$\tau(0,14,0) = 4.2(2)$ μs LF^9
$\tau(0,16,0) = 1.3(3)$ μs LF^{11}
$B_0 = 7.74$ 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]SEP[32]
$\tilde{b}$–$\tilde{a}$ 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 IR	10,20,31
	2	Bend	1352.6	gas	AB	3,27,28
b_2	3	CH a-stretch	2864.97(2)	gas	LD,IR	20,31

$\tau \sim 18$ s[c]
A_0 = 20.118(2); B_0 = 11.205(2); C_0 = 7.069(2) AB[3,27,28]
Barrier to linearity = 9750 [29]

$\tilde{X}\ ^3B_1$ 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, DL	12,16 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]

[a]Value given for $^{13}CH_2$.
[b]The $\tilde{a}\ ^1A_1$ 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 $X\ ^3B_1$ state.[27,28]
[c]Calculated value.[21]
[d]From analysis of perturbations involving combination bands.[31]

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SiH_2

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

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

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

[e] In Fermi resonance with $2\nu_2$, observed for SiH_2 at 1993 cm^{-1} and for SiD_2 at 1445 cm^{-1}.

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NH_2^+

$\tilde{X}\ ^3B_1$ 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	3359.93	gas	LD	3

B_0 = 8.273; C_0 = 7.644 LD[3]

References

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PH_2^+

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

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

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

References

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NH_2

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

T_0 = 11122.6 gas AB[1,8,22]LF[6,21] $\tilde{A}$–$\tilde{X}$ 430–2700 nm
Ar,Kr,Xe[b] AB[2,3,5] $\tilde{A}$–$\tilde{X}$ 344–790 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]
$\tau_{080\Pi}$ = 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 ~100 μs component associatedwith 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 LD	6,15 16,21
			3220w[c]	N_2	IR	5
	2	Bend	1497.32	gas	UV,LF LMR,IR	1,6,8–10 13,20
			1499m	N_2	IR	5
b_2	3	Asym. stretch	3301.11	gas	LD,LF	16,21

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

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

[b]Origin not observed. A detailed comparison of the argon-matrix data of Ref. 2 with gas-phase data has been given in Ref. 22. 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]

References

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SbH_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^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	3213.0	gas	PE,LD	9,11,13
	2	Bend	1408.42	gas	EM,PE	1,5,9
					DL	12
b_2	3	Asym. stretch	3259.03	gas	LD	11

A_0 = 29.037(3); B_0 = 12.417(2); C_0 = 8.468 $LMR^8LD^{11}DL^{12}$
Barrier to linearity = 9187[7]

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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 $CC^{4,5}$

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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

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H_2Cl^+

$\tilde{X}$ 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

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

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6.2. Triatomic Monohydrides

BeOH

gas EM[1] 300–332 nm

A complicated pattern of red-degraded emission bands observed in this spectral region in discharges through a controlled pressure of H_2O or D_2O using beryllium electrodes has been attributed[1] to BeOH and BeOD, respectively.

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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

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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

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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

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

HCC

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

$T_0 < 3800$ Ar AB[21]

In an argon matrix, a complicated absorption band system of HC_2 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] 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 ~5 μs near 500 nm to ~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

$A = \sim 10$ IR[14]
$B_{000} = 1.457$ MW[4,6,7,9] LMR[12]
$B_{020} = 1.451$ LMR[28]

DCC

$\tilde{A}\,^2\Pi$

$T_0 < 3800$ Ar AB[21]

A complicated absorption band system extends to approximately 7500 in argon-matrix studies of DC_2.[21] As for HC_2, 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 color-center laser absorption.[22,29]

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

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

$B_0 = 1.203$ MW[16]

[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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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

References

[1]J. W. Kauffman, R. H. Hauge, and J. L. Margrave, High Temp. Sci. **17**, 237 (1984).

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

References

[1]S. F. Parker, C. H. F. Peden, P. H. Barrett, and R. G. Pearson, J. Am. Chem. Soc. **106**, 1304 (1984).

HFeBr

$\tilde{X}$

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

References

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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
			754m	Ar	IR	1
Σ^+	3	BO stretch	1825.56	gas	DL	2
			1817s	Ar	IR	1

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

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
			2259w	Ar	IR	1
Π	2	Bend	606m	Ar	IR	1
Σ^+	3	BO stretch	1647.69	gas	DL	5
			1648m	Ar	IR	1

B_0 = 1.049 gas MW^4

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[6]J. E. Butler, unpublished data.

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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[1]K. Kawaguchi and E. Hirota, Chem. Phys. Lett. **123**, 1 (1986).
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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

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[1]K. M. Ervin and W. C. Lineberger, J. Phys. Chem. (in press).

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,IB	5,6,15
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 $MW^{1,2}DL^3CC^{4,5}$

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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,IB IR	5,11,12
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

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

T_0 = 38695.5	gas	EM[6]LF[25,26]	$\tilde{B}$–$\tilde{X}$ 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	2589[a]	gas	EM,LF	6,25,26
			2570(30)	Ar	AB	5,11
			2570(30)	CO	AB	5
	2		~1375	gas	LF	25,26
			1375(35)	Ar	AB	5,11
			1375(35)	CO	AB	5
	3		1058	gas	LF	25,26
			1035(35)	Ar	AB	5,11
			1035(35)	CO	AB	5

A_0 = 15.87; B_0 = 1.192; C_0 = 1.107 LF[26]
τ_0 ~ 50 ns gas LF[26]

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

T_0 = 9297(3) gas AB[1,3,8]LF[24] $\tilde{A}$–$\tilde{X}$ 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	UV	1,3,8
	2	Bend	805	gas	UV	1,3,8
	3	CO stretch	1812.2	gas	UV	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
					IR	23
			2483m	Ar	IR	5
			2488m	CO	IR	4
	2	Bend	1080.76	gas	UV	1,3,8
					LS,LMR	9,10
					LF	25
			1087s	Ar	IR	5
			1090s	CO	IR	2,4
	3	CO stretch	1868.17	gas	IR	12,23
					LMR,LF	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

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

T_0 = 9162(3) gas UV[1,3,8]LF[24] $\tilde{A}$–$\tilde{X}$ 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]

[a]The $\tilde{B}(100) - \tilde{X}(000)$ band was previously assigned[6,11] as the origin of the $\tilde{C}$ state. However, the studies of Ref. 25 and 26 have determined that its band contour is identical to that of the origin of the $\tilde{B}\,^2A'$ state.

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HCF

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

T_0 = 17277.47	gas	AB[1]CL[3]LF[5,10]	$\tilde{A}$–$\tilde{X}$ 430–635 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[1]LF[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 < 5140(700) gas PE[12]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	1170(50)	gas	PE	12
	3	CF stretch	1170(50)	gas	PE	12

$\tilde{X}\,^1A'$ C_s Structure: AB[1]LF[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	1180(30)	gas	PE	12
			1181.5m	Ar	IR	2

A_0 = 15.563; B_0 = 1.223; C_0 = 1.130 AB[1]LF[5]SEP[11]

DCF

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

T_0 = 17293.426(3) gas CL[3]LF[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	820(50)	gas	PE	12
	3	CF stretch	1170(50)	gas	PE	12

$\tilde{X}\ ^1A'$ 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	1190(30)	gas	PE	12
			1183m	Ar	IR	2

$A_0 = 8.828$; $B_0 = 1.120$; $C_0 = 0.990$ LF[6]

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HCCl

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

$T_0 < 3990(1050)$ gas PE[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CCl stretch	870(70)	gas	PE	5

$\tilde{X}\ ^1A'$ 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(30)	gas	PE	5
			815s	Ar	IR	2

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

References

[5]K. K. Murray, D. G. Leopold, T. M. Miller, and W. C. Lineberger, J. Chem. Phys. **89**, 5442 (1988).

HCBr

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

$T_0 < 3150(700)$ gas PE[1]

$X\ ^1A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CBr stretch	660(40)	gas	PE	1

References

[1]K. K. Murray, D. G. Leopold, T. M. Miller, and W. C. Lineberger, J. Chem. Phys. **89**, 5442 (1988).

HCl

$\tilde{a}$ C_s

$T_0 < 3150(700)$ gas PE[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	Cl stretch	600(40)	gas	PE	1

References

[1]K. K. Murray, D. G. Leopold, T. M. Miller, and W. C. Lineberger, J. Chem. Phys. **89**, 5442 (1988).

HNO

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

$T_0 =$ 13154.4 gas $AB^{1,4}LF^{13,20}$ $\tilde{A}$–$\tilde{X}$ 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

$\tau = 25(4)$ μs LF[12,14,22]
$A_0 = 22.156$; $B_0 = 1.325$; $C_0 = 1.242$ $AB^{1,4}$MODR[11,17]

DNO

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

$T_0 = 13180.3$ gas AB^1 $\tilde{A}$–$\tilde{X}$ 550–770 nm
Onset of predissociation at 17010(10) LF[18,19]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	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

$\tau_{011} = 32.4(1.6)$ μs gas LF[22]
$A_0 = 12.630$; $B_0 = 1.199$; $C_0 = 1.088$ $AB^{1,4}$

References

[22]S. Mayama, K. Egashira, and K. Obi, Res. Chem. Intermed. **12**, 285 (1989).

HCF^-

Threshold for electron detachment from ground-state HCF^- = 4490(40) gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CF stretch	745(30)	gas	PE	1

DCF^-

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CF stretch	730(30)	gas	PE	1

References

[1]K. K. Murray, D. G. Leopold, T. M. Miller, and W. C. Lineberger, J. Chem. Phys. **89**, 5442 (1988).

$HCCl^-$

Threshold for electron detachment from ground-state $HCCl^-$ = 9790(40) gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CCl stretch	470(30)	gas	PE	1

References

[1]K. K. Murray, D. G. Leopold, T. M. Miller, and W. C. Lineberger, J. Chem. Phys. **89**, 5442 (1988).

$HCBr^-$

Threshold for electron detachment from ground-state $HCBr^-$ = 12550(65) gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CBr stretch	430(40)	gas	PE	1

References

[1]K. K. Murray, D. G. Leopold, T. M. Miller, and W. C. Lineberger, J. Chem. Phys. **89**, 5442 (1988).

HCl^-

Threshold for electron detachment from ground-state HCl^- = 13580(100) gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	Cl stretch	350(40)	gas	PE	1

References

[1]K. K. Murray, D. G. Leopold, T. M. Miller, and W. C. Lineberger, J. Chem. Phys. **89**, 5442 (1988).

HNO^-

Threshold for electron detachment from ground-state HNO^- = 2730(120) gas PE[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH stretch	2750.78	gas	PD	2
	3	NO stretch	1153(170)	gas	PE	1

A_0 = 15.233; $(B_0 + C_0)/2$ = 1.097; $(B_0 - C_0)/2$ = 0.034 PD[2]

DNO^-

Threshold for electron detachment from ground-state DNO^- = 2660(120) gas PE[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	NO stretch	1113(170)	gas	PE	1

References

[1]H. B. Ellis, Jr., and G. B. Ellison, J. Chem. Phys. **78**, 6541 (1983).
[2]H. C. Miller, J. L. Hardwick, and J. W. Farley, J. Mol. Spectrosc. **134**, 329 (1989).

HO_2

$\tilde{X}\,^2A''$ C_s Structure: MW[14]UV[21]LMR[23]ESR[23] IR[31,33]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	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	24
			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
					DL	29,30
			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

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	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.

References

[36]W. E. Thompson and M. E. Jacox, J. Chem. Phys. **91**, 3826 (1989).

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

$\tau^a = 76\ \mu s$ gas LF[6]
$A_0^b = 4.969(7)$; $B_0^b = 0.566$; $C_0^b = 0.507$ LF[7,8]

[a]Measured at 606.0 nm.
[b]Extrapolated from values for 021 and 022.

References

[8]Y. Takehisa and N. Ohashi, J. Mol. Spectrosc. **130**, 221 (1988).

HOI

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3597m	N_2	IR	1
	2	Bend	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.	Type meas.	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).

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.	Type meas.	Refs.
a'	3	SS stretch	610(80)	gas	PE	1

DS_2^-

Threshold for electron detachment from ground-state DS_2^- = 15430(120) gas PE[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	SS stretch	580(90)	gas	PE	1

References

[1]S. Moran and G. B. Ellison, J. Phys. Chem. **92**, 1794 (1988).

FHF^-

$\tilde{X}$ $D_{\infty h}$ Structure: DL[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	583.05	gas	DL	5
Π_u	2	Bend	1286.03	gas	DL	5
			1217m	Ar[a]	IR	1,2
Σ_u^+	3	Asym. stretch	1331.15	gas	DL	5
			1379	Ne	IR	4
			1377.0s	Ar	IR	3,4
			1364vs	Ar[a]	IR	1,2

$B_0 = 0.334$ DL[5]

FDF$^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend 880m	Ar[a]	IR	1,2	
Σ_u^+	3	Asym. stretch	965s	Ar	IR	3,4
			969vs	Ar[a]	IR	1,2

[a]Cs^+ in adjacent site.

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).

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.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	260[ab]	Ar	IR	1-3
Σ_u^+	3	Asym. stretch	722.90	gas	DL	5
			696s[a]	Ar	IR	1-3

B_0 = 0.0974 DL[5]

ClDCl$^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	267[a]c	Ar	IR	1-3
Σ_u^+	3	Asym. stretch	463[a]	Ar	IR	1-3

[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]Assignment deduced from weak to moderately intense combination with 696 cm^{-1} fundamental that appears at 956 cm^{-1}.
[c]Assignment deduced from weak to moderately intense combination with 463 cm^{-1} fundamental that appears at 730 cm^{-1}.

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).
[4]M. Kneba and J. Wolfrum, J. Phys. Chem. **83**, 69 (1979).
[5]K. Kawaguchi, J. Chem. Phys. **88**, 4186 (1988).
[6]J. Hacaloglu and L. Andrews, Chem. Phys. Lett. **160**, 274 (1989).

6.3. Triatomic Nonhydrides

Li_3

$2^2E'$ D_{3h}[a]

T_0 = 14583 gas MPI[2] $2^2E'$–$\tilde{X}$ 660–690 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	326	gas	MPI	2

$\tilde{X}$ D_{3h}[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	303	Xe	Ra	1

[a]Subject to dynamic Jahn-Teller distortion. Structure in the $2^2E'$ state is characterized by a radial frequency ω_0 = 191 and linear and quadratic Jahn-Teller parameters k = 0.77 and g = 0.15. In the $\tilde{X}$ state, as well, a complicated pattern of absorptions accompanies the absorption attributed to ν_1.

References

[1]M. Moskovits and T. Mejean, Surf. Sci. **156**, 756 (1985).
[2]J.-P. Wolf, G. Delacrétaz, and L. Wöste, Phys. Rev. Lett. **63**, 1946 (1989).

Na_3

Evidence for a predissociated state near 420 nm was obtained from the depletion of the single-photon ionization signal of Na_3^+, with a corresponding increase in the Na_2^+ signal, as this region was scanned by a second laser.[4,5]

$\tilde{C}\ ^2E''$ D_{3h}[a]

T_0 = 20813 gas MPI[2,4,6,8]PF[8] $\tilde{C}$–$\tilde{X}$ 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]

$\tilde{B},\tilde{B}'\ ^2E'$ D_{3h}[a]

T_0 = 15996 gas MPI[1-6] $\tilde{B},\tilde{B}'$–$\tilde{X}$ 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]

$\tilde{A}\ ^2E''$ D_{3h}[a]

T_0 = 14896.5 gas MPI[1,2,4-6] $\tilde{A}$–$\tilde{X}$ 660–675 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	128.5	gas	MPI	4,6
	2	Bend	47	gas	MPI	4,6

τ_0 = 60(10) ns gas MPI[7]

$\tilde{X}\ ^2E'$ D_{3h}[a]

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]Distorted by Jahn-Teller interaction.

References

[7]M. Broyer, G. Delacrétaz, N. Guoquan, J. P. Wolf, and L. Wöste, Chem. Phys. Lett. **145**, 232 (1988).
[8]M. Broyer, G. Delacrétaz, G.-Q. Ni, R. L. Whetten, J.-P. Wolf, and L. Wöste, J. Chem. Phys. **90**, 843 (1989).
[9]M. Broyer, B. Delacrétaz, G.-Q. Ni, R. L. Whetten, J.-P. Wolf, and L. Wöste, J. Chem. Phys. **90**, 4620 (1989).
[10]M. Broyer, G. Delacrétaz, G.-Q. Ni, R. L. Whetten, J.-P. Wolf, and L. Wöste, Phys. Rev. Lett. **62**, 2100 (1989).

Ag_3

In argon, krypton, and xenon matrices, absorption bands near 40660, 43130, and 45020 have been attributed[2,3] to Ag_3.

$^2E''$ D_{3h}[a]

T_0 = 26971(10) gas MPI[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	158.2(1.9)	gas	MPI	4

Extensive vibronic structure has been assigned[4] to energy levels derived from excitation of ν_2 (e'), perturbed by dynamic Jahn-Teller interaction.

In argon, krypton, and xenon matrices, an absorption maximum near 23700 has been attributed[2,3] to Ag_3.

$\tilde{X}$[b]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	120.5(5)	Kr	Ra	1

[a]Distorted by Jahn-Teller interaction.
[b]Possibly the ground state of a linear isomer.

References

[1]W. Schulze, H. U. Becker, R. Minkwitz, and K. Manzel, Chem. Phys. Lett. **55**, 59 (1978).
[2]W. Schulze, H. U. Becker, and H. Abe, Chem. Phys. **35**, 177 (1978).
[3]G. A. Ozin, H. Huber, and S. A. Mitchell, Inorg. Chem. **18**, 2932 (1979).
[4]K. LaiHing, P. Y. Cheng, and M. A. Duncan, Z. Phys. D **13**, 161 (1989).

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	~150	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

[1]K. D. Bier, T. L. Haslett, A. D. Kirkwood, and M. Moskovits, J. Chem. Phys. **89**, 6 (1988).

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)[a]	gas	LF	3

[a]Tentative assignment.

References

[1]M. Moskovits and J. E. Hulse, J. Chem. Phys. **66**, 3988 (1977).
[2]M. Moskovits and D. P. DiLella, J. Chem. Phys. **72**, 2267 (1980).
[3]J. R. Woodward, S. H. Cobb, and J. L. Gole, J. Phys. Chem. **92**, 1404 (1988).
[4]K. M. Ervin, J. Ho, and W. C. Lineberger, J. Chem. Phys. **89**, 4514 (1988).

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_0^0 band.

References

[1]Z. Fu, G. W. Lemire, Y. M. Hamrick, S. Taylor, J.-C. Shui, and M. D. Morse, J. Chem. Phys. **88**, 3524 (1988).

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

References

[1]T. C. Devore, J. R. Woodward, and J. L. Gole, J. Phys. Chem. **92**, 6919 (1988).

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)[a]	Ar	AB	15
Σ_u^+	3	Asym. stretch	780(30)[ab]	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]

$\tilde{A}\ ^1\Pi_u$ $D_{\infty h}$ 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[c]	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[d]	gas	AB	6
Σ_u^+	3	Asym. stretch	~840[a]	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 $\tau \leqslant 10$ ns.
B_0 = 0.430 UV[6]

$\tilde{a}\ ^3\Pi_u$ $D_{\infty h}$

T_0 =	17080	Ne	EM[5]LF[11]	$\tilde{a}$–$\tilde{X}$ 585–631 nm
	16930	Ar	EM[5]	
τ ~ 0.02 s		Ne	EM[5]	

$\tilde{X}\ ^1\Sigma_g^+$ $D_{\infty h}$ Structure: UV[6]

This state of C_3 is highly anharmonic. The term values of 144 excited vibrational energy levels have been determined in SEP[21] and LF[23] studies.

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[e]	Ar	IR	19
			1234[c]	N_2	IR	19
Π_u	2	Bend	63.7[f]	gas	UV,DL	6,22,23
					SEP	24
			~70[g]	Ne,Ar	AB	5
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 = 0.430 UV[6]IR[16]DL[18]

[a] $\frac{1}{2}(2\nu_i)$.
[b] Alternate assignment gives 1320.
[c] In the LF studies,[11] a second site was observed with T_0 = 24408.
[d] 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.
[e] $(\nu_1 + \nu_3) - \nu_3$.
[f] ~45 in $X(011)$.[22]
[g] 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[5]AB[11]

T_0 =	20085.505	gas	EM[1]AB[3,11]LF[4]	$\tilde{A}$–$\tilde{X}$ 402–507 nm
	20142	Ne	AB[2]LF[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	1464	gas	EM,AB	1,3,4,
					LF	11
			1462	Ne	AB,LF	2,4
			1457	Ar	AB	9
	2	CSi s-stretch	979	gas	AB,LF	3,4
			1011	Ne	AB,LF	2,4
			1021	Ar	AB	9
b_2	3	CSi a-stretch	228[a]	gas	EM,AB	1,3,4,
					LF	11
			231[a]	Ne	AB,LF	2,4
			224[a]	Ar	AB	9

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[5]MW[6,7]AB[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CC stretch	1742	gas	EM	1
			1746s	Ne	IR,LF	2,4
			1741.3	Ar	IR	8,14
	2	CSi s-stretch	837	gas	EM	1,10
			836m	Ne	IR,LF	2,4
			824.3	Ar	IR	8,14
b_2	3	CSi a-stretch	177[a]	gas	LF	4
			186(11)	gas	MW	13
			172[a]	Ne	LF	4
			160.4	Ar	IR	14

$A_0 = 1.750$; $B_0 = 0.439$; $C_0 = 0.348$ MW[6,7,12,13]AB[11]

[a] $\frac{1}{2}(2\nu_3)$.

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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	658wm	Ar	IR	1
b_2	3	Asym. stretch	1189s	Ar	IR	1

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AlCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1872s	Ar	IR	1

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CCN

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

$T_0 =$ 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	~475	gas	AB	1
Σ^+	3	Stretch	1241.64	gas	AB	1
			1225(2)	Ar	LF	2

$\tau = 170$ 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
			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

$A = 41.76$; $\epsilon\omega_2 = 132.8$ gas LF^8
$B_0 = 0.398$ $AB^1LF^{4,6}$

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NCN

$\tilde{A}\ ^3\Pi_u$ $D_{\infty h}$ 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

$A = -37.56$; $\epsilon\omega_2 = -85.7$[b]	gas	AB^1
$\tau_0 = 183(6)$ ns	gas	LF^8
$B_0 = 0.396$ AB^1		

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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

$\tilde{B}\,^3\Sigma^-$? $C_{\infty v}$

$T_0 \leqslant$ 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^6LF^{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

τ_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	CN stretch	2824	Ar	LF	8
			2847m	Ar[c]	IR	3
			2856m	N_2	IR	3,4,7,12
Π	2	Bend	394	Ar	LF	8
			393	Ar[c]	IR	3
			394	N_2	IR	4,7
Σ^+	3	NN stretch	1235	Ne	EM	5
			1235	Ar	LF	8
			1241	Ar[c]	IR	3
			1252	N_2	IR	3,4,7

B_0 = 0.414(10)[b] LF^{11}

[a]Possibly 2440(40).[10]
[b]Approximate value, used in simulation.
[c]N_2 trapped in adjacent site.

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BO_2

$\tilde{A}\,^2\Pi_u$ $D_{\infty h}$ Structure: UV^1

T_0 = 18291.597	gas	$UV^1LF^{3-5,14}$		$\tilde{A}$–$\tilde{X}$ 396–700 nm
17915[c]	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	2357[b]	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^1LF^{14}
B_0 = 0.311 $UV^1LF^{13,14}$

$\tilde{X}\,^2\Pi_g$ $D_{\infty h}$ 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[d]	gas	UV,LF	1,3–5, 14
Σ_u^+	3	Asym. stretch	1278.26	gas	DL,IR	8,12
			1276	Ar	IR	2

$A = -148.6$; $\epsilon\omega_2 = -86.91$ gas $UV^1LF^{3,7,14}$
B_0 = 0.329 $UV^1LF^{3,7,13,14}DL^8IR^{12}$

[a]Estimated from isotopic shifts.
[b]$\frac{1}{2}(2\nu_2)$.
[c]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.
[d]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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NCO

$\tilde{A}\,^2\Sigma^+$ $C_{\infty v}$ Structure: UV[20]

T_0 = 22754.0	gas	AB[1]	$\tilde{A}$–$\tilde{X}$ 360–450 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	1272.97[b]	gas	LF,LMR	14,15 17,19
			1275vw	Ar	IR,LF	3,8
Π	2	Bend	535.4	gas	UV,LF	1,7,15
			529.5[c]	Ar	LF	8
Σ^+	3	Asym. stretch	1921.30	gas	LMR	10,14
					LF,DL	15,21
			1923m	Ar	IR,LF	3,8
			1935	N_2	IR	3

A_{010} = −94.19; $\epsilon\omega_2$ = −76.9 gas UV[7]
B_0 = 0.390 UV[1]MW[16]LMR[22]

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NCS

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

T_0 = 26971.01 gas EM[1]AB[2]LF[4] $\tilde{B}$–$\tilde{X}$ 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^2LF[4] $\tilde{A}$–$\tilde{X}$ 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[6]
A = −91.58(1); $|\epsilon\omega_2|$ = 103(5) gas AB^2LF[4]
B_0 = 0.193 AB^2LF[4]

$\tilde{X}\,^2\Pi$ $C_{\infty v}$ 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	387(10)	gas	AB,LF	2,4
Σ^+	3	CS Stretch	765.8	gas	SEP	5

A = −323.4; $|\epsilon\omega_2|$ = 55(15) gas AB^2LF[4]
B_0 = 0.206 AB^2LF[4]

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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 = 28500.5 gas EM[2,11] $\tilde{A}$–$\tilde{X}$ 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 = −95.86; $\epsilon\omega_2$ = −42.6 gas EM[11]
B_0 = 0.350 EM[2,11]

$\tilde{X}\ ^2\Pi_g$ $D_{\infty h}$ 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			
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)[b]	gas	PE	10
Σ^+	3	CS stretch	803.8[c]	gas	PF	9

τ_0 = 93(9) ns[d] gas PEFCO[5]
τ_0 (Ω = 3/2) = 105(3) ns; τ_0 (Ω = 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[e]	gas	PF	9
Π	2	Bend	476(16)	gas	PE	10
Σ^+	3	CO stretch	2038.98[f]	gas	DL	11

A = −367.2 gas EF[1]PF[9]
B_0[f] = 0.201 DL[11]

[a]Ref. 10 gives value of 742(7).
[b]$\frac{1}{2}(2\nu_2)$.
[c]816.9 for Ω = 1/2.[9]
[d]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.
[e]699.7 for Ω = 1/2.[9]
[f]Measured for Ω = 1/2.

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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,MP	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)[c]	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]	gas	EM	3
			621	Ne	LF	6,7
Π_u	2	Bend	~275[c]	gas	EM	3
			280[c]	Ne	LF	6,7
Σ_u^+	3	Asym. stretch	1644[c]	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	3
			618[a]	Ne	LF	6,7
Π_u	2	Bend	348[c]	gas	EM	3
			349[c]	Ne	LF	6,7
Σ_u^+	3	Asym. stretch	1203[c]	gas	EM,PE	3,14
			1224[c]	Ne	LF	6,7

A = −440.39(3) gas EM[1,2]
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] $\frac{1}{2}(2\nu_i)$.

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ClCN$^+$

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

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]

$\tilde{X}\,^2\Pi_{3/2}$ $C_{\infty v}$ 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	376[a]	gas	LF	10
Σ^+	3	CCl stretch	827(2)	gas	EF,LF	8–10

B_0 = 0.205 LF[11]

[a]Tentative assignment.

References

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BrCN$^+$

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

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)[a]	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]

$\tilde{X}\ ^2\Pi_{3/2}$ $C_{\infty v}$ 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)[a]	gas	EF,LF	7,10
Σ^+	3	CBr stretch	649.4(5)	gas	EF,LF	7,10

$A = -1477(2)$ gas EF^3PIFCO^4
$B_0 = 0.142$ gas $LF^{10,11}$

[a] $\frac{1}{2}(2\nu_2)$.

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N_3

$\tilde{B}\ ^2\Sigma_u^+$ $D_{\infty h}$ Structure: AB^2

T_0[a] = 36738.750(2) gas $AB^{1,2}LF^3$ $\tilde{B}$–$\tilde{X}$ 260–273 nm

All bands above 37000 are diffuse.

An absorption maximum was observed at 272 nm in mixed argon-nitrogen matrix studies.[6]

$\tau \leqslant 20$ ns gas LF^3
$B_0 = 0.432$ 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	~1320	gas	LF	3
			1287[b]	N_2[c]	IR	4
Π_u	2	Bend	~457	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

References

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Sb_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	217.5(3)	Ar	Ra	1
			217.0(5)	Kr	Ra	1

References

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N_2O^+

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

$T_0 = 38440(100)$[a] gas PE^1PF^{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]	gas	PE	1

$\tilde{A}\ ^2\Sigma^+$ $C_{\infty v}$ Structure: EM^3PF^{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

$\tau = 230(10)$ ns gas $EF^{2,9}PIFCO^4PEFCO^7ID^8EM^{12}HFD^{13}$
$B_0 = 0.433$ $EM^{3,14}PF^{10,11}$

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$ 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
Π	2	Bend	452.42	gas	EM,PF	3,11,14
Σ^+	3	Asym. stretch	1737.6	gas	EM	3

$A = -132.434$; $\epsilon\omega_2 = -90.2$ gas $EM^{3,14}PF^{11,16}$
$B_0 = 0.412$ $EM^3PF^{10,11,16}$

[a]Calculated using first ionization potential of 12.886(2) eV, from Ref. 5.
[b]Somewhat irregular band spacings.

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NNS^+

$\tilde{B}\ ^2\Pi^a$ $C_{\infty v}$

$T_0 \sim 41500$ 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^+		N-S stretch	~500	gas	PE	1

$A \sim 400$ gas PE[1]

[a]Tentative assignment.

References

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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
II	2	Bend	502	Ne	IR	1
			493	Ar	IR	1

$B_0 = 0.312$ DL,MW[2]

References

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NCO^-

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

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).

NCS^-

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

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).

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

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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

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N_3^-

Threshold for electron detachment from ground-state N_3^- is 22270(350).[1]

$\tilde{X}\ ^1\Sigma_g^+$ $D_{\infty h}$ 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.

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PNO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med. meas.	Type	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

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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
			2030	Ar	IR	1

$B_0 = 0.216$ gas IR^2

References

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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.

Emission which is observed between 240 and 380 nm on excitation of BCl_3 by radiation of wavelength shorter than 118 nm has been attributed[4,5] to BCl_2, as has been a similar chemiluminescence emission observed[1,2] on reaction of H atoms with BCl_3.

Emission which is observed between 280 and 380 nm on excitation of BCl_3 by radiation of wavelength shorter than 124 nm has been attributed[4,5] to BCl_2.

Emission which is observed between 380 and 500 nm on excitation of BCl_3 by radiation of wavelength shorter than 138 nm has been attributed[4,5] to 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	966vs	Ar	IR	3

References

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$AlCl_2$

$\tilde{X}$ 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

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$GaCl_2$

$\tilde{X}$ 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

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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).

PO_2

$^2B_1$? C_{2v}

$T_0 = 30378(3)$ gas AB^1LF^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

$\tau \sim 500$ ns gas LF^3
$\tau_{cont} \sim 4.5$ μs gas LF^3

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

[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).
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$NSBr^+$

$\tilde{D}\ ^2A'$ 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).

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

$\tilde{A}\ ^1B_1$ C_{2v} Structure: AB[10]

T_0 = 37226 gas EM[1]AB[2,3,5,10] $\tilde{A}$–$\tilde{X}$ 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	4,6,16
					LF	17
			496(2)	N_2	LF	17

τ_0 = 61(3) ns gas LF[20,21,28]EM[32]
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[31] $\tilde{A}$–$\tilde{X}$ 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

$\tau \sim 1$ 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	23,30
					PE	31
			1220	Ne	IR,LF	12,17
			1222vs	Ar	IR,LF	6,11,17
	2	Bend	667	gas	UV,PE	1,10,31
			668vw	Ar	IR,LF	6,11,17
b_2	3	Asym. stretch	1114.44	gas	IR,DL	7,13
						27,30
			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 $\tilde{C}$ 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.

References

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CFCl

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

T_0 = 25283(5) gas LF[6,7] $\tilde{A}$–$\tilde{X}$ 359–390 nm
24983 Ar UV[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	1263	gas	LF	7
	2	Bend	394(3)	gas	LF	6
			392(1)	Ar	LF	3
	3	CCl stretch	726(6)	gas	LF	6,7
			712(2)	Ar	LF	3

τ_0 = 650(40) ns gas LF[4-6]EM[8]
330(20) ns Ar LF[3]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CF stretch	1158(10)	gas	LF	6,7
			1146vs	Ar	IR	1
	2	Bend	448(6)	gas	LF	6,7
			442	Ar	LF	2,3
	3	CCl stretch	750(6)	gas	LF	6,7
			742s	Ar	IR	1

References

[7]T.-X. Xiang, Chem. Phys. Lett. **147**, 183 (1988).
[8]T. Ibuki, A. Hiraya, and K. Shobatake, J. Chem. Phys. **90**, 6290 (1989).

CCl_2

$\tilde{A}\ ^1B_1$ C_{2v} Structure: LF[16]

T_0 = 16913(3) gas CL[8]LF[7,9,10,15,16]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	644	gas	LF	10,15
			624	Ar	LF	6
	2	Bend	308	gas	LF	9,10,15
			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_{020} = 3.745; B_{020} = 0.106; C_{020} = 0.103 LF[16]

$\tilde{X}\ ^1A_1$ C_{2v} Structure: MW[14]LF[16]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	730(40)	gas	PE	12
			721wm	Ar	IR,LF	1–3,5,6
	2	Bend	340(40)	gas	PE	12
			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]

References

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[3]M. E. Jacox and D. E. Milligan, J. Chem. Phys. **53**, 2688 (1970).
[4]J. S. Shirk, J. Chem. Phys. **55**, 3608 (1971).
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[12]K. K. Murray, D. G. Leopold, T. M. Miller, and W. C. Lineberger, J. Chem. Phys. **89**, 5442 (1988).
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[16]D. J. Clouthier and J. Karolczak, J. Phys. Chem. **93**, 7542 (1989).

CBr_2

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

T_0 = 14885 gas LF[5] $\tilde{A}$–$\tilde{X}$ 614–663 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	460	gas	LF	5
			468	Ar	LF	4
	2	Bend	189	gas	LF	5
			186	Ar	LF	4

τ = 14.5(1.5) μs Ar LF[4]

References

[5]S. K. Zhou, M. S. Zhan, J. L. Shi, and C. X. Wang, Chem. Phys. Lett. **166**, 547 (1990).

$SiCl_2$

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

T_0 = 30013.4(1.0) gas AB[4]EM[5]–7LF[8,10] $\tilde{A}$–$\tilde{X}$ 308–430 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	435(5)	gas	LF	8
	2	Bend	149.9(5)	gas	UV,LF	3,7,8

τ_{070} = 77(3) ns gas LF[8]
A_{060} = 0.909; B_{060} = 0.076; C_{060} = 0.069 LF[10]

$\tilde{X}\ ^1A_1$ 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	526.5	gas	LF	8
			518.7	Ne	IR	2
			512.5s	Ar	IR	1,2
	2	Bend	201.2	gas	EM,LF	7,8
			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]

References

[9]M. Tanimoto, H. Takeo, C. Matsumura, M. Fujitake, and E. Hirota, J. Chem. Phys. **91**, 2102 (1989).
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$GeCl_2$

$\tilde{B}$

$T_0 \sim 30969$ gas AB[2] 330–314 nm[a]

Structured absorption is superposed on a continuum with maximum near 32280, presumably due to predissociation of $GeCl_2$ into GeCl + Cl.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	95(5)	gas	AB	2

$\tau = 89.7(6.8)$ ns gas EM[10]

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

$T_0 = 22388$ gas CL[1] 410–490 nm[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	312(15)	gas	CL	1
	2	Bend	116(9)	gas	CL	1

$\tau = 17.4(6)$ gas EM[10]

References

[10]T. Ibuki, Chem. Phys. Lett. **169**, 64 (1990).

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
	2	Bend	776(30)	gas	PE	4
b_2	3	NO stretch	1244	Ar	IR	1,2

References

[1]D. E. Milligan, M. E. Jacox, and W. A. Guillory, J. Chem. Phys. **52**, 3864 (1970).
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[4]K. M. Ervin, J. Ho, and W. C. Lineberger, J. Phys. Chem. **92**, 5405 (1988).

PO_2^-

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	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.	Type meas.	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.	Type meas.	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

[1]M. Binnewies, M. Lakenbrink, and H. Schnöckel, Z. Anorg. Allg. Chem. **497**, 7 (1983).
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BrPO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	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

[1]M. Binnewies, M. Lakenbrink, and H. Schnöckel, High Temp. Sci. **22**, 83 (1986).
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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).

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	185[a]	Ar	IR	1
	3	PBr stretch	372	Ar	IR	1

[a] $\frac{1}{2}(2\nu_2)$.

References

[1]H. Schnöckel and S. Schunck, Z. Anorg. Allg. Chem. **552**, 155 (1987).

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).

NSBr

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

[1]S. C. Peake and A. J. Downs, J. Chem. Soc., Dalton Trans. 859 (1974).
[2]A. W. Allaf, G. Y. Matti, R. J. Suffolk, and J. D. Watts, J. Electron Spectrosc. Relat. Phenom. **48**, 411 (1989).

NSI

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NS stretch	1295[a]	gas	IR	1

[a] Tentative assignment.

References

[1]A. W. Allaf, G. Y. Matti, R. J. Suffolk, and J. D. Watts, Chem. Phys. Lett. **155**, 32 (1989).

SSO

$\tilde{A}\ ^1A'$ C_s Structure: AB^{11}

$T_0 =$ 29689.6 gas $AB^{1,7,11}LF^{12,13,16}$ Ã–X̃ 250–395 nm
29285(20) Xe AB^4 Ã–X̃ 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}
$\tau \sim 10$ ns gas LF^{13}

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

$A_0 = 1.398$; $B_0 = 0.169$; $C_0 = 0.150$ $MW^{2,5,6}DL^{14}$

References

[16]D. J. Clouthier and M. L. Rutherford, Chem. Phys. **127**, 189 (1988).

Se_3

$\tilde{X}$ 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

References

[1]H. Schnöckel, H.-J. Göcke, and R. Elsper, Z. Anorg. Allg. Chem. **494**, 78 (1982).

Te_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	203[a]	N_2	Ra	1

[a] ^{130}Te.

References

[1]H. Schnöckel, Z. Anorg. Allg. Chem. **510**, 72 (1984).

CF_2^-

Threshold for electron detachment from ground-state CF_2^- = 1440(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	1	CF stretch	860(30)	gas	PE	1

References

[1]K. K. Murray, D. G. Leopold, T. M. Miller, and W. C. Lineberger, J. Chem. Phys. **89**, 5442 (1988).

CCl_2^-

Threshold for electron detachment from ground-state CCl_2^- = 12930(65) gas PE[1]

References

[1]K. K. Murray, D. G. Leopold, T. M. Miller, and W. C. Lineberger, J. Chem. Phys. **89**, 5442 (1988).

PF_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		PF_2 stretch	852.1ms	Ar	IR	1
		PF_2 stretch	831.4s	Ar	IR	1

References

[1]J. K. Burdett, L. Hodges, V. Dunning, and J. H. Current, J. Phys. Chem. **74**, 4053 (1970).

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]

References

[1]Y. Ni, X. Wang, M. Suto, and L. C. Lee, J. Phys. B **21**, 1821 (1988).
[2]C. Ye, M. Suto, L. C. Lee, and T. J. Chuang, J. Phys. B **22**, 2527 (1989).

O_3^-

Threshold for electron detachment from ground-state O_3^- = 16970(20) gas PE^7PD^9

$\tilde{X}\ ^2B_1$ 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[a]	Ar	Ra	3,5
			1011[b]	Ar	Ra	3,5
	2	Bend	590(10)	gas	PD,PF	7,8
			600w[a]	Ar	IR	4
b_2	3	Asym. stretch	796.3	Ne	IR	10
			789s[a]	Ar	IR	2,4
			802s			
			802s[b]	Ar	IR	1,2,4

[a] Cs^+ present.
[b] Na^+ present.

References

[9]L. J. Wang, S. B. Woo, and E. M. Helmy, Phys. Rev. A **35**, 759 (1987).
[10]W. E. Thompson and M. E. Jacox, J. Chem. Phys. **91**, 3826 (1988)

FOO

$\tilde{X}$ 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 $DL^7IR^9MW^{10}$

References

[10]M. Bogey, P. B. Davies, C. Demuynck, and J. L. Destombes, Mol. Phys. **67**, 1033 (1989).

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

References

[1]D. E. Tevault, N. Walker, R. R. Smardzewski, and W. B. Fox, J. Phys. Chem. **82**, 2733 (1978).
[2]S. D. Allen, M. Poliakoff, and J. J. Turner, J. Mol. Struct. **157**, 1 (1987).
[3]W. Levason, J. S. Ogden, M. D. Spicer, and N. A. Young, J. Am. Chem. Soc. **112**, 1019 (1990).

SF_2

Ẽ 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

C̃

gas MPI $\tilde{C}$–$\tilde{X}$ 165–175 nm

B̃ $^1B_1$ (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

Ã

T_0 = 18500(1200) gas CL[7,8] 550–860 nm

Chemiluminescence in the reaction of F_2 with CS_2, originally assigned[7,8] to FCS, has been reassigned[9] to SF_2.

$\tilde{X}$ 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
			834	Ne	IR	3
			832vs	Ar	IR	3
			825	N_2	IR	3
	2	Bend	357(2)	gas	MW,CL	2,7–9
			358	Ne	IR	3
			358m	Ar	IR	3
			358	N_2	IR	3
b_2	3	Asym. stretch	813.04	gas	IR	5
			807.5	Ne	IR	3
			804vs	Ar	IR	3
			795	N_2	IR	6

A_0 = 0.898; B_0 = 0.307; C_0 = 0.228 MW[1,2]

References

[1]D. R. Johnson and F. X. Powell, Science **164**, 950 (1969).
[2]W. H. Kirchhoff, D. R. Johnson, and F. X. Powell, J. Mol. Spectrosc. **48**, 157 (1973).
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[4]Y. Endo, S. Saito, E. Hirota, and T. Chikaraishi, J. Mol. Spectrosc. **77**, 222 (1979).
[5]J.-C. Deroche, H. Burger, P. Schulz, and H. Willner, J. Mol. Spectrosc. **89**, 269 (1981).
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[9]R. J. Glinski and C. D. Taylor, Chem. Phys. Lett. **155**, 511 (1989).
[10]R. D. Johnson III and J. W. Hudgens, J. Phys. Chem. **94**, 3273 (1990).

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 $2\nu_2$.

References

[1]H. Willner, Z. Naturforsch. **39B**, 314 (1984).

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).

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	225[ae]	Ar	Ra	2
			253[b]	Ar	Ra	2
			258[c]	Ar	Ra	2
			276[d]	Ar	Ra	2
Σ_u^+	3	Asym. stretch	327[a]	Ar	IR,Ra	2
			340[b]	Ar	IR,Ra	2
			345[c]	Ar	IR,Ra	2
			375[d]	Ar	IR,Ra	2
			374[f]	Kr	IR	1

[a]Cs^+ present.
[b]Rb^+ present.
[c]K^+ present.
[d]Na^+ present.
[e]Tentative assignment.
[f]Attributed in Ref. 1 to the uncharged species. Reassigned by Ref. 4 to the anion.

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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^5EF^7

References

[1]J. A. Mangano, J. H. Jacob, M. Rokni, and A. Hawryluk, Appl. Phys. Lett. **31**, 26 (1977).
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6.4. Four-Atomic Trihydrides

BH_3

$\tilde{X}\,^1A_1'$ D_{3h}

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	2808w	Ar	IR	1

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	2112?	Ar	IR	1

References

[1]A. Kaldor and R. F. Porter, J. Am. Chem. Soc. **93**, 2140 (1971).
[2]K. Kawaguchi, J. E. Butler, C. Yamada, S. H. Bauer, T. Minowa, H. Kanamori, and E. Hirota, J. Chem. Phys. **87**, 2438 (1987).

SiH_3^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	820(40)	gas	PE,PI	1,2

References

[1]J. M. Dyke, N. Jonathan, A. Morris, A. Ridha, and M. J. Winter, Chem. Phys. **81**, 481 (1983).
[2]J. Berkowitz, J. P. Greene, H. Cho, and B. Ruscic, J. Chem. Phys. **86**, 1235 (1987).

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

***4p* $^2A_2''$** D_{3h}

T_0 = 69853.44(13) gas MPI[15]
B_0 = 9.90 gas MPI[15]

***X̃* $^2A_2''$** D_{3h} Structure: $AB^2IR^{9,18}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	CH stretch	3004.8(2)	gas	CAR,Ra	13,16
a_2''	2	OPLA	606.453	gas	IR,DL	5,9
			617vs	Ne	IR	4
			603[c]	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[d]	Ar	IR	8

B_0 = 9.578 AB^2DL^9; C_0 = 4.742 DL^9

CD_3

***4p* $^2A_2''$** D_{3h}

T_0 = 69777.40(4) gas MPI[15]
B_0 = 4.846(2) gas MPI[15]

***3p* $^2A_2''$** D_{3h} Structure: MPI[12]

T_0 = 59886 gas $MPI^{12,17}$

Higher members of Rydberg series observed (MPI^{12}) at 69789, 73645, and 75557.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	CD stretch	2031[e]	gas	MPI	12,17
a_2''	2	OPLA	1032	gas	MPI	12,17

B_0 = 4.76(2); C_0 = 2.38 $MPI^{12,17}$

***X̃* $^2A_2''$** 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[c]	Ar	IR	3,8
			463	N_2	IR	3
e'	3	CD stretch	2381.09	gas	IR	21
			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] $\frac{1}{2}(2\nu_2)$.
[c]Band center. Rotational structure assigned.[8]
[d] $^RR(0_0)$ transition.
[e]Approximate value; perturbed by Fermi resonance.

References

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[15]J. F. Black and I. Powis, J. Chem. Phys. **89**, 3986 (1988).
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[21]W. M. Fawzy, T. J. Sears, and P. B. Davies, J. Chem. Phys. **92**, 7021 (1990).

SiH_3

M̃* $^2A_2''$ *(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

J̃* $^2A_2''$ *(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

Ẽ* $^2A_2''$ *(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)[a]	gas	MPI	7

***X̃* $^2A_1$** 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[b]	gas	DL,MPI	3,6,7
			721.05[c]	gas	DL,MPI	3,6,7

Barrier to inversion = 1935 gas PE^4MPI^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

$\tilde{N}\ ^2E'$ (4f) 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	615(3)	gas	MPI	7

$\tilde{J}\ ^2A_2''$ (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

$\tilde{H}\ ^2E'$ (4p) D_{3h}

$T_0 \sim 50000$ 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

$\tilde{E}\ ^2A_2''$ (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)[a]	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[b]	gas	MPI	7
			542[c]	gas	MPI	7

Barrier to inversion = 1925 gas MPI[7]

[a] $\frac{1}{2}(2\nu_4)$.
[b] $1^- - 0^+$ transition.
[c] $1^+ - 0^-$ transition.

References

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[8] R. D. Johnson, III, and J. W. Hudgens, J. Chem. Phys. (in press).

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

[1] R. D. Johnson III, B. P. Tsai, and J. W. Hudgens, J. Chem. Phys. **89**, 4558 (1988).

NH_3^+

$\tilde{X}\ ^2A_2''$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	NH stretch	~2740	gas	PE	3
a_2''	2	OPLA	903.536	gas	PE,DL	3,6
e'	3	NH stretch	3388.65	gas	LD	5

B_0 = 10.644; C_0 = 5.246 LD[5]

References

[5]M. G. Bawendi, B. D. Rehfuss, B. M. Dinelli, M. Okumura, and T. Oka, J. Chem. Phys. **90**, 5910 (1989).
[6]S. Lee and T. Oka, Paper RA14, 44th Symposium on Molecular Spectroscopy, Columbus, Ohio, June 1989.

AsH_3^+

$\tilde{X}\ ^2A_1$ 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).

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
e	3	OH stretch	3535.96[c]	gas	CC	1,4,10
			3519.40[d]	gas	CC	1,4,10
	4	Deformation	1625.95[c]	gas	DL	11
			1638.53[d]	gas	DL	11

B(0^+) = 11.254; (C–B)(0^+) = −4.91(6) IR,MW[9,12]

D_3O^+

$\tilde{X}$

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[c]	gas	LD	13
			2624.24[d]	gas	LD	13

B(0^+) = 5.675 DL[8]LD[13]

[a]$1^- - 0^+$ transition.
[b]$1^+ - 0^-$ transition. For H_3O^+, $0^S - 0^+$ = 55.35 cm^{-1}[1,6,12] and for D_3O^+, 15.39 cm^{-1}[1,8]
[c]$1^+ - 0^+$ transition.
[d]$1^- - 0^-$ 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	D	1,3

B_0 = 4.895; C_0 = 4.228 $LD^{1,3}DL^2$

References

[1]T. Nakanaga and T. Amano, Chem. Phys. Lett. **134**, 195 (1987).
[2]T. Amano, K. Kawaguchi, and E. Hirota, J. Mol. Spectrosc. **126**, 177 (1987).
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6.5. Four-Atomic Dihydrides

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 2956.1	Ar	IR	1
	2	CH_2 scissors	1341.5 1339.1	Ar	IR	1
	3	ZnC stretch	513.7 512.0	Ar	IR	1
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 697.4	Ar	IR	1,2
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 $CL^1LF^{3,4}$ $\tilde{B}$–$\tilde{X}$ 620–650 nm
$A = 14.6(2)$; $\frac{1}{2}(B + C) = 0.304$ LF^4

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

$T_0 = 15464$ gas $CL^1LF^{3,4}$ $\tilde{A}$–$\tilde{X}$ 620–650 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CaN stretch	520(10)	gas	F	3

$A = 11.4$; $\frac{1}{2}(B + C) = 0.304$ LF^7

$\tilde{X}\ ^2A_1$ 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	F	3

$A = 13.0$; $B^a = 0.301$; $C^a = 0.293$ $LF^{2,4}$

[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).
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$CuNH_2$

$\tilde{X}$

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).

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
Σ^+	3	BN stretch	1786.19	gas	L	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
Σ^+	2	BD stretch	2730	Ar	IR	3
Σ^+	3	BN stretch	1734	Ar	IR	3
Π	4	Bend	360	Ar	IR	3

References

[1]N. C. Baird and R. K. Datta, Inorg. Chem. **11**, 17 (1972).
[2]D. R. Armstrong and D. T. Clark, Theor. Chim. Acta **24**, 307 (1972).
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[4]Y. Kawashima, K. Kawaguchi, and E. Hirota, J. Chem. Phys. **87**, 6331 (1987).

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
		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
		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
		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
		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
		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
		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).

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
		^{63}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
		^{63}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).

$H_2C=C$

$\tilde{b}\ ^3A_2$ 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

$D_2C=C$

$\tilde{a}\ ^3B_2$ 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

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_2 s-stretch	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

[6]K. M. Ervin, J. Ho, and W. C. Lineberger, J. Chem. Phys. **91**, 5974 (1989).

$HCNH^+$

$\tilde{X}$ $C_{\infty v}$ Structure: LD[3]

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	6,7
Π	4	HCN bend	801.59	gas	DL	4
	5	HNC bend	645.92	gas	DL	5

B_0 = 1.236 LD[1,2]

References

[1]R. S. Altman, M. W. Crofton, and T. Oka, J. Chem. Phys. **80**, 3911 (1984).
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[6]M. Kajita, K. Kawaguchi, and E. Hirota, J. Mol. Spectrosc. **127**, 275 (1988).
[7]D.-J. Liu, S.-T. Lee, and T. Oka, J. Mol. Spectrosc. **128**, 236 (1988).

$H_2C{=}C^-$

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).

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
		^{69}GaO stretch	646.4[a]	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
		^{69}GaO stretch	644.6	Ar	IR	1
		DGaO bend	582.9	Ar	IR	1

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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

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H_2CSe

$\tilde{A}\ ^1A_2$ C_{2v} Structure: LF[7]

$T_0 \sim 13555$ gas LF[5,6] $\tilde{A}$–$\tilde{X}$ 685–720 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	~355	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 $AB^1CL^3LF^{5,6}$ $\tilde{a}$–$\tilde{X}$ 658–822 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
b_1	4	OPLA	297[b]	gas	AB,LF	1,5,6
b_2	6	HCSe bend	812[c]	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	3	C=Se stretch	~901	gas	LF	6

A_0 = 9.690; B_0 = 0.414; C_0 = 0.396 $MW^{2,4}LF^7$

D_2CSe

$\tilde{A}\ ^1A_2$ C_{2v}

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	563[c]	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	~789	gas	LF	6

A_0 = 4.87(2); B_0 = 0.344; C_0 = 0.321 MW^4LF^7

[a] $v_4 = 1$.
[b] From fit to double minimum potential. Barrier to inversion 13.1 for H_2CSe, 16.2 for D_2CSe.[6]
[c] $\frac{1}{2}(2\nu_i)$.

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[1] R. H. Judge and D. C. Moule, J. Am. Chem. Soc. **106**, 5406 (1984).
[2] R. D. Brown, P. D. Godfrey, and D. McNaughton, Chem. Phys. Lett. **118**, 29 (1985).
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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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[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).

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] 1847	Ar	IR	1,2
	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. meas.	Type	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

References

[1]R. Withnall and L. Andrews, J. Phys. Chem. **94**, 2351 (1990).

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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[1]J. W. Kauffman, 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. 355–362.
[2]R. Withnall and L. Andrews, J. Phys. Chem. **94**, 2351 (1990).

HSnOH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	SnH stretch	1608.0 1597.7	Ar	IR	1
	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_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

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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

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[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_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

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H_2Cl

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	~3050	gas	IR	2
		CH_2 scissors	~1330	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

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[2]S. L. Baughcum and S. R. Leone, J. Chem. Phys. **72**, 6531 (1980).

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

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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.
			~550	gas	PE	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			~300[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).

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[a]	Ar	IR	1
			3234	N_2	IR	3
	2	NH_2 scissors	1568[a]	Ar	IR	1
			1564	N_2	IR	3
	3	NH_2 wag	1244[a]	Ar	IR	1
			1241	N_2	IR	3
			1233			
	4	NF stretch	934[a]	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[a]	Ar	IR	1
	2	ND_2 scissors	1151[a]	Ar	IR	1
	3	ND_2 wag	968[a]	Ar	IR	1
	4	NF stretch	924[a]	Ar	IR	1

A_0 = 4.612; B_0 = 0.784; C_0 = 0.726 MW^2

[a]HF or DF trapped in adjacent site.

References

[1]L. Andrews and R. Lascola, J. Am. Chem. Soc. **109**, 6243 (1987).
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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).

H_2O_2

Continuous absorption, 120–300 nm.[1,2,7,12]

$\tilde{X}$ C_2 Structure: IR[4,19]MW[8]

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
	2	OH s-bend	1393.5	gas	Ra	10
			1385	Ar	Ra	11
	3	OO stretch	863.5	gas	Ra	10
			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]MW[8,13–15]

D_2O_2

$\tilde{X}$ 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

$\tilde{X}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
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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6.6. Four-Atomic Monohydrides

CaCCH

References

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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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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	3238.0[a]	Ar	IR	5
	2	C_3 a-stretch	1832.3 1824.8	Ar	IR	1,5
	3	C_3 s-stretch	1167br 1159.7	Ar	IR	5
Π	4	HCC bend	28[b]	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	2424.2[a]	Ar	IR	5
	2	C_3 a-stretch	1779.3 1770.6	Ar	IR	1,5
	3	C_3 s-stretch	1148.0 1140.3	Ar	IR	5

$A = 12.53$ gas MW^4
$B_0 = 0.337$ MW^4

[a]Tentative assignment.
[b]$^2\Sigma^\mu$ component.

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HNCN

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

$T_0 = 28994.1$ gas AB^1 $\tilde{A}$–$\tilde{X}$ 344 nm
$A_0 = 22.438$; $B_0 = 0.376$; $C_0 = 0.369$ AB^1

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

$A_0 = 21.220$; $B_0 = 0.370$; $C_0 = 0.362$ AB^1

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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.

$\tilde{X}$ C_s Structure: MW^2

$A_0 = 41.5(1.5)$; $B_0 = 0.363$; $C_0 = 0.359$ MW^2

DCCO

$\tilde{X}$ C_s

$A_0 = 21.75(12)$; $B_0 = 0.331$; $C_0 = 0.325$ MW^2

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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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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	~555	gas	AB	4

$A \sim 4.37$; $B \sim 0.388$; $C \sim 0.357$ 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[7]IR[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

$T_0 \leqslant 35053$ 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
	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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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

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$HOCO^+$

$\tilde{X}$ 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	~2300	gas	PI	6
	3	OCO s-stretch	~1500	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

$A_0 = 14.44$; $B_0 = 0.339$; $C_0 = 0.331$ $MW^{4,5}$

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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

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$HONN^+$

$\tilde{X}$

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

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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

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t-HOCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3602.9	Ar	IR	2
			3456	CO	IR	1
	2	C=O stretch	1843.6	Ar	IR	2
			1833	CO	IR	1
	3	HOC bend	1211.2	Ar	IR	2
			1261	CO	IR	1
	4	C-O stretch	1064.6	Ar	IR	2
			1077	CO	IR	1
	5	OCO bend	615	CO	IR	1
a"	6	Torsion	515	Ar	IR	2

t-DOCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2558	CO	IR	1
	2	C=O stretch	1841.7	Ar	IR	2
			1825	CO	IR	1
	3	C-O stretch + DOC bend	1092.6	Ar	IR	2
			1117	CO	IR	1
	5	OCO bend	610m	CO	IR	1
a"	6	Torsion	472wm	CO	IR	1

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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
			3558	N_2	IR	7
	2	N=O stretch	1699.76s	gas	IR,LS DL	4,5,8,14 16-18
			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
			1298	N_2	IR	7
	4	O-N stretch	790.12s	gas	IR	4,5,8,16 17
			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]

t-DONO

$\tilde{X}$ $^1A''$ 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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c-HONO

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	3426.22w	gas	IR	4,5,8,16 17
			3412	Ar	IR	9
			3410	N_2	IR	7
	2	N=O stretch	1640.52m	gas	IR,LS	4,5,8,14 16
			1632.6	Ar	IR	9,19
			1633	N_2	IR	7
	3	HON bend	1261w	gas	IR	8
			1263.3	Ar	IR	9,19
	4	O-N stretch	851.94s	gas	IR,DL	4,5,8 16–18
			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]

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	~660	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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[15]W. C. Bowman, F. C. DeLucia, and P. Helminger, J. Mol. Spectrosc. **88**, 431 (1981).
[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).
[19]J. N. Crowley and J. R. Sodeau, J. Phys. Chem. **93**, 4785 (1989).

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

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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	2912.5	gas	IR	1
	2	CO stretch	1798.4[a]	gas	IR	1
	3	H deform.	1271.2[b]	gas	IR	1
	4	BrCO deform.	646.0	gas	IR	1
a″	6	OPLA	894vw	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	2207.1	gas	IR	1
	2	CO stretch	1748.6	gas	IR	1
	3	D deform.	975.8[c]	gas	IR	1
	4	BrCO deform.	605.9	gas	IR	1
a″	6	OPLA	747vw	gas	IR	1

[a]In Fermi resonance with $2\nu_6$.
[b]In Fermi resonance with $2\nu_4$.
[c]In Fermi resonance with $(\nu_4 + \nu_5)$.

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6.7. Four-Atomic Nonhydrides

C_4

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1543.4	Ar	IR	1

References

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$CNCN^+$ [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

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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	1897.8	Ar	IR	1,2
Π_u	5	Bend	213	Ar	IR	1,2

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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	975[a]	gas	IR	1
			979.2	Ar	IR	2
Π	4	Bend	463.5[a]	gas	IR	2
			468.5	Ar	IR	2
			467.2			
	5	Bend	194.75	gas	IR	1
			~200[b]	Ar	IR	1

$B_0 = 0.173$ IR[1,3]MW[1,3,4]

[a]Preliminary value.
[b]From combination bands.

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[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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CNNC

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1996.4[a]	Ar	IR	1

[a]Tentative assignment.

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).

CCCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ	1		2243s	Ar	IR	1,2
	2		1907w	Ar	IR	2
Π	4		580w	Ar	IR	2

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[1]R. L. DeKock and W. Weltner, Jr., J. Am. Chem. Soc. **93**, 7106 (1971).
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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	~2076[a]	Ne	IR	4
			526(30)[b]	gas	PD	2
b_u	5	CO a-stretch	2056.6	Ne	IR	3,4

[a]Calculated using observed values for asymmetrically substituted species.
[b]Tentative assignment.

References

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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	~2283[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^+

$\tilde{B}\,^2A_1$ T_d

T_0[a] = 21860(500) gas PE[1,2]
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	540(40)	gas	PE	1,2
			550(10)	Ar	AB	3

$\tilde{A}\,^2T_2$[b] T_d

T_0[a] = 8880(800) gas PE[1,2]

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^+.

Jahn-Teller splitting ~ 1130 gas PE[1,2]

$\tilde{X}\,^2E$[b] T_d

Jahn-Teller splitting ~ 2820 gas PE[1,2]

[a]The first ionization potential of P_4 is taken as 9.10(5) eV, as in Ref. 2. T_0 values are given with respect to onset of the transition.
[b]Ref. 2 reverses the assignment of these two bands.

References

[3]L. Andrews and Z. Mielke, J. Phys. Chem. **94**, 2348 (1990).

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	1–3
			804.7	N_2	IR	1
b_{3u}	6	SiO stretch	766.7	Ne	IR	2
			768.2	Ar	IR	1–3
			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	666	Ar	IR	1
			667	N_2	IR	1
B_{3u}	6	GeO stretch	601	Ar	IR	1
			599	N_2	IR	1

References

[1]J. S. Ogden and M. J. Ricks, J. Chem. Phys. **52**, 352 (1970).

Sb_4

$\tilde{X}$ 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

$\tau \sim 1.5$ 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

References

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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.

References

[1]M. E. Jacox and W. E. Thompson, Res. Chem. Intermed. **12**, 33 (1989).
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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	~1800	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	~800	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).

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
			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 1778.7	Ne	IR	12
			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]

[a]From observation of $\nu_5 - \nu_4 = 1700.8\ cm^{-1}$.

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$(PO)_2$

$\tilde{X}$

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).

C_2F_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	CF stretch	1149[a]	gas	IR	1
			1341[a]	Ar	IR	2

[a]Tentative value. Further experimental studies are needed to resolve this conflicting assignment.

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[2]J. C. Brahms and W. P. Dailey, J. Am. Chem. Soc. **111**, 8940 (1989).

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).

CINCO

$\tilde{X}$ 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

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[2]H. H. Eysel and E. Nachbaur, Z. Anorg. Allg. Chem. **381**, 71 (1971).
[3]W. H. Hocking and M. C. L. Gerry, J. Mol. Spectrosc. **42**, 547 (1972).
[4]W. H. Hocking, M. L. Williams, and M. C. L. Gerry, J. Mol. Spectrosc. **58**, 250 (1975).
[5]T. C. DeVore, J. Mol. Struct. **162**, 287 (1987).

BrNCO

In the gas phase, an absorption maximum has been observed at 292 nm.[1]

$\tilde{X}$ C_s Structure: MW[2,3]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]

References

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[2]H. M. Jemson, W. Lewis-Bevan, N. P. C. Westwood, and M. C. L. Gerry, Chem. Phys. Lett. **108**, 496 (1984).
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[4]T. C. DeVore, J. Mol. Struct. **162**, 287 (1987).
[5]M. Gerke, G. Schatte, and H. Willner, J. Mol. Spectrosc. **135**, 359 (1989).

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

$A_0 = 1.354$; $B_0 = 0.057$; 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).
[2]T. C. DeVore, J. Mol. Struct. **162**, 287 (1987).

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).
[2]T. C. DeVore, J. Mol. Struct. **162**, 287 (1987).

BrSCN

$\tilde{X}$

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

References

[1]T. C. DeVore, J. Mol. Struct. **162**, 287 (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

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BCl_3^+

$\tilde{D}\ ^2E'$ 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 330 and 420 nm on excitation of BCl_3 by radiation of wavelength shorter than 81 nm has been attributed to the $\tilde{D}$–$\tilde{X}$ transition of BCl_3^+, and emission between 420 and 580 nm, with vibrational spacings of ~445, has been attributed to the $\tilde{D}$–$\tilde{A},\tilde{B}$ transitions of this species.[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

References

[3]L. C. Lee, J. C. Han, and M. Suto, J. Chem. Phys. **91**, 2036 (1989).

NO_3

$\tilde{X}\ ^2A_2'$ 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	8,9
a_2''	2	OPLA	762.33	gas	IR	12
e'	3	NO stretch[a]	1492.39	gas	LF,DL IR	8,9,11 12
	4	Deformation	360	gas	LF	8,9

$B_0 = 0.459$ DL[11,13] IR[12]

[a]Arguments of Ref. 3 suggest that NO_3 should have a very low-lying $\tilde{A}\ ^2E''$ state. Ref. 12 presents experimental evidence consistent with the presence of such a state. Ref. 13 has suggested that the 1492 cm^{-1} absorption may possibly be contributed by the $\tilde{A}$ state.

References

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PO_3

$\tilde{B}^2E'$ [a] D_{3h}

$T_0 = 14378$ Ar AB^2 $\tilde{A}$–$\tilde{X}$ 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 photo dissociation 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] 1320.3[b]	Ne Ne	IR IR	4 4
b_u	5	O=O a-stretch	1164.4	Ne	IR	4

[a]$(\nu_1 + \nu_5) - \nu_5$.
[b]In a neon matrix, almost as intense as ν_5, and with very similar isotopic shift pattern. Probably results from interaction of ν_5 with combination bands of B_u symmetry.

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[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).

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).

ClONO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		N=O stretch	1714.0	gas	IR	2
			1714s	Ar	IR	1
			1717	N_2	IR	3
		ClO stretch	856m	Ar	IR	1
		ONO bend	390ms	Ar	IR	1
a''		Torsion	398m	Ar	IR	1

References

[1]D. E. Tevault and R. R. Smardzewski, J. Chem. Phys. **67**, 3777 (1977).
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$BrNO_2$

$\tilde{X}$ 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	~1660	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.

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[3]B. J. Finlayson-Pitts, F. E. Livingston, and H. N. Berko, J. Phys. Chem. **93**, 4397 (1989).

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).

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[a]	Ar	IR	2
			1005.5[a]	N_2	IR	2

[a] ^{80}Se.

References

[1]N. J. Brassington, H. G. M. Edwards, D. A. Long, and M. Skinner, J. Raman Spectrosc. **7**, 158 (1978).
[2]A. K. Brisdon and J. S. Ogden, J. Mol. Struct. **157**, 141 (1987).

CF_2Cl

3p Rydberg state C_{2v}

$T_0 \leqslant 49220$ 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).

$CFCl_2$

3p Rydberg state C_{2v}

$T_0 \leqslant 49850$ 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

X̃ 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

[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**, 5568 (1978).
[3]B. P. Tsai, R. D. Johnson, III, and J. W. Hudgens, J. Phys. Chem. **93**, 5334 (1989).

CCl_3

M̃ $^2E'$ (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

L̃ $^2A_2''$ (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

K̃ $^2E'$ (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

J̃ $^2A_1'$ (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

G̃ $^2E'$ (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

F̃ $^2A_2''$ (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

Ẽ $^2E'$ (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	Sym. stretch	544(6)	gas	MPI	9
a_2''	2	OPLA	509(21)	gas	MPI	9

$A = 33(5)$ gas MPI[9]

An unstructured gas-phase absorption between 195 and 260 nm, with a maximum at 211(2) nm, has been assigned[8] to CCl_3.

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.

X̃ $^2A_1$ C_{3v} Structure: ESR[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2	2	Umbrella	290[b] 251	gas	MPI	9
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).
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[3]J. H. Current and J. K. Burdett, J. Phys. Chem. **73**, 3504 (1979).
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SiF_3

Unstructured emission bands between 350 and 800 nm and between 290 and 340 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[3] 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[4] 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]M. Suto, J. C. Han, L. C. Lee, and T. J. Chuang, J. Chem. Phys. **90**, 2834 (1989).
[4]W. B. Griffith, Jr., and C. W. Mathews, private communication.

$GeCl_3$

$\tilde{X}$

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).

$OPCl_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		P=O stretch	1300[a]	Ar	IR	1
		PCl_2 a-stretch	621[a]	Ar	IR	1

[a]Tentative assignment.

References

[1]B. W. Moores and L. Andrews, J. Phys. Chem. **93**, 1902 (1989).

$OPBr_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			558[a]	Ar	IR	1

[a]Tentative assignment.

References

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$t\text{-}O_4^-$

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[c]	Ar	IR	10
	2	O···O stretch	287[a]	Ar	Ra	6
			298[b]	Ar	Ra	6
			305[c]	Ar	Ra	5
b_u	5	O=O a-stretch	973.1	Ne	IR	11
			1001[a]	Ar	IR	4
			992[b]	Ar	IR	3
			993[c]	Ar	IR	3,10
			1001[d]	Ar	IR	2,4
			991			
	6	Asym. bend	131[c]	Ar	IR	10

[a]Cs^+ present.
[b]Rb^+ present.
[c]K^+ present.
[d]Na^+ present.

References

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SO_3^-

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		S=O stretch	1191[a]	Ar	IR	1
		S-O stretch	1093[a]	Ar	IR	1
			1091[a]			
		S-O stretch	965[a]	Ar	IR	1
			585[a]	Ar	IR	1
			504[a]	Ar	IR	1
			474?[a]	Ar	IR	1

[a]Cs^+ trapped in adjacent site.

References

[1]D. M. Stanbury, T. A Holme, Z. H. Kafafi, and J. L. Margrave, Chem. Phys. Lett. **129**, 181 (1986).

ClOOCl

An unstructured gas-phase absorption with maximum at 40800 (245 nm) has been assigned[1,4] to ClOOCl.

$\tilde{X}$ 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).

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			

References

[1]M. Hawkins, L. Andrews, A. J. Downs, and D. J. Drury, J. Am. Chem. Soc. **106**, 3076 (1984).

6.8. H_5^+ and Five-Atomic Tetra- and Trihydrides

H_5^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	H-H stretch	3910	gas	VP[a]	1
	2	Ring s-stretch	3532	gas	VP	1

[a]Vibrational predissociation of mass-selected beam.

References

[1]M. Okumura, L. I. Yeh, and Y. T. Lee, J. Chem. Phys. **83**, 3705 (1985).

SiH_4^+

$\tilde{X}$ [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

References

[5]M. N. Paddon-Row and S. S. Wong, J. Chem. Soc., Chem. Commun. 1585 (1987).
[6]R. F. Frey and E. R. Davidson, J. Chem. Phys. **89**, 4227 (1988).

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
	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

References

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$CaCH_3$

$\tilde{B}\,^2A_1$ 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)[b]	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)[b]	gas	LF	1

$A_0 = 5.448$; $B_0 = 0.252$ LF[2]

[a]Predissociated above ~ 16200.[1]
[b] $\frac{1}{2}(2\nu_6)$.

References

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$ZnCH_3$

$\tilde{B}\,^2E$ C_{3v}

$T_0 = 36510$ gas AB[1] $\tilde{B}$–$\tilde{X}$ 260–274 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 deform.	~950	gas	AB	1

$\tilde{A}\,^2E$ C_{3v}

$T_0 = 23949$ gas AB[1] $\tilde{A}$–$\tilde{X}$ 379–418 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 deform.	~1060	gas	AB	1
	3	ZnC stretch	~265	gas	AB	1

References

[1]P. J. Young, R. K. Gosavi, J. Connor, O. P. Strausz, and H. E. Gunning, J. Chem. Phys. **58**, 5280 (1973).

$CdCH_3$

$\tilde{B}\,^2E$ C_{3v}

$T_0 = 34916$ gas AB[1] $\tilde{B}$–$\tilde{X}$ 264–287 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 deform.	~960	gas	AB	1
	3	CdC stretch	~360	gas	AB	1

$\tilde{A}\,^2E$ C_{3v}

$T_0 = 22507$ gas AB[1] $\tilde{A}$–$\tilde{X}$ 400–445 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 deform.	~1000	gas	AB	1
	3	CdC stretch	~400	gas	AB	1

References

[1]P. J. Young, R. K. Gosavi, J. Connor, O. P. Strausz, and H. E. Gunning, J. Chem. Phys. **58**, 5280 (1973).

$HFeNH_2$

$\tilde{X}$

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

References

[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

References

[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

References

[1]D. W. Ball, R. H. Hauge, and J. L. Margrave, Inorg. Chem. **28**, 1599 (1989).

$C_2H_3^+$

$\tilde{X}$ C_{2v} (bridged) Structure: $CE^1LD^{2,3}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
A_{1u}^+		CH stretch	3142.2	gas	LD	3

$B_0 = 1.142$; $C_0 = 1.046$ $LD^{2,3}$

References

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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

$\tilde{X}$ 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]

References

[2]R. A. Shepherd, T. J. Doyle, and W. R. M. Graham, J. Chem. Phys. **89**, 2738 (1988).
[3]A. Fahr and A. H. Laufer, J. Phys. Chem. **92**, 7229 (1988).
[4]H. Kanamori, Y. Endo, and E. Hirota, J. Chem. Phys. **92**, 197 (1990).

CH_3N

$\tilde{A}\ ^3E$ C_{3v} Structure: EM[4]

T_0 = 31823.915(7) gas AB[1],EM[1,2,4,5] $\tilde{A}$–$\tilde{X}$ 288–356 nm
31576(20) N_2 AB[3] $\tilde{A}$–$\tilde{X}$ 284–317 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CN stretch	758(4)	gas	UV	1,2
			755(22)	N_2	AB	3
e	6	CH_3 rock	728(4)	gas	EM	5

A = −22.872(7) gas EM[4]
B_0 = 0.846 EM[4]

$\tilde{X}\ ^3A_2$ C_{3v} Structure: EM[4]

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

B_0 = 0.931 EM[4]

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] $\tilde{A}$–$\tilde{X}$ 295–318 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CN stretch	759(4)	gas	UV	1,2
			805(53)	N_2	AB	3
		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 $A(CD_3N) = A(CH_3N)$.

References

[5]E. L. Chappell and P. C. Engelking, J. Chem. Phys. **89**, 6007 (1988).

$HSiNH_2$

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

References

[1]G. Maier, J. Glatthaar, and H. P. Reisenauer, Chem. Ber. **122**, 2403 (1989).

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]

References

[1]J. M. Dyke, A. R. Ellis, N. Jonathan, N. Keddar, and A. Morris, Chem. Phys. Lett. **111**, 207 (1984).
[2]T. Amano and H. E. Warner, Astrophys. J. **342**, L99 (1989).

CH_3O

$3s\ ^2A_1$ C_{3v}

Resonance-enhanced MPI spectrum of CH_3O between 313 and 328 nm has been tentatively assigned to a two-photon absorption into this Rydberg state, accompanied by a single-photon ionization.[15]

$\tilde{A}\ ^2A_1$ C_{3v} Structure: LF[23,24]

ν_0 = 31614.51(4) gas EM[1,2,11,12]AB[5] LF[6,8,19,20,23-25] $\tilde{A}$-$\tilde{X}$ 271–421 nm

31291(3) Ar LF[22] $\tilde{A}$-$\tilde{X}$ 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	20
	2	Umbrella	1315	gas	LF	20
			1308(4)	Ar	LF	22
	3	CO stretch	660	gas	AB,EM LF	5,12,20
			657(2)	Ar	LF	22
e	4	CH_3 stretch	2962	gas	LF	20
	5	CH_2 scissors	1407	gas	LF	20
			1410(3)	Ar	LF	22
	6	HCO deform.	595	gas	LF	20

τ = 2.2(2)μs gas EM[2,9]LF[4,14,16,17,19,21]

A_0 = 4.981(3); B_0 = 0.743 LF[23-25]

$\tilde{X}\ ^2E$ C_{3v}[a] Structure: LMR[3,7]MW[10,18]LF[23]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 stretch	2840	gas	LF	20
	2	CH_3 umbrella	1362	gas	LF	20
			1356(2)	Ar	LF	22
	3	CO stretch	1047	gas	LF,EM	6,9,12 20
			1044(2)	Ar	LF	22
e	4	CH_3 stretch	2774[b]	gas	LF	20
			2758(3)	Ar	LF	22
	5	CH_2 scissors	1487	gas	LF	20
			1406(2)	Ar	LF	22
	6	HCO deform.	653	gas	LF	20

A = −61.97(7) gas LMR[7]MW[10]EM[11,12]LF[20,23,24]

A_0 = 5.206(4); B_0 = 0.932 LMR[7]MW[10,18]LF[23,24]

CD_3O

$3s\ ^2A_1$ C_{3v}

Resonance-enhanced MPI spectrum of CD_3O between 313 and 328 nm has been tentatively assigned to a two-photon absorption into this Rydberg state, accompanied by a single-photon ionization.[15]

$\tilde{A}\ ^2A_1$

T_0 = 31554 gas LF[6,20]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	20
	2	CD_3 umbrella	971	gas	LF	20
	3	CO stretch	663	gas	EM,LF	12,20
e	5	CD_2 scissors	1047	gas	LF	20

$\tilde{X}\ ^2E$ C_{3v}[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CO stretch	1000[b]	gas	LF	20
	3	CD_3 umbrella	893[b]	gas	LF	20
e	5	CD_2 scissors	1174	gas	LF,EM	6,12,20
	6	DCO deform.	496	gas	LF	20

A = −56(2) gas EM[12]

B_0 = 0.740 MW[18]

[a]Somewhat distorted by Jahn-Teller coupling.

[b]Tentative assignment.

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[24]J. Kappert and F. Temps, Chem. Phys. **132**, 197 (1989).

[25]X. Liu, S. C. Foster, J. M. Williamson, L. Yu, and T. A. Miller, Mol. Phys. **69**, 357 (1990).

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

Threshold for photodecomposition into H_2CO + H near 280 nm.[1,2]

3s Rydberg state C_s

T_0 = 35050 gas AB[5] $3s$-$\tilde{X}$ 243–285 nm

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]

References

[5]P. Pagsberg, J. Munk, A. Sillesen, and C. Anastasi, Chem. Phys. Lett. **146**, 375 (1988).

[6]P. Pagsberg, J. Munk, C. Anastasi, and V. Simpson, Chem. Phys. Lett. **157**, 271 (1989).

CH_3S

$\tilde{A}\ ^2A_1$ C_{3v} Structure: LF[9]

$T_0 = 26399$ gas EM[2]LF[6,9] $\tilde{A}$-$\tilde{X}$ 365–520 nm

Predissociation threshold $\leqslant 27300$.[6] *In an argon matrix,* CH_2SH *is formed.*[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CS stretch	401	gas	EM,LF	2,6,9

$\tau_0 = 310(20)$ ns gas LF[6]; 760(60) ns gas LF[8]
$A_0 = 5.343(47)$; $B_0 = 0.346$ 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	2	CH_3 umbrella	1316(4)	gas	PD,LF	4,6
	3	CS stretch	740(4)	gas	EM,PE PD,LF	2–4,6

$A = -255.5$ gas LF[9]
$A_0 = 5.68(4)$; $B_0 = 0.450$ MW[7]LF[9]

References

[9]Y.-C. Hsu, X. Liu, and T. A. Miller, J. Chem. Phys. **90**, 6852 (1989).

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.	~1100	gas	AB	2

References

[1]J. Connor, G. Greig, and O. P. Strausz, J. Am. Chem. Soc. **91**, 5695 (1969).

[2]P. J. Young, R. K. Gosavi, J. Connor, O. P. Strausz, and H. E. Gunning, J. Chem. Phys. **58**, 5280 (1973).

CH_3I^+

$\tilde{A}\ ^2A_1$ 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

Spin-orbit splitting = 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

Spin-orbit splitting = 5036 gas PF[11]

[a]From vertical ionization potential.
[b]From study of band at 16978 in $\tilde{A} \leftarrow \tilde{X}\ ^2E_{1/2}$ transition.
[c]Identified for $^2E_{1/2}$, but not for $^2E_{3/2}$.

References

[11]K. Walter, R. Weinkauf, U. Boesl, and E. W. Schlag, J. Chem. Phys. **89**, 1914 (1988).

CH_3S^-

Threshold for electron detachment from ground-state CH_3S^- = 15020(30) gas PD^2PE[1,3]

$\tilde{X}$ C_{3v}

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

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).

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).

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. sym.	No.	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. sym.	No.	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. sym.	No.	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. sym.	No.	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. sym.	No.	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. sym.	No.	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. sym.	No.	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. sym.	No.	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-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.
			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]

cyc-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*-C_3H_2.

References

[7]J. W. Huang and W. R. M. Graham, J. Chem. Phys. **93**, 1583 (1990).

$H_2C{=}C{=}C$:

Photoisomerization to HCCCH occurs at 254 nm.[1,2]

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

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]Singlet state.

References

[2]J. W. Huang and W. R. M. Graham, J. Chem. Phys. **93**, 1583 (1990).

HCCCH

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

References

[6]G. Maier, H. P. Reisenauer, W. Schwab, P. Carsky, V. Spirko, B. A. Hess, Jr., and L. J. Schaad, J. Chem. Phys. **91**, 4763 (1989).
[7]J. W. Huang and W. R. M. Graham, J. Chem. Phys. **93**, 1583 (1990).

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

$\tilde{X}\,^1B_1$ 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

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).

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).

$Ca(OH)_2$

$\tilde{X}$

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

[1]J. W. Kauffman, R. H. Hauge, and J. L. Margrave, High Temp. Sci. **18**, 97 (1984).

$Ba(OH)_2$

$\tilde{X}$

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

References

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

$Ni(OH)_2$

$\tilde{X}$

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

References

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

H_2CCN^-

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.
			951(10)	gas	PD	4
b_1	5	H_2CC deform.	692(10)	gas	PD	4

$A_0 = 9.510$; $B_0 = 0.341$; $C_0 = 0.329$ PD[3]

References

[4]D. M. Wetzel and J. I. Brauman, J. Chem. Phys. **90**, 68 (1989).

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 ($\nu_2 + \nu_8$) combination band.
[b]Both ND-stretching frequencies presumed equal.

References

[1]S. T. King and J. H. Strope, J. Chem. Phys. **54**, 1289 (1971).
[2]M. Birk and M. Winnewisser, Chem. Phys. Lett. **123**, 386 (1986).
[3]M. Winnewisser and M. Birk, J. Chem. Soc., Faraday Trans. 2 **84**, 1341 (1988).
[4]M. Birk, M. Winnewisser, and E. A. Cohen, J. Mol. Spectrosc. **136**, 402 (1989).

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	~599	Ar	IR	1
	7	Bend	~523	Ar	IR	1
	8	Bend	~383	Ar	IR	1
	9	Bend	~346	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	2586.8v	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

References

[1]R. Hochstrasser and J. Wirz, Angew. Chem. **101**, 183 (1989); Angew. Chem. Int. Ed. Engl. **28**, 181 (1989).

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

References

[1]A. Krantz and J. Laureni, J. Am. Chem. Soc. **96**, 6768 (1974).
[2]A. Krantz and J. Laureni, J. Am. Chem. Soc. **103**, 486 (1981).
[3]M. Hawkins, M. J. Almond, and A. J. Downs, J. Phys. Chem. **89**, 3326 (1985).

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	657m[b]	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.
[b]Tentative. See Refs. 5 and 6.

References

[1]J. Laureni, A. Krantz, and R. A. Hajdu, J. Am. Chem. Soc. **98**, 7872 (1976).
[2]A. Krantz and J. Laureni, J. Am. Chem. Soc. **99**, 4842 (1977).
[3]M. Torres, A. Clement, J. E. Bertie, H. E. Gunning, and O. P. Strausz, J. Org. Chem. **43**, 2490 (1978).
[4]M. Torres, I. Safarik, A. Clement, J. E. Bertie, and O. P. Strausz, Nouv. J. Chim. **3**, 365 (1979).
[5]A. Krantz and J. Laureni, J. Org. Chem. **44**, 2730 (1979).

[6]A. Krantz and J. Laureni, J. Am. Chem. Soc. **103**, 486 (1981).
[7]M. Hawkins, M. J. Almond, and A. J. Downs, J. Phys. Chem. **89**, 3326 (1985).
[8]W. D. Allen, J. E. Bertie, M. V. Falk, B. A. Hess, Jr., G. B. Mast, D. A. Othen, L. J. Schaad, and H. F. Schaefer III, J. Chem. Phys. **84**, 4211 (1986).

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

References

[1]J. W. Kauffman, 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. 355–362.

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

References

[1]J. W. Kauffman, 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. 355–362.

$CHBr=CH$

$\tilde{X}$ 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

References

[1]A. Engdahl and B. Nelander, J. Chem. Soc., Perkin Trans. 2, 1747 (1985).

$CH_2=NCl$

$\tilde{X}$ 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

References

[1]Y. Amatatsu, Y. Hamada, and M. Tsuboi, J. Mol. Spectrosc. **129**, 364 (1988).

$CH_2=PCl$

$\tilde{X}$ 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

$A_0 = 0.758$; $B_0 = 0.156$; $C_0 = 0.108$ $MW^{1,2}$

$CD_2{=}PCl$

$\tilde{X}$ 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]

References

[1]H. W. Kroto, J. F. Nixon, O. Ohashi, K. Ohno, and N. P. C. Simmons, J. Mol. Spectrosc. **103**, 113 (1984).
[2]B. Bak, N. A. Kristiansen, and H. Svanholf, Acta Chem. Scand. A **36**, 1 (1982).
[3]K. Ohno, E. Kurita, M. Kawamura, and H. Matsuura, J. Am. Chem. Soc. **109**, 5614 (1987).

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).

6.10. Five-Atomic Monohydrides

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	6
	2	C≡C stretch	2083.9wm	Ar	IR	6
	3	C≡C stretch	2060.6ms	Ar	IR	1,6

$B_0 = 0.165$ MW[2-5]

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	6
	2	C≡C stretch	2056.5wm	Ar	IR	6
	3	C≡C stretch	2049.6ms	Ar	IR	1,6

References

[6]L. N. Shen, T. J. Doyle, and W. R. M. Graham, J. Chem. Phys. **93**, 1597 (1990).

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).

HCOCN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	C≡N stretch	2229	gas	IR	2
	3	C=O stretch	1716	gas	IR	2
	5	C-C stretch	914	gas	IR	2
	7	CCN bend	230	gas	LF,IR	1,2
a''	9	CCN bend	278	gas	LF	1

A_0 = 2.251; B_0 = 0.167; C_0 = 0.155 MW[3]

References

[3]M. Bogey, J. L. Destombes, Y. Vallee, and J. L. Ripoll, Chem. Phys. Lett. **146**, 227 (1988).

HC(O)OO

(Formylperoxy)

$\tilde{X}$

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).

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	1624?	Ar	IR	1
		CF stretch	1217wm	Ar	IR	1
		NF stretch	968wm	Ar	IR	1

References

[1]R. D. Hunt and L. Andrews, Inorg. Chem. **26**, 3051 (1987).

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]

References

[1]M. J. Hopkinson, H. W. Kroto, J. F. Nixon, and N. P. C. Simmons, J. Chem. Soc., Chem. Commun. 513 (1976).
[2]H. W. Kroto, Chem. Soc. Rev. **11**, 435 (1982).
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HCF_3^+

$\tilde{D},\tilde{E}\ ^2E,^2A_1$ C_{3v}

$T^a \sim 54400$ 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] 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

References

[5]L. C. Lee, J. C. Han, C. Ye, and M. Suto, J. Chem. Phys. **92**, 133 (1990).

$HOPO_2$

$\tilde{X}$ 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

References

[1]R. Withnall and L. Andrews, J. Phys. Chem. **91**, 784 (1987).

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).
[2]R. Withnall and L. Andrews, J. Phys. Chem. **92**, 4610 (1988).

$HOAsO_2$

$\tilde{X}$

Vib. No. sym.	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. No. sym.	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

[1]L. Andrews, R. Withnall, and B. W. Moores, J. Phys. Chem. **93**, 1279 (1989).

$HSbO_3$

$\tilde{X}$

Vib. No. sym.	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. No. sym.	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. No. sym.	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. No. sym.	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).

$HOSO_2$

$\tilde{X}$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	OH stretch	3539.9wm	Ar	IR	1,2
	SO_2 a-stretch	1309.2m	Ar	IR	1,2
	SO_2 s-stretch	1097.3m	Ar	IR	1,2
	S—OH stretch	759.5m	Ar	IR	1,2

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).

6.11. Five-Atomic Nonhydrides

C_5

$\tilde{X}\ ^3\Sigma_g^-$ $D_{\infty h}$ Structure: ESR[2]

Vib. No. sym.		Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	2169.441	gas	IR,DL	4–7
			2168(3)	Ne	IR	2
			2164	Ar	IR	1–3
Π_g	5	Bend	~218(13)	gas	DL	7
Π_u	7	Bend	~118(3)	gas	DL	7

$B_0 = 0.0853$ 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).
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[7]N. Moazzen-Ahmadi, A. R. W. McKellar, and T. Amano, J. Chem. Phys. **91**, 2140 (1989).

C_4O

$\tilde{X}$

Vib. No. sym.	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).

$N{\equiv}C{-}CNO$

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

Vib. No. sym.	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. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		~2280vs	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).
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[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. No. sym.	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).

P_4O

$\tilde{X}$ C_{3v}

Vib. No. sym.		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. No. sym.	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).

As_4O

$\tilde{X}$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		981.5[a]	Ar	IR	1

[a]Tentative assignment.

References

[1]L. Andrews and Z. Mielke, Inorg. Chem. **28**, 4001 (1989).

br-As_4O

$\tilde{X}$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	AsOAs a-stretch	590.3s	Ar	IR	1
		565.4s			
	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).

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.

$\tilde{X}$ C_s Structure: MW^3

Vib. No. sym.		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. Liege **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).
[6]E. M. Nour, L.-H. Chen, and J. Laane, J. Phys. Chem. **87**, 1113 (1983).
[7]M. E. Jacox and W. E. Thompson, J. Chem. Phys. **93** (in press).

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 to O_2N-NO.[1,3]

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

Vib. No. sym.		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	Sym. O=NO bend	366s	N_2	IR	1
a_2	5	Torsion	140	NO	Ra	2
b_1	6	Torsion	105[a]	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

$\tilde{X}$ — Continued

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
8	N—O a-stretch	877vw	N_2	IR	1
		865vw	NO	IR	2
9	Asym. O=NO bend	704vw	N_2	IR	1
		705vw	NO	IR	2

[a] $\frac{1}{2}(2\nu_6)$.

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**, (in press).

ON—NSO

$\tilde{X}$

Vib. No. sym.	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]

$\tilde{X}$

Vib. No. sym.	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).

cyc-F_2SiO_2

$\tilde{X}$

Vib. No. sym.	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. No. sym.	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. No. sym.	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. No. sym.	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).

$BrONO_2$

$\tilde{X}$ 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

[1]W. W. Wilson and K. O. Christe, Inorg. Chem. **26**, 1573 (1987).

Cl_2O_3

An unstructured gas-phase absorption with maximum at 37700 (265 nm) has been assigned[2,4] 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).
[3]B.-M. Cheng and Y.-P. Lee, J. Chem. Phys. **90**, 5930 (1989).
[4]J. B. Burkholder, J. J. Orlando, and C. J. Howard, J. Phys. Chem. **94**, 687 (1990).

CF_3O

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF_3 stretch	1221.6	Ar	IR	1,2

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).

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

Spin-orbit splitting = +16(1) EF[6-8]
τ = 9.0(9) ns gas EF[1]EM[9]
$B_0 \sim 0.168$[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.

References

[1]J. E. Hesser and K. Dressler, J. Chem. Phys. **47**, 3443 (1967).
[2]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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[8]R. N. Dixon and R. P. Tuckett, Chem. Phys. Lett. **140**, 553 (1987).
[9]I. R. Lambert, S. M. Mason, R. P. Tuckett, and A. Hopkirk, J. Chem. Phys. **89**, 2683 (1988).
[10]L. C. Lee, J. C Han, C. Ye, and M. Suto, J. Chem. Phys. **92**, 133 (1990).

CF_3Cl^+

$\tilde{D}\ ^2E$ C_{3v}

T_0^a= 39720(400) gas PE[1,2,4]

Broad emission bands in the 200–600 nm spectral region which appear on excitation of CF_3Cl by synchrotron radiation of wavelength less than about 62 nm have been tentatively attributed[8] to transitions arising from the $\tilde{D}$ state of CF_3Cl^+.

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

References

[8]L. C. Lee, J. C. Han, C. Ye, and M. Suto, J. Chem. Phys. **92**, 133 (1990).

CF_3Br^+

$\tilde{D}\ ^2E$ 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

References

[6]L. C. Lee, J. C. Han, C. Ye, and M. Suto, J. Chem. Phys. **92**, 133 (1990).

$CF_2Cl_2^+$

$\tilde{D}\ ^2B_2$ 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

References

[8]Z. J. Jabbour and K. Becker, J. Chem. Phys. **90**, 4819 (1989).

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

Spin-orbit splitting = +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_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]

References

[1]J. E. Hesser and K. Dressler, J. Chem. Phys. **47**, 3443 (1967).
[2]T. P. Fehlner and D. W. Turner, Inorg. Chem. **13**, 754 (1974).
[3]D. R. Lloyd and P. J. Roberts, J. Electron Spectrosc. Relat. Phenom. **7**, 325 (1975).
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[7]S. M. Mason and R. P. Tuckett, Mol. Phys. **60**, 771 (1987).
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[9]S. M. Mason and R. P. Tuckett, Mol. Phys. **62**, 175 (1987).
[10]H. van Lonkhuyzen and J. F. M. Aarts, Chem. Phys. Lett. **140**, 434 (1987).
[11]R. N. Dixon and R. P. Tuckett, Chem. Phys. Lett. **140**, 553 (1987).
[12]I. R. Lambert, S. M. Mason, R. P. Tuckett, and A. Hopkirk, J. Chem. Phys. **89**, 2683 (1988).

SiCl‡

$\tilde{D}\ ^2A_1$ 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	~290	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‡. 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‡.

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‡. 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	717[b]	Ar	IR	4

[a]From vertical ionization potential.
[b]Tentative assignment.

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]P. J. Bassett and D. R. Lloyd, J. Chem. Soc. A 641 (1971).
[3]R. G. Egdell, I. L. Fragala, and A. F. Orchard, J. Electron Spectrosc. Relat. Phenom. **17**, 267 (1979).
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SiBr‡

$\tilde{D}\ ^2A_1$ 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‡, 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‡.

$\tilde{B}\ ^2E$ 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.

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).

GeF‡

$\tilde{D}\ ^2A_1$ 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‡, 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]	

[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

[7]I. R. Lambert, S. M. Mason, R. P. Tuckett, and A. Hopkirk, J. Chem. Phys. **89**, 2683 (1988).

GeCl‡

$\tilde{D}\ ^2A_1$ 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‡. 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‡.

$\tilde{B}\ ^2E$

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).
[2]P. J. Bassett and D. R. Lloyd, J. Chem. Soc. A 641 (1971).
[3]I. R. Lambert, S. M. Mason, R. P. Tuckett, and A. Hopkirk, J. Chem. Phys. **89**, 2675 (1988).
[4]I. R. Lambert, S. M. Mason, R. P. Tuckett, and A. Hopkirk, J. Chem. Phys. **89**, 2683 (1988).

GeBr‡

$\tilde{D}\ ^2A_1$ 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‡, 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‡.

$\tilde{B}\ ^2E$ 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).

$SClF_3$

$\tilde{X}$

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).

6.12. Six-Atomic Molecules

$B_2H_4^{\ddagger}$

$\tilde{X}$ 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. Ruščic, 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).

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
	2	BH stretch	2495	gas	IR	2
	3	NH_2 scissors	1625	gas	IR	2
	4	BN stretch	1337.47	gas	IR	2
	5	BH_2 scissors	1225	gas	IR	2
a_2	6	Torsion	~820[a]	gas	IR	3
b_1	7	NH_2 wag	1005	gas	IR	2
	8	BH_2 wag	612s	gas	IR	3
b_2	9	NH stretch	3534	gas	IR	2
	10	BH stretch	2564	gas	IR	2
	11	NH_2 rock	1131	gas	IR	2
	12	BH_2 rock	~742vw	gas	IR	3

$A_0 = 4.610$; $B_0 = 0.917$; $C_0 = 0.763$ MW[1]

[a]Value estimated from appearance of perturbation.

References

[1]M. Sugie, H. Takeo, and C. Matsumura, Chem. Phys. Lett. 64, 573 (1979).
[2]M. C. L. Gerry, W. Lewis-Bevan, A. J. Merer, and N. P. C. Westwood, J. Mol. Spectrosc. **110**, 153 (1985).
[3]W. D. Anderson, M. C. L. Gerry, W. Lewis-Bevan, A. J. Merer, and D. M. Steunenberg, 41st Symposium on Molecular Spectroscopy, Columbus, Ohio, June 1986.

$CH_2NH_2^+$

$\tilde{X}\ ^1A_1$ 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).

SiH_3OH [a]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Si—O stretch	859	Ar	IR	1

SiD_3OD [a]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Si—O stretch	874	Ar	IR	1

[a]Tentative identification.

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).

$SrOCH_3$

References

[3]L. C. O'Brien, C. R. Brazier, and P. F. Bernath, J. Mol. Spectrosc. **130**, 33 (1988).

CH_2CCH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	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

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

[b]Ref. 4 presents arguments for the reassignment of this absorption to *cyc*-C_3H_3.

References

[4]J. W. Huang and W. R. M. Graham, J. Chem. Phys. **93**, 1583 (1990).

$CH_2{=}C{=}NH^+$

$\tilde{B}\ ^2A'$ 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).

$CH_2{=}C{=}NH$

$\tilde{X}$ 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).
[3]M. E. Jacox, Chem. Phys. **43**, 157 (1979).
[4]M. Rodler, R. D. Brown, P. D. Godfrey, and L. M. Tack, Chem. Phys. Lett. **110**, 447 (1984).
[5]M. Rodler, R. D. Brown, P. D. Godfrey, and B. Kleibömer, J. Mol. Spectrosc. **118**, 267 (1986).
[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).
[3]K. Ohno, H. Matsuura, D. McNaughton, and H. W. Kroto, J. Mol. Spectrosc. **124**, 82 (1987).
[4]K. Ohno, H. Matsuura, D. McNaughton, and H. W. Kroto, J. Mol. Spectrosc. **126**, 245 (1987).

$HCr(OH)_2$ [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 $\times > 1$.

References

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

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
	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	~400	gas	IR	1,4

$A_0 = 2.258$; $B_0 = 0.396$; $C_0 = 0.336$ MW[2,3,5]

References

[1]S. Califano and W. Lüttke, Z. Phys. Chem. **6**, 83 (1956).
[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).

CH_3O_2

On photolysis of CH_3NNCH_3:O_2 or CH_4:O_2:Cl_2 mixtures, an unstructured absorption which has been assigned[1,3,4,6,7] to CH_3O_2 appears between 200 and 280 nm, with a maximum at ~240 nm. In an argon matrix, CH_3O_2 photolyzes on exposure to 254-nm radiation.[5]

References

[7]P. Dagaut and M. J. Kurylo, J. Photochem. Photobiol. A: Chem. **51**, 133 (1990).

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).

$CH_3S_2^-$

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_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[a]	Ar	IR	1
		HNF rock	1282s[a]	Ar	IR	1
		NH_2 wag	1091w[a]	Ar	IR	1
		NF stretch	1013w,br[a]	Ar	IR	1

[a]Molecule hydrogen-bonded to HF.

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}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	3	PH_3 deform.	1262w	gas	IR	1
	4	PF_2 a-stretch	759vs	gas	IR	1
			755	Ar	IR	2
e'	5	PH_3 a-stretch	2500m	gas	IR	1
			2480w,br	Ar	IR	2
	6	PH_3 deform.	970s	gas	IR	1
			974	Ar	IR	2

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

References

[1]F. Seel and K. Velleman, Z. Anorg. Allg. Chem. **385**, 123 (1971).
[2]L. Andrews and R. Withnall, Inorg. Chem. **28**, 494 (1989).

$C_4H_2^+$

$\tilde{B}$

$T_0 = 51960(160)$ gas PE[2]

$\tilde{A}\ ^2\Pi_u$ $D_{\infty h}$ Structure: LF[9]

T_0 = 19722.610(2) gas EM[1]EF[7]LF[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≡Cstretch	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[3]PEFCO[5]LF[6]
A_0 = −31.1(2.0) gas EM[1]LF[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[1]LF[4,9]EF[7]
B_0 = 0.147 EM[1]EF[7]LF[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[1]LF[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.	418[ab]	Ne	LF	4

τ = 79(4) ns gas EF[5]PEFCO[5]LF[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
Σ_u^+	4	CD stretch	2180(40)[b]	gas	PE	2
Π_g	7	Deformation	412.8[b]	gas	EM	1
			414(2)[b]	Ne	LF	4

A = −33.3(2.0) gas EF[7]LF[9]
B_0 = 0.127 EF[7]LF[9]

[a]Alternate assignment in which values of ν_3 and $2\nu_7$ are interchanged is also possible.
[b] $\frac{1}{2}(2\nu_i)$.

References

[9]J. Lecoultre, J. P. Maier, and M. Rösslein, J. Chem. Phys. **89**, 6081 (1988).

$HCCCNH^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NH stretch	3513.96	gas	LD	1

B_0 = 0.144 LD[1]

References

[1]S. K. Lee and T. Amano, Astrophys. J. **323**, L145(1987).

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. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	Ca stretch	355(10)	gas	LF	1

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

Vib. No. sym.	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. No. sym.	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. No. sym.	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. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	Sr stretch	278(10)	gas	LF	1

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

Vib. No. sym.	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. No. sym.	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).

$H_2C{=}C{=}C{=}O$

$\tilde{X}$ C_s Structure: MW[2]

Vib. No. sym.	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
	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).
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$H_2C=C=C=Se$

$\tilde{X}$

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

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HC≡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).

t-HN=CHCN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	C≡N stretch	2250	gas	IR	1
	4	C=N stretch	~1605	gas	IR	1
	5	CH bend	1387	gas	IR	1
	6	CNH bend	1218	gas	IR	1
	7	CC stretch	~900	gas	IR	1
a"	10	Torsion	1095	gas	IR	1
	11	CH OPLA	~800	gas	IR	1

References

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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

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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	~200[a]	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. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	OCF deform.	491	gas	PD	1
	Torsion	172[a]	gas	PD	1

$\tilde{X}$ C_s

Vib. No. sym.	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

[a] $\frac{1}{2}(2\nu_i)$.

References

[1]J. Marks, J. I. Brauman, R. D. Mead, K. R. Lykke, and W. C. Lineberger, J. Chem. Phys. **88**, 6785 (1988).

H_2SiO_3

$\tilde{X}$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type	Refs. meas.
	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. No. sym.	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. No. sym.	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. No. sym.	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).

$HOONO_2$

In the gas phase, the threshold for unstructured absorption 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. No. sym.	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
		941.0w	gas	IR	1,3
		922.1w	gas	IR	1,3
		919.2w	gas	IR	1,3
6	N–O stretch	802.7m	gas	IR	1–4,7,9
12	NO_2 torsion	145(6)	gas	MW	8

A_0 = 0.400; B_0 = 0.156; C_0 = 0.113 gas MW[8]

References

[1]H. Niki, P. D. Maker, C. M. Savage, and L. P. Breitenbach, Chem. Phys. Lett. **45**, 564 (1977).
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[3]R. A. Graham, A. M. Winer, and J. N. Pitts, Jr., Chem. Phys. Lett. **51**, 215 (1977).

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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).
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[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).

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]

$\tilde{X}$ V_h Structure: ED[1]

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		79	gas	IR[a]	6
b_{1g}	5		1718(3)	Xe	Ra	8
	6		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
b_{2u}	9		1758	gas	IR	6
			1749.2s	Ar	IR	2,3,9
			1735s			
			1761	N_2	IR	4
			1737			
			1750	O_2	IR	3
			1735			
b_{3u}	11		1264	gas	IR	2,6
			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]From analysis of sequence bands near 540 cm^{-1}.

References

[1]D. W. Smith and K. Hedberg, J. Chem. Phys. **25**, 1282 (1956).
[2]W. G. Fateley, H. A. Bent, and B. Crawford, Jr., J. Chem. Phys. **31**, 204 (1959).
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$ONO—NO_2$

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.

$\tilde{X}$ (Structure D)

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

$\tilde{X}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		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

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[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).

$(SiO)_3$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	4	Deformation	74[a]	Ar	IR	2
e'	5	SiO stretch	971.9s	Ar	IR	1,2
			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

[a]Tentative assignment.

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).

$(GeO)_3$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	5	GeO stretch	824s	Ar	IR	1
			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).

$(PN)_3$

$\tilde{X}$ 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

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$F_2C=C=C=O$

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

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1914.5m	Ar	IR	1
			1779.9m	Ar	IR	1
			1761.2m	Ar	IR	1
			1285.5s	Ar	IR	1
			1071.4w	Ar	IR	1
			860.2w	Ar	IR	1
			699.6w	Ar	IR	1
			656.0w	Ar	IR	1

References

[1]J. C. Brahms and W. P. Dailey, J. Am. Chem. Soc. **111**, 8940 (1989).

$OPCl_2OCl$

$\tilde{X}$

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

$\tilde{X}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			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	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).
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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).

6.13. Seven-Atomic Molecules

$B_2H_5^{\pm}$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			~1290	gas	PI	1

References

[1]B. Ruscic, M. Schwarz, and J. Berkowitz, J. Chem. Phys. **91**, 4183 (1989).

$C_2H_5^{\pm}$

$\tilde{X}$ 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. sym.	No.	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 stretc	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

References

[1]H. R. Wendt, D. Wyrsch, and H. E. Hunziker, Ber. Bunsenges. Phys. Chem. **78**, 201 (1974).
[2]J. Pacansky, G. P. Gardini, and J. Bargon, J. Am. Chem. Soc. **98**, 2665 (1976).
[3]D. A. Parkes and C. P. Quinn, J. Chem. Soc., Faraday Trans. 1 **72**, 1952 (1976).
[4]J. Pacansky and M. Dupuis, J. Am. Chem. Soc. **104**, 415 (1982).
[5]J. Pacansky and B. Schrader, J. Chem. Phys. **78**, 1033 (1983).
[6]H. R. Wendt and H. E. Hunziker, J. Chem. Phys. **81**, 717 (1984).
[7]J. Munk, P. Pagsberg, E. Ratajczak, and A. Sillesen, J. Phys. Chem. **90**, 2752 (1986).
[8]G. Chettur and A. Snelson, J. Phys. Chem. **91**, 3483 (1987).
[9]A. D. Sappey and J. C. Weisshaar, J. Phys. Chem. **91**, 3731 (1987).

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

References

[1]L. Manceron and L. Andrews, J. Phys. Chem. **90**, 4514 (1986).

$H_5O_2^+$

$\tilde{X}$ 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

References

[1]L. I. Yeh, M. Okumura, J. D. Myers, J. M. Price, and Y. T. Lee, J. Chem. Phys. **91**, 7319 (1989).

$HFeC_2H_3$

$\tilde{X}$

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
	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

$\tilde{X}$ — Continued

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	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

References

[1]Z. H. Kafafi, R. H. Hauge, and J. L. Margrave, J. Am. Chem. Soc. **107**, 7550 (1985).

AlC_2H_4

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

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CH stretch	~3094	Ar	IR	1
	CH stretch	~2980	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 s-stretch	352ms	Ar	IR	1
	AlC 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	~2337	Ar	IR	1
	CD stretch	~2194	Ar	IR	1
	CD stretch	~2175	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 s-stretch	337ms	Ar	IR	1
	AlC a-stretch	212m	Ar	IR	1

References

[1]L. Manceron and L. Andrews, J. Phys. Chem. **93**, 2964 (1989).

$HNiOCH_3$

$\tilde{X}$

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	Refs. meas.
		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

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

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

$B_0 = 0.287$ LD[1]

References

[1]T. Amano, Astrophys. J. **330**, L137 (1988).

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

[1]R. Withnall and L. Andrews, J. Am. Chem. Soc. **108**, 8118 (1986).
[2]R. Withnall and L. Andrews, J. Phys. Chem. **92**, 594 (1988).

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	284[a]	gas	LF	3
	10	CCl bend	184[a]	gas	LF	3

$\tau_1 = 19(3)$ ns gas EF^2
$\tau_2 = 600(200)$ 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	318[b]	gas	EF	3
	10	CCl bend	271[a]	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	263[a]	gas	LF	3
	10	CCl bend	155[a]	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	311[b]	gas	EF	3
	10	CCl bend	222[b]	gas	EF	3

[a] $\frac{1}{2}(2\nu_i)$.
[b]Tentative assignment.

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 E. Kloster-Jensen, J. Electron Spectrosc. Relat. Phenom. **18**, 251 (1980).
[3]D. Klapstein, R. Kuhn, J. P. Maier, M. Ochsner, and T. Wyttenbach, Chem. Phys. **101**, 133 (1986).

$CH_3C{\equiv}CBr^+$

$\tilde{B}\ ^2A_1$ 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	207[a]	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	335[b]	gas	EF	3
	10	CBr bend	259[a]	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	195[a]	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	243[a]	gas	EF	3

[a] $\frac{1}{2}(2\nu_i)$.
[b]Tentative assignment.

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 E. Kloster-Jensen, J. Electron Spectrosc. Relat. Phenom. **18**, 251 (1980).
[3]D. Klapstein, R. Kuhn, J. P. Maier, M. Ochsner, and T. Wyttenbach, Chem. Phys. **101**, 133 (1986).

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

$\tilde{X}$ — Continued

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
		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).

$(HO)_2HPO$

$\tilde{X}$

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).

$H(C{\equiv}C)_2CN^+$

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

T_0 = 27350(160) gas PE[1]

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

T_0 = 21860(160) gas PE[1]

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

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	Refs. meas.
Σ^+		C≡C stretch	1870(160)	gas	EF	1
	6	C–C stretch	600(160)	gas	EF	1

τ_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

References

[1]G. Bieri, E. Kloster-Jensen, S. Kvisle, J. P. Maier, and O. Marthaler, J. Chem. Soc., Faraday Trans. 2 **76**, 676 (1980).

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).
[2]F. Holland, M. Winnewisser, G. Maier, H. P. Reisenauer, and A. Ulrich, J. Mol. Spectrosc. **130**, 470 (2988).

$O_2N{-}O{-}NO_2$

$\tilde{X}$ 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	~614m	gas	IR	2
	5	NON s-stretch	~353vs	gas	IR	2
b_1	9	NO_2 wag	557s	gas	IR	2,5
	10	NO_2 twist	~50w,br	gas	IR	9
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	~353vs	gas	IR	2,9

[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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6.14. Eight-Atomic Molecules

Ga_2H_6

$\tilde{X}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{1u}	8	GaH_t stretch	1998m	gas	IR	1
			2015m	Ar	IR	1
			1996m			
			2000m	N_2	IR	1
	9	GaH_2 rock?	659m	Ar	IR	1
			655m			
			653m			
			648m			
			655s	N_2	IR	1
			647w			
b_{2u}	13	GaH_b stretch	1267s	gas	IR	1
			1283s	Ar	IR	1
			1278m			
			1253m			
			1282m	N_2	IR	1
	14	GaH_2 rock	760w	gas	IR	1
			773m	Ar	IR	1
			761m			
			770m	N_2	IR	1

$\tilde{X}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{3u}	16	GaH_t stretch	~1976	gas	IR	1
			1985s	Ar	IR	1
			1968m			
			1985m	N_2	IR	1
	17	GaH_b stretch	~1200m	gas	IR	1
			1213m	Ar	IR	1
			1208m			
			1195m			
			1220s	N_2	IR	1
	18	GaH_2 bend	~671vs	gas	IR	1
			676vs	Ar	IR	1
			666s			
			673vs	N_2	IR	1

Ga_2D_6

$\tilde{X}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{1u}	8	GaD_t stretch	1446m	gas	IR	1
			1434m,sh			
	9	GaD_2 rock	439wm	gas	IR	1
b_{2u}	13	GaD_b stretch	914s	gas	IR	1
	14	GaD_2 rock	545m	gas	IR	1
b_{3u}	16	GaD_t stretch	~1416m	gas	IR	1
	17	GaD_b stretch	~860m	gas	IR	1
	18	GaD_2 bend	~484vs	gas	IR	1

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cyc-$C_3H_5^{\ddagger}$

$\tilde{X}$ 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

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

gas AB^2 $\tilde{B}$–$\tilde{X}$ 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.

3s $^2A_1$ C_{2v}

T_0 = 40056.8(2.0) gas MPI[7,8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		C_3 bend	394(3)	gas	MPI	7,8
a_2		CH_2 a-twist	529(3)	gas	MPI	8
b_1		CH_2 s-twist	491(7)	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}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3107m	Ar	IR	4,5
		CH stretch	3051w	Ar	IR	4,5
		CH stretch	3040w	Ar	IR	4
		CH stretch	3019m	Ar	IR	4,5
			1602m	Ar	IR	4
			1477m	Ar	IR	4,5
			1463m	Ar	IR	4,5
			1403vw	Ar	IR	5
			1388s	Ar	IR	4,5
			1317vw	Ar	IR	4
			1283w	Ar	IR	4,5
			1242w	Ar	IR	4,5
			1182w	Ar	IR	4
			983.6s	Ar	IR	4,5,9
			972m	Ar	IR	4
			810w	Ar	IR	5
a_1		C_3 bend	427(5)	gas	MPI	7,8
a_2		CH_2 a-twist	547(15)	gas	MPI	8
b_1			801.1vs	Ar	IR	3–5,9
		CH_2 s-twist	508(12)	gas	MPI	7,8
			510.1s	Ar	IR	4,5,9

CD_2CDCD_2

3s $^2A_1$ C_{2v}

T_0 = 40125(30) gas MPI[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		C_3 bend	342(60)	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		C_3 bend	380(225)	gas	PE	6
b_1			646.5	Ar	IR	9

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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	~1359	gas	IR	3
			1358s	Ar	IR	1
	9	CH deform.	1102	gas	IR	3
			1106s	Ar	IR	1
	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
	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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$C_2H_3NH_2$

$\tilde{X}$ C_1[a]

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	~1625	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
			570[c]	gas	IR	2,4
			470[d]	gas	IR	4
			425[e]	gas	IR	4
	16	C=C torsion	379[b]	gas	IR	4
			~334[c]	gas	IR	4
			~332[d]	gas	IR	4
			287[e]	gas	IR	4

$A_0 = 1.879$; $B_0 = 0.335$; $C_0 = 0.286$ $MW^{1,3}$

[a]The barrier to inversion about the N atom is estimated to be between 400 and 800 cm^{-1}, [3,4] leading to splittings in a number of the vibrational band centers.
[b] $1^- - 0^+$.
[c] $1^- - 0^-$.
[d] $1^+ - 0^+$.
[e] $1^+ - 0^-$.

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$H_2C{=}NCH_3$

$\tilde{X}$ 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			
	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.	1425w[a]	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	1026vs	gas	IR	3
			1026vvs	Ar	IR	2–4
			1030	N_2	IR	4
	17	C=N torsion	686w	gas	IR	3
	18	CH_3 twist	220w[a]	Ar	IR	3

$A_0 = 1.752$; $B_0 = 0.356$; $C_0 = 0.313$ MW[1]

[a]Tentative assignment.

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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

$\tau_0 = 1.7(2)$ 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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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

$\tau = 75$ 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

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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).

$H_2C=(cyc\text{-}C_3H_2)$

$\tilde{X}$

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

References

[1]W. E. Billups, L-J. Lin, and E. W. Casserly, J. Am. Chem. Soc. **106**, 3698 (1984).
[2]G. Maier, M. Hoppe, K. Lanz, and H. P. Reisenauer, Tetrahedron Lett. **25**, 5645 (1984).

cyc-C_4H_4

$\tilde{X}$ D_{2h} Structure: IR[3-5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{1u}		CH stretch	3105wm	Ar	IR	5
		C=C stretch	1526w	Ar	IR	4,5
		CH deform.	1028vw	Ar	IR	5
b_{2u}		CH stretch	3073w	Ar	IR	5
		CH deform.	1242s	Ar	IR	1-5
		Ring deform.	719wm	Ar	IR	4,5
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

[1]O. L. Chapman, C. L. McIntosh, and J. Pacansky, J. Am. Chem. Soc. **95**, 614 (1973).
[2]C. Y. Lin and A. Krantz, J. Chem. Soc., Chem. Commun. 1111 (1972).
[3]G. Maier, H.-G. Hartan, and T. Sayrac, Angew. Chem. **88**, 252 (1976); Angew. Chem., Int. Ed. Engl. **15**, 226 (1976).
[4]S. Masamune, F. A. Souto-Bachiller, T. Machiguchi, and J. E. Bertie, J. Am. Chem. Soc. **100**, 4889 (1978).
[5]G. Maier, Angew. Chem. **100**, 317 (1988); Angew. Chem. Int. Ed. Engl. **27**, 309 (1988).

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

$\tilde{X}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		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.	629.2[a]	Ar	IR	1
			626.0	Xe	IR	1

[a]Tentative assignment.

References

[1]K. A. Singmaster and G. C. Pimentel, J. Mol. Struct. **194**, 215 (1989).

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	~2900	gas	IR	1
		OOH bend	~1350	gas	IR	1
		CO stretch	1050	gas	IR	1
		OO stretch	~820	gas	IR	1

References

[1]F. Su, J. G. Calvert, J. H. Shaw, H. Niki, P. D. Maker, C. M. Savage, and L. P. Breitenbach, Chem. Phys. Lett. **65**, 221 (1979).
[2]H. Niki, P. D. Maker, C. M. Savage, and L. P. Breitenbach, Chem. Phys. Lett. **75**, 533 (1980).

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

$\tilde{X}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			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).
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[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)[a]	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	244[a]	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)[a]	gas	LF	3

[a]Tentative assignment.

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).

$CF_2{=}PCF_3$

$\tilde{X}$ 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).

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).

$(CH_3)_2CH$

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

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}.

References

[1]D. A. Parkes and C. P. Quinn, Chem. Phys. Lett. **33**, 483 (1975).
[2]D. A. Parkes and C. P. Quinn, J. Chem. Soc., Faraday Trans. 1 **72**, 1952 (1976).
[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.	303[ab] 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.	313[ab] 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	284[ab]	gas	EF	4

τ_0 = 53(3) ns gas EF[1]PEPICO[3]

$\tilde{A}\ ^2B_1$ 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

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C_6 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.
		C_6 deform.	519s	Ar	IR	2,5

References

[1]G. Porter and B. Ward, Proc. Roy. Soc. (London) **A287**, 457 (1965).
[2]J. Pacansky and J. Bargon, J. Am. Chem. Soc. **97**, 6896 (1975).
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[4]J. H. Miller, L. Andrews, P. A. Lund, and P. N. Schatz, J. Chem. Phys. **73**, 4932 (1980).
[5]M. E. Jacox, J. Phys. Chem. **86**, 670 (1982).
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$C_6H_6^+$

$\tilde{G}\ ^2A_{1g}$ 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]

$T_0 \sim$ 19840[c] Ar LF[3]AB[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)[c]	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[d]	gas	PF	9
e_{2g}	16 (8)	Ring stretch	1520(100)[c]	gas	PE	1
	17 (9)	CH bend	1140[d]	gas	PF	9
	18 (6)	Ring deform.	645(100)[e]	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)[c]	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)[e]	gas	PE	1,6
			1480(10)[c]	Ar	LF	3
	17 (9)	CH bend	1230(15)[e]	gas	PE,MPI	1,6,8
	18 (6)	Ring deform.	660(15)[e]	gas	PE,MPI	1,6,8
			630(10)[c]	Ar	LF	3
			340(10)[f]	gas	PE	6
e_{2u}	20 (16)	Ring deform.	295(5)	gas	PE,MPI	6,8

$B_0 \sim 0.2$ gas PE[7]

$C_6D_6^+$

$\tilde{G}\,^2A_{1g}$ D_{6h}

$T^a \sim 62000$ 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}

$T^a \sim 50000$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1[b] (2)	CD stretch	~1610	gas	PE	1

$\tilde{C}\,^2A_{2u}$ D_{6h}

$T_0 \sim 19930$[c] Ar LF[3]AB[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)[c]	Ar	AB	4

$\tilde{B}\,^2E_{2g}$ D_{6h}

$T^a \sim 18600$ 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
e_{2g}	16 (8)	Ring stretch	1565(100)	gas	PE	1
			1460(10)[c]	Ar	LF	3
	18 (6)	Ring deform.	637(20)[e]	gas	PE	1,6
			590(10)[c]	Ar	LF	3
			343(20)[f]	gas	PE	6
e_{2u}	20 (12)	Ring deform.	278(20)	gas	PE	6

[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]Tentative assignment.

[d]From analysis of combination bands.

[e] $j = 1/2$.

[f] $j = 3/2$.

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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	248[a]	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.	327[a]	gas	EF	7
e_g	20	Skel. deform.	237[a]	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	230[a]	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.	217[a]	gas	EF	7

[a] $\frac{1}{2}(2\nu_i)$.

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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-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
			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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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

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$C_6H_5CH_2$ [a]

$\tilde{E}$

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. 15. 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

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

T_0 = 22460(30) gas AB[11]EM[11]
Vibronically coupled to modes of b_2 symmetry in the $\tilde{A}$ state.[11]

$\tilde{A}\ ^2A_2$ C_{2v}

T_0 = 22001.5 gas EM[1,3,5,10]AB[4]LF[12] $\tilde{A}$-$\tilde{X}$ 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
			798	Ar	LF	13
	6a	Ring deform.	433	gas	AB	11,17
			433	Ne	AB	6
			456	Ar	LF	13
			388	gas	AB	11,16,17
			402	Ne	AB	6
			328	gas	AB	11,16,17
			344	Ne	AB	6

τ_{6a} = 880(10) ns gas LF[14]
$A_0 \sim 0.180^b$; $B_0 = 0.089^b$; $C_0 = 0.059^b$ EM[10,16,18]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	8a	Ring stretch	1603	gas	EM	5,8,17
	19a	Ring stretch	1431	gas	EM	5,8,17
			1423	Ar	LF	13
	7a	C-CH_2 stretch	1258	gas	EM	5,7,17
	9a	CH deform.	1181	gas	EM	5,8
	18a	CH deform.	1046	gas	EM	17
	1	Ring breathing	987.4	gas	EM	5,8,10 17
			982	Ar	LF	13
	12a	Ring deform.	818	gas	EM	5,8,17
	6a	Ring deform.	524	gas	EM	5,8,10
			520	Ar	LF	13
a_2	17a	CH deform.	963	gas	EM	17
	10a	CH deform.	860	gas	EM	8,17
	16a	Ring deform.	393	gas	EM	8
b_1	16b	Ring deform.	430	gas	EM	8
b_2	8b	Ring stretch	1549	gas	EM	5,8,17
			1530	Ar	LF	13
	9b	CH deform.	1152	gas	EM	5,8,17
	15	CH deform.	1089	gas	EM	5,8

$\tilde{X}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	6b	Ring deform.	615	gas	EM	5,8,10 17
			612	Ar	LF	13
	18b	CH deform.	356	gas	EM	5,8,17
			357	Ar	LF	13

$A^\circ \sim 0.185$[b]; $B_0 = 0.090$[b]; $C_0 = 0.060$[b] EM[10,16,18]

$C_6D_5CD_2$

$\tilde{B}\ ^2B_1$ 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

$\tau \sim 1340$ ns gas LF[14]

$\tilde{X}\ ^2B_1$ 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 rotational band contours.

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$C_6H_5CH_2^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			945	gas	MPD	1

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p-$CH_3C_6H_4CH$:

(p-Tolylmethylene)

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

$\tilde{X}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1454w	Ar	IR	1,2
			1449m	Ar	IR	1,2
			1380w	Ar	IR	1,2
			1116w	Ar	IR	1,2
			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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m-$CH_3C_6H_4CH$:

(*m*-Tolylmethylene)

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
			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

$\tilde{X}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			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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o-$CH_3C_6H_4CH$:

(*o*-Tolylmethylene)

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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[1]R. J. McMahon and O. L. Chapman, J. Am. Chem. Soc. **109**, 683 (1987).
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o-$(CH_2)_2C_6H_4$

(*o*-Xylylene)

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

$CH_3SiH=CH_2$

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.

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[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).
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$(CH_3)_2Ge$

In an argon matrix, an absorption maximum has been observed[1,2] at 420 nm.

$\tilde{X}$

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

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[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).

$(CH_3)_2Sn$

$\tilde{X}$ 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

$(CD_3)_2Sn$

$\tilde{X}$ 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

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$(CH_3)_2Si=CH_2$ [a]

$\tilde{X}$ Structure: ED[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type	Refs. meas.
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.

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$C_5SiH_6^+$

(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

$\tilde{X}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1354vs	Ar	IR	1,2
			1259vs	Ar	IR	1,2
			1069wm	Ar	IR	2
			886m	Ar	IR	1,2
			720wm	Ar	IR	2
			716			
			700vs	Ar	IR	2
			698			
			568vs	Ar	IR	1,2
			565			
			419s	Ar	IR	1,2

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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

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[1]G. Maier, G. Mihm, and H. P. Reisenauer, Angew. Chem. **92**, 58 (1980); Angew. Chem. Int. Ed. Engl. **19**, 52 (1980).
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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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$CH_3(C{\equiv}C)_2Cl^+$

$\tilde{B}$ 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	319[b]	gas	LF	3
	13	CCCl bend	235(2)	gas	LF	3
	14	Skel. bend	87[b]	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)[b]	gas	EF	2

[a]From vertical ionization potential.
[b]Tentative assignment.

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$CH_3(C{\equiv}C)_2Br^+$

$\tilde{B}$ 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	2141[b]	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	306[b]	gas	LF	3
	13	CCBr bend	203(2)	gas	LF	3
	14	Skel. bend	76(2)	gas	LF	3

A = −720(80) gas PE[1]EF[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)[b]	gas	EF	3

A = −400(80) gas PE[1]EF[3]

[a]From vertical ionization potential.
[b]Tentative assignment.

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[1]E. Heilbronner, V. Hornung, J. P. Maier, and E. Kloster-Jensen, J. Am. Chem. Soc. **96**, 4252 (1974).
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1,3,5-$C_6H_3F_3^+$

$\tilde{B}\ ^2A_2''$ D_{3h}

T_0 = 21867.479 gas EF[1,12]EM[5]LF[3,9,15,16] $\tilde{B}$–$\tilde{X}$ 457–571 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
	2		954	gas	LF	9
			959	Ne	LF	7

$\tilde{B}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	13		489.99	gas	LF	3,8,9
						16
			484	Ne	LF	7,14
	14		323.81	gas	LF	8,9,16
			327	Ne	LF	7
	17		198[a]	gas	LF	9
			209[a]	Ne	LF	7

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[16]

$\tilde{X}\ ^2E''$ 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[16]

1,3,5-$C_6D_3F_3^+$

$\tilde{B}\ ^2A_2''$ 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		198[a]	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	EM	7
	13		532.3	gas	EM,EF	6,15
			541	Ne	LF	7,14
	14		334	Ne	LF	7,14

[a] $\frac{1}{2}(2\nu_i)$.

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$CF_3(C{\equiv}C)_2F^+$

$\tilde{A}\ ^2E$ 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	CC 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

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$CF_3(C{\equiv}C)_2CF_3^+$

$\tilde{B}$

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[2]PEPCO[3]

$\tilde{X}\ ^2E_g$ D_{3d}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1	CC 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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$C_6F_6^+$

$\tilde{C}\ ^2B_{2u}$ D_{6h}

$T_0 \sim 32300$ gas PE[10]
$\tau_0 < 15$ 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
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_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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[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_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

$\tilde{X}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1388m	Ar	IR	1
			1248m	Ar	IR	1
			1228m	Ar	IR	1
			1188s	Ar	IR	1
			1182s	Ar	IR	1
			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).

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

References

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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.

References

[1]W. Sander, Spectrochim. Acta **43A**, 637 (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. Adta **43A**, 637 (1987).

$H_2C{=}CH{-}CH{=}NH$ [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	~2885	gas	IR	2
	6	C=N stretch	1651	gas	IR	2
	7	C=C stretch	1600	gas	IR	2
	8	CH_2 scissors	~1416	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	~855	gas	IR	2

$\tilde{X}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
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

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[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	~2941	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
	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	~1452w	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	~523w	gas	IR	1

$\tilde{X}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
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	~3015	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	~1430	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
a″	16	CH_2 twist	1142	gas	IR	2
	17	CH_2 twist	1102s	gas	IR	1,2
	18	CH_2 rock	~1038	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	~1615m	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	~1108	gas	IR	1
	22	1-CH OPLA	~993	gas	IR	1
	24	NH_2 wag	675m	gas	IR	1

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[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	~2928	gas	IR	1
	6	CH_3 s-stretch	~2868	gas	IR	1
	7	C=C stretch	1655s	gas	IR	1
	8	CH_3 deform.	1495	gas	IR	1
	9	NH bend	1465	gas	IR	1
	10	CH_2 scissors	~1430	gas	IR	1
	11	CH_3 s-deform.	1405	gas	IR	1
	12	CCH bend	1315	gas	IR	1
	13	CNC a-stretch	1230 1223	gas	IR	1
	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	~2822	gas	IR	1
	20	CH_3 deform.	~1445	gas	IR	1
	21	CH_3 rock	~1063	gas	IR	1
	22	CH OPLA	966	gas	IR	1
	23	CH_2 OPLA	795s 788s	gas	IR	1
	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).

$(CH_3)_2C{=}C{=}NH$

(3,3-Dimethylketenimine)

$\tilde{X}$

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

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[1]S. T. Collins and G. C. Pimentel, J. Phys. Chem. **88**, 4258 (1984).

$CH_3C{\equiv}C{-}NH(CH_3)$

(N-Methyl-1-amino-1-propyne)

$\tilde{X}$

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

$\tilde{X}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			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

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[1]H.-H. Nam and G. E. Leroi, J. Am. Chem. Soc. **110**, 4096 (1988).

$CH_3(C{\equiv}C)_2CN^+$

$\tilde{C}\ ^2E$ 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

$\tau_0 = 8(2)$ 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).

$(C_6F_5)N$

$\tilde{X}$ 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).

$NC(C{\equiv}C)_2CN^+$

$\tilde{E}\ ^2\Pi_u$ $D_{\infty h}$

$T_0 = 30420(160)$ 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

$T^a \sim 29530$ 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

$\tau_0 < 6$ 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).

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 ~ 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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[4]J. Bai, H. Okabe, and J. B. Halpern, Chem. Phys. Lett. **149**, 37 (1988).

$(CH_3)_2SiO$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Si=O stretch	1209.6	Ar	IR	1–3

References

[1]C. A. Arrington, R. West, and J. Michl, J. Am. Chem. Soc. **105**, 6176 (1983).
[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 identification.

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).

cyc-$C_4H_4O^+$

(Furan Cation)

$\tilde{X}\ ^2A_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1776	gas	LF	2
			1585	gas	LF	2
			1409	gas	PE,LF	1,2
			1225	gas	LF	2
			1068	gas	PE,LF	1,2
			846	gas	PE,LF	1,2
			644	gas	LF	2
			459	gas	LF	2
			287	gas	LF	2
			133	gas	LF	2

References

[1]P. J. Derrick, L. Åsbrink, O. Edqvist, B. O. Jonsson, and E. Lindholm, Int. J. Mass Spectrom. Ion Phys. **6**, 161 (1971).
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(*cyc*-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).

$(CH_2)_3C{=}C{=}Se$

(Trimethyleneselenoketene)

$\tilde{X}$

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).

C_6H_5O

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

	gas AB[1,2]		$\tilde{B}$–$\tilde{X}$ 380–395 nm
T_0 = 25175(10)	Ar AB[4]		$\tilde{B}$–$\tilde{X}$ 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

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

$T_0 \sim$ 16360	gas AB[2,3]		$\tilde{A}$–$\tilde{X}$ 559–612 nm
	Ar AB[4]		$\tilde{A}$–$\tilde{X}$ 573–629 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			~500	gas	AB	3
			504(10)	Ar	AB	4

C_6D_5O

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

T_0 = 25240(10)	Ar AB[4]		$\tilde{B}$–$\tilde{X}$ 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

References

[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).
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C_6H_5S

$\tilde{C}$

$T_0 \sim 32260$ gas AB[1]

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

$T_0 = 19328(4)$ gas LF[2] $\tilde{B}$–$\tilde{X}$ 490–600 nm

Vib. sym.	No.	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

$\tau_0 < 20$ ns gas LF[2]

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

Vib. sym.	No.	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. sym.	No.	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).

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.

References

[1]M. A. Kesselmayer and R. S. Sheridan, J. Am. Chem. Soc. **108**, 844 (1986).

$C_2H_5O_2$

An unstructured gas-phase absorption between 215 and 280 nm, with maximum at 235 nm, has been assigned[1,3–5] 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

[1]D. A. Parkes, D. M. Paul, C. P. Quinn, and R. C. Robson, Chem. Phys. Lett. **23**, 425 (1973).
[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).
[5]J. Munk, P. Pagsberg, E. Ratajczak, and A. Sillesen, J. Phys. Chem. **90**, 2752 (1986).
[6]G. Chettur and A. Snelson, J. Phys. Chem. **91**, 3483 (1987).

$(CH_3)_2CHO_2$

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	AR	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

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[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).

$CH_3O_4CH_3$

$\tilde{X}$

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)

(Methyl(nitrosomethyl)amine—Conformer 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

$\tilde{X}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		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)

(Methyl(nitrosomethyl)amine—Conformer 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
		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).

$HOCH_2OONO_2$

$\tilde{X}$

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
		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).

7. Master Index

Formula	*Structure*	*Page Nos.*
$BrNO_2$	BrONO	V-1005
$BrNO_3$	$BrONO_2$	S-1478
$BrNS^+$	$NSBr^+$	S-1418
BrNS	NSBr	V-976,S-1422
BrN_3^+	BrN_3^+	E-397
BrNeXe	NeXeBr	E-351
BrOP	BrPO	S-1421
BrO_2	BrOO	V-977
BrO_2	OBrO	V-979
BrPS	BrPS	S-1422
BrS_2	SSBr	V-978
$BrXe_2$	Xe_2Br	E-351
Br_2Cl^-	$BrClBr^-$	V-983
Br_2Cl^-	$ClBrBr^-$	V-983
Br_2F	BrBrF	V-980
Br_2F_2	Br_2F_2	V-1009
Br_2Ge^+	$GeBr_2^+$	E-330
$Br_2GeH_2^+$	$GeH_2Br_2^+$	E-439
Br_2H^-	$BrHBr^-$	V-962
Br_2HN^+	$HNBr_2^+$	E-384
$Br_2H_2Si^+$	$SiH_2Br_2^+$	E-438
Br_2N	NBr_2	V-976
Br_2O	BrOBr	V-979,S-1423
Br_2O	BrBrO	V-980
Br_2OP	$OPBr_2$	S-1455
Br_2P	PBr_2	V-976
Br_2S^+	SBr_2^+	V-978
Br_2S	SBr_2	V-979
$Br_2S_2^+$	$S_2Br_2^+$	E-413
Br_2S_2	$SSBr_2$	V-1009
Br_2Se^+	$SeBr_2^+$	E-347
Br_2Si	$SiBr_2$	V-975,E-339
Br_3^-	Br_3^-	V-983
Br_3P^+	PBr_3^+	E-409
Br_3PO^+	Br_3PO^+	E-463
Br_3PS^+	Br_3PS^+	E-465
Br_3Sb^+	$SbBr_3^+$	E-411
Br_4Ge^+	$GeBr_4^+$	S-1481
Br_4Si^+	$SiBr_4^+$	S-1480
CAsN	AsCN	E-314
CAlO	AlCO	S-1410
CBaN	BaCN	E-308
$CBrCl^+$	$CClBr^+$	V-972
CBrCl	CClBr	V-974,E-337
$CBrCl_2^+$	CCl_2Br^+	V-1003
$CBrCl_2$	CCl_2Br	V-1007
$CBrClF_2^-$	CF_2ClBr^-	V-1021
CBrF	CFBr	V-973,E-336
$CBrF_2^+$	CF_2Br^+	V-1002
$CBrF_2$	CF_2Br	V-1006
$CBrF_2^-$	CF_2Br^-	V-1008
$CBrF_3^+$	CF_3Br^+	V-1018,E-454,S-1479
$CBrF_3^-$	CF_3Br^-	V-1021
$CBrF_4$	CF_3BrF	V-1029,E-505
$CBrN^+$	$BrCN^+$	V-969,E-323,S-1414
CBrN	BrNC	V-971
$CBrNO^+$	$BrNCO^+$	E-393
CBrNO	BrCNO	S-1452
CBrNO	BrNCO	S-1451
$CBrNS^+$	$BrSCN^+$	V-999,E-394
CBrNS	BrSCN	S-1451
$CBrNSe^+$	$BrSeCN^+$	V-1000,E-395
CBr_2^+	CBr_2^+	V-972
CBr_2	CBr_2	V-974,E-337,S-1420
CBr_2Cl^+	$CClBr_2^+$	V-1003
CBr_2Cl	$CClBr_2$	V-1007
CBr_2F^+	$CFBr_2^+$	V-1003
CBr_2F	$CFBr_2$	V-1006
$CBr_2F_2^+$	$CF_2Br_2^+$	V-1019,E-457
$CBr_2F_2^-$	$CF_2Br_2^-$	V-1021
CBr_3^+	CBr_3^+	V-1003
CBr_3	CBr_3	V-1007
CBr_3F^+	$CFBr_3^+$	V-1019,E-458
CBr_3F^-	$CFBr_3^-$	V-1021
CBr_4^+	CBr_4^+	V-1019,E-459
CCaN	CaCN	E-308
CCaNO	CaNCO	E-386
CClF	CFCl	V-973,E-335,S-1419
CClFOS	ClFCSO (I)	S-1477
CClFOS	ClFCSO (II)	S-1478
$CClFS^+$	$FClCS^+$	E-403
$CClF_2^+$	CF_2Cl^+	V-1002
$CClF_2$	CF_2Cl	V-1006,S-1453
$CClF_2NO^+$	CF_2ClNO^+	E-503
$CClF_3^+$	CF_3Cl^+	V-1018,E-454,S-1479
$CClF_3^-$	CF_3Cl^-	V-1020
$CClF_4$	CF_3ClF	V-1029,E-504
$CClN^+$	$ClCN^+$	E-322,S-1414
CClN	ClNC	V-970
$CClNO^+$	$ClNCO^+$	E-392
CClNO	ClCNO	S-1451
CClNO	ClNCO	S-1450
$CClNS^+$	$ClSCN^+$	V-999,E-394
CClNS	ClSCN	S-1451
$CClNSe^+$	$ClSeCN^+$	V-1000,E-395
CClO	ClCO	V-971
CCl_2^+	CCl_2^+	V-972
CCl_2	CCl_2	V-974,E-336,S-1420
CCl_2^-	CCl_2^-	S-1423
CCl_2F^+	$CFCl_2^+$	V-1003
CCl_2F	$CFCl_2$	V-1006,S-1454
CCl_2FNO^+	$CFCl_2NO^+$	E-504
$CCl_2F_2^+$	$CF_2Cl_2^+$	V-1019,E-456,S-1479
$CCl_2F_2^-$	$CF_2Cl_2^-$	V-1021
CCl_2I	CCl_2I	V-1007
CCl_2O^+	Cl_2CO^+	E-401
CCl_2S^+	Cl_2CS^+	E-403
CCl_2Se	Cl_2CSe	V-1002
CCl_3^+	CCl_3^+	V-1003
CCl_3	CCl_3	V-1006,S-1454
CCl_3F^+	$CFCl_3^+$	V-1019,E-457
CCl_3F^-	$CFCl_3^-$	V-1021
CCl_3NO^+	CCl_3NO^+	E-504
CCl_3O_2	CCl_3O_2	S-1492

Formula	*Structure*	*Page Nos.*
CCl_4^+	CCl_4^+	V–1019,E–458
CFI	CFI	V–973
CFI_2^+	CFI_2^+	V–1003
CFI_2	CFI_2	V–1006
CFN^+	FCN^+	E–322
CFN	FNC	V–970
CFNO	FNCO	S–1450
$CFNS^+$	$FSCN^+$	V–999,E–393
CFN_2	FNCN	V–999
CFO^+	FCO^+	V–970
CFO	FCO	V–971,E–327
CFO_2^-	FCO_2^-	V–1002
CFP^+	FCP^+	V–969,E–325
CF_2^+	CF_2^+	V–971,E–328
CF_2	CF_2	V–973,E–334,S–1419
CF_2^-	CF_2^-	S–1423
CF_2I^+	CF_2I^+	V–1002
CF_2I	CF_2I	V–1006
CF_2N	F_2CN	V–1001,E–400
CF_2NOP^+	PF_2NCO^+	E–503
CF_2NP^+	PF_2CN^+	E–452
CF_2NPS^+	PF_2NCS^+	E–503
$CF_2N_2^+$	$CF_2N_2^+$	E–452
CF_2O^+	F_2CO^+	E–401
CF_2OS	F_2CSO	S–1477
CF_2S^+	F_2CS^+	E–402
CF_2Se^+	F_2CSe^+	E–404
CF_3^+	CF_3^+	V–1002
CF_3	CF_3	V–1005,E–407
CF_3I^+	CF_3I^+	V–1018,E–455
CF_3I^-	CF_3I^-	V–1021
CF_3IO	CF_3IO	S–1494
CF_3IO	CF_3OI	S–1495
CF_3NO^+	CF_3NO^+	E–503
CF_3NO_3	CF_3ONO_2	S–1508
CF_3O	CF_3O	S–1478
CF_3O^-	CF_3O^-	V–1020
CF_3O_2	CF_3O_2	V–1028,S–1492
CF_4^+	CF_4^+	E–453,S–1478
CF_4I	CF_3IF	V–1029,E–505
CF_4O^+	CF_3OF^+	E–504
CHBr	HCBr	S–1403
$CHBr^-$	HCBr−	S–1404
$CHBrCl^+$	$HCClBr^+$	V–995
CHBrCl	HCClBr	V–998
$CHBrF^+$	$HCFBr^+$	V–994
CHBrF	HCFBr	V–997
CHBrO	HCOBr	S–1446
$CHBr_2^+$	$HCBr_2^+$	V–995
$CHBr_2$	$HCBr_2$	V–998
$CHBr_3^+$	$HCBr_3^+$	E–444
$CHCaO_2$	HCOOCa	S–1471
CHCl	HCCl	V–957,E–298,S–1403
$CHCl^-$	$HCCl^-$	S–1404
$CHClF^+$	$HCFCl^+$	V–994
CHClF	HCFCl	V–997
$CHClF_2^+$	HCF_2Cl^+	E–443
$CHClO^+$	$HCOCl^+$	E–379
CHClO	HCOCl	V–994
$CHCl_2^+$	$HCCl_2^+$	V–994,E–380
$CHCl_2$	$HCCl_2$	V–998,E–383
$CHCl_2F^+$	$HCFCl_2^+$	E–443
$CHCl_3^+$	$HCCl_3^+$	E–444
CHF^+	HCF^+	V–957
CHF	HCF	V–957,E–297,S–1402
CHF^-	HCF^-	S–1404
$CHFI^+$	$HCFI^+$	V–994
CHFI	HCFI	V–998
CHFN	HFCN	S–1443
$CHFO^+$	$HFCO^+$	E–378
CHF_2^+	HCF_2^+	V–994
CHF_2	HCF_2	V–997
CHF_2N	*c*-HFC=NF	S–1472
CHF_2P	CF_2=PH	S–1472
CHF_3^+	HCF_3^+	E–443,S–1473
CHI	HCI	S–1403
CHI^-	HCI^-	S–1404
CHI_2	HCI_2	V–998
CHN^+	HCN^+	E–292
CHN	HNC	V–955,E–295
$CHNO^+$	$HNCO^+$	E–375
$CHNO^+$	$HCNO^+$	E–376
CHNO	HNCO	S–1441
CHNO	HOCN	V–992,S–1441
CHNO	HCNO	S–1442
CHNO	HONC	S–1442
CHNP	HPCN	E–375
$CHNS^+$	$HNCS^+$	E–375
CHN_2	HCNN	V–992,S–1440
CHN_2	HNCN	E–374,S–1440
CHO^+	HCO^+	V–955,S–1400
CHO^+	HOC^+	S–1401
CHO	HCO	V–956,E–296,S–1402
$CHOS^+$	$HOCS^+$	S–1443
CHO_2^+	$HOCO^+$	S–1443
CHO_2	*c*-HOCO	V–993
CHO_2	*t*-HOCO	V–993,S–1444
CHO_2Sr	HCOOSr	S–1471
CHO_3	HC(O)OO	V–1016,S–1472
CHP^+	HCP^+	V–954,E–293
CHS^+	HCS^+	S–1400
CH_2	CH_2	V–951,E–279,S–1395
CH_2^-	CH_2^-	E–282
CH_2Br^+	H_2CBr^+	V–989
CH_2Br	H_2CBr	V–990
CH_2BrF^+	CH_2FBr^+	V–1015
CH_2BrI	H_2CBr-I	E–440
$CH_2Br_2^+$	$CH_2Br_2^+$	V–1015,E–437
CH_2CaNO	HCONHCa	S–1488
CH_2Cl^+	H_2CCl^+	V–988
CH_2Cl	H_2CCl	V–990,S–1437
CH_2ClF^+	CH_2FCl^+	V–1015,E–436
CH_2ClI	H_2CCl-I	E–439
CH_2ClN	CH_2=NCl	S–1470

Formula	*Structure*	*Page Nos.*
CH_2ClP	$CH_2{=}PCl$	S-1470
$CH_2Cl_2^+$	$CH_2Cl_2^+$	V-1015,E-436
CH_2Cl_2Si	$CH_2{=}SiCl_2$	V-1026,E-491
CH_2Cu	$CuCH_2$	S-1430
CH_2F+	H_2CF+	V-988
CH_2F	H_2CF	V-989,E-367
CH_2FI^+	CH_2FI^+	V-1015
$CH_2F_2^+$	$CH_2F_2^+$	V-1015,E-435
CH_2Fe	$FeCH_2$	S-1429
CH_2Fe	$HFeCH$	S-1430
CH_2I	H_2CI	V-990,S-1437
$CH_2I_2^+$	$CH_2I_2^+$	E-437
CH_2I_2	$H_2CI{-}I$	E-400
CH_2N^+	$HCNH^+$	V-987,S-1433
CH_2N	H_2CN	E-360
CH_2NOSr	$HCONHSr$	S-1489
CH_2NO_2	CH_2NO_2	V-1026,E-485
$CH_2N_2^+$	$CH_2N_2^+$	E-431
$CH_2N_2^+$	*cyc*-$CH_2N_2^+$	E-432
$CH_2N_2^+$	NH_2CN^+	E-431
CH_2N_2	$HN{=}C{=}NH$	V-1013,S-1468
CH_2N_2O	H_2NNCO	S-1490
CH_2O^+	H_2CO^+	E-361
CH_2OS^+	H_2CSO^+	E-435
CH_2OS	H_2CSO	V-1014
$CH_2O_2^+$	$HCOOH^+$	E-434
CH_2S^+	H_2CS^+	V-987,E-362
CH_2S	H_2CS	V-988,E-363
CH_2S^-	H_2CS^-	S-1437
CH_2Se^+	H_2CSe^+	E-362
CH_2Se	H_2CSe	E-365,S-1434
CH_2Si	H_2CSi	E-359
CH_2Zn	$ZnCH_2$	S-1429
CH_2Zn	$HZnCH$	S-1429
CH_3^+	CH_3^+	V-985,E-352
CH_3	CH_3	V-985,E-352,S-1426
CH_3^-	CH_3^-	E-355
CH_3BO^+	BH_3CO^+	E-473
CH_3BaO	$BaOCH_3$	E-477
CH_3Br^+	CH_3Br^+	E-423
CH_3BrF	CH_3BrF	S-1487
CH_3Ca	$CaCH_3$	E-416,S-1457
CH_3CaO	$CaOCH_3$	E-475
CH_3Cd	$CdCH_3$	S-1457
CH_3Cl^+	CH_3Cl^+	E-422
CH_3ClF	CH_3ClF	S-1487
CH_3ClO^+	CH_3OCl^+	E-483
CH_3ClSi	$CH_2{=}SiHCl$	V-1024,E-482
CH_3ClSi	CH_3SiCl	V-1025,E-482
CH_3F^+	CH_3F^+	E-422
CH_3FI	CH_3IF	S-1487
CH_3I^+	CH_3I^+	E-423,S-1461
CH_3IO	CH_3IO	S-1486
CH_3IO	CH_3OI	S-1486
CH_3IO	ICH_2OH	S-1486
CH_3N^+	CH_2NH^+	E-417
CH_3N	CH_3N	E-418,S-1459
CH_3N	CH_2NH	V-1010,E-418
CH_3NO^+	CH_3NO^+	E-478
CH_3NO^+	H_2CNOH^+	E-479
CH_3NO^+	$HCONH_2^+$	E-479
CH_3NO	CH_3NO	V-1025
CH_3NO	CH_2NOH	S-1485
CH_3NO_2	*c*-$CH_2(NO)OH$	V-1033
CH_3NO_2	*t*-$CH_2(NO)OH$	V-1033
CH_3NO_5	$HOCH_2OONO_2$	S-1535
CH_3NS^+	$HCSNH_2^+$	E-480
CH_3O^+	CH_2OH^+	S-1459
CH_3O	CH_3O	V-1010,E-419,S-1459
CH_3O	CH_2OH	V-1011,E-420,S-1460
CH_3O^-	CH_3O^-	V-1012
CH_3OSr	$SrOCH_3$	E-476,S-1484
CH_3O_2	CH_3O_2	E-482,S-1485
CH_3S	CH_3S	V-1011,E-421,S-1460
CH_3S	CH_2SH	V-1011
CH_3S^-	CH_3S^-	V-1012,S-1462
CH_3S_2	CH_3S_2	S-1485
$CH_3S_2^-$	$CH_3S_2^-$	S-1486
CH_3Sr	$SrCH_3$	E-417
CH_3Te	CH_3Te	S-1461
CH_3Zn	$ZnCH_3$	S-1457
CH_4^+	CH_4^+	E-415
CH_4Fe	$HFeCH_3$	S-1482
CH_4N^+	$CH_2NH_2^+$	S-1483
CH_4Ni	$HNiCH_3$	S-1482
CH_4NiO	$HNiOCH_3$	S-1497
CH_4NiO	CH_3NiOH	S-1497
CH_4O^+	CH_3OH^+	E-471
CH_4OSi	HCH_3SiO	S-1497
CH_4O_3	HO_2CH_2OH	S-1506
CH_4S^+	CH_3SH^+	E-472
CH_4Si^+	$CH_2{=}SiH_2^+$	V-1022
CH_4Si	$CH_2{=}SiH_2$	V-1022,E-470
CH_4Si	CH_3SiH	V-1023,E-471
CH_6OSi	CH_3SiH_2OH	S-1530
CIN^+	ICN^+	E-324
$CINO^+$	$INCO^+$	E-393
$CINO$	$INCO$	S-1451
$CINS^+$	$ISCN^+$	E-395
$CINS$	$ISCN$	S-1451
CI_3	CI_3	V-1007
CNO^+	NCO^+	V-966,E-314
CNO	CNO	E-325
CNO	NCO	V-968,E-318,S-1412
CNO^-	NCO^-	S-1416
$CNOSr$	$SrNCO$	E-386
CNP	PCN	E-313
CNS	NCS	V-968,E-319,S-1412
CNS^-	NCS^-	S-1416
$CNSr$	$SrCN$	E-308
CN_2	NCN	V-966,E-313,S-1410
CN_2	CNN	V-966,E-314,S-1410
CN_2O^+	$ONCN^+$	E-388
CN_2O	$NCNO$	E-388

Formula	*Structure*	*Page Nos.*
CN_4^+	N_3CN^+	E-446
COS^+	OCS^+	V-968,E-320,S-1413
COSi	SiCO	V-966,E-312
CO_2^+	CO_2^+	V-968,E-320,S-1412
CO_2^-	CO_2^-	V-971,S-1418
CO_3	CO_3	V-1000,E-397
CO_3^-	CO_3^-	V-1001
CS_2^+	CS_2^+	V-969,E-321,S-1413
CSi_2	Si_2C	V-965,S-1410
C_2BrCl^+	$ClCCBr^+$	E-390
C_2BrN	BrCCN	V-999
$C_2Br_2^+$	$C_2Br_2^+$	V-1044,E-390
$C_2ClF_3^+$	$CF_2{=}CFCl^+$	E-501
C_2ClN	ClCCN	V-999
$C_2Cl_2^+$	$C_2Cl_2^+$	V-1044,E-389
$C_2Cl_2F_2^+$	$CF_2{=}CCl_2^+$	E-501
$C_2Cl_2O^+$	Cl_2CCO^+	V-1017,E-452
C_2Cl_2O	Cl_2CCO	V-1017
$C_2Cl_2O_2^+$	*t*-$(ClCO)_2^+$	E-499
$C_2Cl_4^+$	$C_2Cl_4^+$	E-502
$C_2F_2^+$	$C_2F_2^+$	E-389
C_2F_2	C_2F_2	V-1000,S-1450
$C_2F_2N_2$	$F_2C{=}C{=}N{=}N$	S-1494
$C_2F_2O_2^+$	*t*-$(FCO)_2^+$	E-499
$C_2F_4^+$	$C_2F_4^+$	E-500
C_2F_5	C_2F_5	V-1035
C_2F_5P	$CF_2{=}PCF_3$	S-1508
C_2H	HCC	V-954,E-291,S-1398
C_2H^-	HCC^-	S-1400
C_2HBr^+	$HCCBr^+$	V-1044,E-373
C_2HCa	CaCCH	E-370,S-1439
C_2HCl^+	$HCCCl^+$	V-1044,E-372
$C_2HClF_2^+$	$CHCl{=}CF_2^+$	E-494
$C_2HCl_3^+$	$CHCl{=}CCl_2^+$	E-494
$C_2HF_3^+$	$CHF{=}CF_2^+$	E-493
C_2HF^+	$HCCF^+$	E-372
C_2HI^+	$HCCI^+$	E-374
C_2HN	HCCN	V-992,E-370
C_2HNO	HCOCN	E-442,S-1472
C_2HO	HCCO	E-370,S-1440
C_2HS	HCCS	E-371
C_2HS	HSCC	E-371
C_2HSr	SrCCH	E-370
$C_2H_2^+$	$C_2H_2^+$	E-357
C_2H_2	$H_2C{=}C$	V-987,E-359,S-1433
$C_2H_2^-$	$H_2C{=}C^-$	S-1434
C_2H_2Br	$CHBr{=}CH$	S-1470
$C_2H_2ClF^+$	$CH_2{=}CFCl^+$	E-488
$C_2H_2ClN^+$	CH_2ClCN^+	E-485
$C_2H_2Cl_2^+$	$CH_2{=}CCl_2^+$	E-488
$C_2H_2Cl_2^+$	*c*-$CHCl{=}CHCl^+$	E-489
$C_2H_2Cl_2^+$	*t*-$CHCl{=}CHCl^+$	E-489
C_2H_2F	*t*-$CHF{=}CH$	V-1014
$C_2H_2FN^+$	CH_2FCN^+	E-485
$C_2H_2FO^-$	CH_2COF^-	S-1490
$C_2H_2F_2^+$	$CH_2{=}CF_2^+$	E-486
$C_2H_2F_2^+$	*c*-$CHF{=}CHF^+$	V-1026,E-486
$C_2H_2F_2^+$	*t*-$CHF{=}CHF^+$	E-487
C_2H_2Fe	HFeCCH	S-1464
C_2H_2Li	LiC_2H_2	S-1464
C_2H_2N	H_2CCN	S-1467
C_2H_2N	H_2CNC	S-1467
$C_2H_2N^-$	H_2CCN^-	E-430,S-1468
$C_2H_2N^-$	H_2CNC^-	E-430
$C_2H_2N_2$	*t*-$HN{=}CHCN$	S-1490
$C_2H_2N_2O_2$	$HON{=}CHCNO$	S-1507
$C_2H_2N_2O_2$	$HON{=}CHNCO$	S-1507
C_2H_2Ni	C_2H_2Ni	E-427
C_2H_2Ni	$NiC{=}CH_2$	E-427
$C_2H_2O^+$	H_2CCO^+	E-429
C_2H_2O	HCCOH	S-1469
C_2H_2OS	CHOCHS	V-1026
$C_2H_2O_2^+$	$(HCO)_2^+$	E-484
$C_2H_2O_3$	$(HCO)_2O$	V-1034
$C_2H_2S^+$	H_2CCS^+	V-1012,E-430
C_2H_2S	H_2CCS	V-1013,E-433
C_2H_2S	HCCSH	V-1013,S-1469
C_2H_2S	*cyc*-C_2H_2S	V-1014,S-1469
$C_2H_2S_2$	$HS{-}CH{=}C{=}S$	V-1026
$C_2H_3^+$	$C_2H_3^+$	S-1458
C_2H_3	C_2H_3	E-417,S-1458
$C_2H_3Cl^+$	$CH_2{=}CHCl^+$	E-481
C_2H_3ClO	CH_3OCCl	V-1032,S-1499
$C_2H_3F^+$	$CH_2{=}CHF^+$	E-480
$C_2H_3N^+$	CH_3CN^+	E-474
$C_2H_3N^+$	CH_3NC^+	E-474
$C_2H_3N^+$	$CH_2{=}C{=}NH^+$	S-1484
C_2H_3N	$CH_2{=}C{=}NH$	V-1023,S-1484
C_2H_3N	$HCCNH_2$	S-1484
C_2H_3NO	CH_3CNO	S-1498
C_2H_3NO	$HOCH_2CN$	S-1499
$C_2H_3NO_2$	CH_3ONCO	S-1506
C_2H_3O	CH_3CO	V-1024,E-477
C_2H_3O	CH_2CHO	V-1024,E-477
$C_2H_3O^-$	CH_2CHO^-	V-1024,E-481
$C_2H_3O_3$	CH_3COO_2	S-1507
$C_2H_3P^+$	CH_3CP^+	V-1023,E-475
C_2H_3P	CH_3CP	S-1485
$C_2H_4^+$	$C_2H_4^+$	E-468
C_2H_4Al	AlC_2H_4	S-1496
C_2H_4F	FCH_2CH_2	V-1032
C_2H_4Fe	$HFeC_2H_3$	S-1496
C_2H_4FeO	$CH_2{=}CHFeOH$	S-1506
C_2H_4FeO	*cyc*-C_2H_4OFe	S-1505
C_2H_4Li	C_2H_4Li	S-1496
$C_2H_4Li_2$	1,2-$C_2H_4Li_2$	S-1505
$C_2H_4N^+$	CH_3CNH^+	S-1497
C_2H_4O	$CH_2{=}CHOH$	V-1032
$C_2H_4O_3$	1,2,3-*cyc*-$C_2H_4O_3$	V-1059
$C_2H_4O_3$	1,2,4-*cyc*-$C_2H_4O_3$	V-1059
$C_2H_4O_3$	*c*-$HCOOCH_2OH$	V-1060
$C_2H_4O_3$	*t*-$HCOOCH_2OH$	V-1061
$C_2H_4S^+$	CH_3CHS^+	V-1032
$C_2H_5^+$	$C_2H_5^+$	V-1031,S-1495

Formula	*Structure*	*Page Nos.*
C_2H_5	C_2H_5	V-1031,S-1495
C_2H_5N	*c*-$CH_3CH{=}NH$	S-1503
C_2H_5N	*t*-$CH_3CH{=}NH$	S-1502
C_2H_5N	$C_2H_3NH_2$	S-1503
C_2H_5N	$H_2C{=}NCH_3$	S-1504
$C_2H_5NO_2$	*c*-$CH_3CH(NO)OH$	S-1535
C_2H_5O	C_2H_5O	V-1036,S-1504
$C_2H_5O_2$	$C_2H_5O_2$	S-1533
C_2H_5S	C_2H_5S	S-1504
C_2H_6Ge	$(CH_3)_2Ge$	S-1520
$C_2H_6N_2O$	CH_3NHCH_2NO(A)	S-1535
$C_2H_6N_2O$	CH_3NHCH_2NO(B)	S-1535
C_2H_6OSi	$(CH_3)_2SiO$	V-1062,S-1530
C_2H_6OSi	$CH_2{=}Si(OH)CH_3$	S-1531
C_2H_6OSi	CH_3OSiCH_3	S-1531
C_2H_6OSi	$CH_3OSiH{=}CH_2$	S-1531
$C_2H_6O_2Si$	$(CH_3O)_2Si$	S-1534
$C_2H_6O_2Si$	$CH_3SiOOCH_3$	S-1534
$C_2H_6O_4$	$CH_3O_4CH_3$	S-1535
C_2H_6Si	$(CH_3)_2Si$	V-1056,S-1519
C_2H_6Si	$CH_3SiH{=}CH_2$	V-1056,S-1520
C_2H_6Sn	$(CH_3)_2Sn$	V-1058,S-1520
$C_2H_7^+$	$C_2H_7^+$	S-1508
$C_2H_7^+$	*br*-$C_2H_7^+$	S-1508
C_2H_8OSi	$(CH_3)_2SiHOH$	S-1531
$C_2I_2^+$	$C_2I_2^+$	V-1044,E-391
C_2N	CCN	V-965,E-310,S-1410
C_2N	CNC	V-965,E-311
$C_2N_2^+$	$NCCN^+$	E-387
$C_2N_2^+$	$CNCN^+$	S-1446
C_2N_2	CNCN	S-1447
C_2N_2	CNNC	S-1447
$C_2N_2O^+$	$NCNCO^+$	E-447
C_2N_2O	NC−CNO	S-1475
C_2N_2O	NC−NCO	S-1475
$C_2N_2S^+$	$S(CN_2^+)$	E-447
$C_2N_2S^+$	$NCNCS^+$	E-448
C_2N_2S	NC−NCS	S-1475
$C_2N_2S_2^+$	$(SCN)_2^+$	V-1027,E-497
$C_2N_2Se^+$	$Se(CN)_2^+$	E-451
C_2O	CCO	V-965,E-312
C_2O^-	CCO^-	V-967,E-316
$C_2O_2^+$	*t*-$OCCO^+$	S-1447
$C_2O_2^-$	*t*-$OCCO^-$	S-1449
C_2O_2Si	$Si(CO)_2$	V-1017
C_2Si	SiCC	V-964,E-309,S-1409
C_3	C_3	V-964,E-308,S-1408
C_3BrN^+	$BrCCCN^+$	E-450
C_3ClN^+	$ClCCCN^+$	E-449
C_3FN^+	$FCCCN^+$	E-448
C_3F_2O	$F_2C{=}C{=}C{=}O$	S-1493
C_3F_2O	*cyc*-$(CF{=}CFC){=}O$	S-1494
$C_3F_6^+$	$C_3F_6^+$	V-1054
C_3F_7	*n*-C_3F_7	V-1054
C_3F_7	*i*-C_3F_7	V-1055
C_3H	HC_3	V-992,S-1440
C_3HN^+	$HCCCN^+$	E-441
C_3HF_3S	CF_3H(*cyc*-CCS)	V-1037
C_3H_2	HCCCH	V-1012,E-428,S-1466
C_3H_2	*cyc*-C_3H_2	E-427,S-1466
C_3H_2	$H_2C{=}C{=}C$:	E-428,S-1466
C_3H_2	$HCCH{=}C$:	S-1467
$C_3H_2N^+$	$HCCCNH^+$	S-1488
$C_3H_2O^+$	$H_2C{=}C{=}C{=}O^+$	S-1489
C_3H_2O	$H_2C{=}C{=}C{=}O$	S-1489
C_3H_2S	$H_2C{=}C{=}C{=}S$	S-1490
C_3H_2Se	$H_2C{=}C{=}C{=}Se$	S-1490
C_3H_2Se	HCC−CHSe	S-1490
C_3H_3	CH_2CCH	V-1023,E-473,S-1484
$C_3H_3Br^+$	CH_3CCBr^+	S-1498
$C_3H_3Cl^+$	CH_3CCCl^+	S-1497
C_3H_4Li	CH_3CCHLi	S-1505
C_3H_4O	*cyc*-$(H_2COC){=}CH_2$	S-1506
C_3H_4S	HCH_3(*cyc*-CCS)	V-1037
$C_3H_5^+$	$CH_2CHCH_2^+$	V-1036
$C_3H_5^+$	*cyc*-$C_3H_5^+$	S-1501
C_3H_5	CH_2CHCH_2	V-1036,S-1501
C_3H_5N	$H_2C{=}CH{-}CH{=}NH$	S-1526
C_3H_5N	$H_2C{=}C{=}NCH_3$	S-1526
C_3H_5N	$H_2C{=}CHN{=}CH_2$	S-1526
C_3H_5N	*cyc*-C_3H_5N	S-1527
C_3H_6O	*t*-CH_3C-OCH_3	S-1530
C_3H_6O	*c*-CH_3C-OCH_3	S-1530
$C_3H_7^+$	1-$C_3H_7^+$	S-1508
$C_3H_7^+$	2-$C_3H_7^+$	V-1038,S-1508
C_3H_7	$CH_3CH_2CH_2$	V-1038
C_3H_7	$(CH_3)_2CH$	V-1038,S-1508
C_3H_7N	$CH_3CH{=}CHNH_2$	S-1527
C_3H_7N	$C_2H_3NHCH_3$	S-1527
C_3H_7O	*n*-C_3H_7O	S-1530
C_3H_7O	$(CH_3)_2CHO$	S-1530
$C_3H_7O_2$	$(CH_3)_2CHO_2$	S-1534
$C_3H_8Si^+$	$(CH_3)_2Si{-}CH_2^+$	V-1056
C_3H_8Si	$(CH_3)_2Si{=}CH_2$	V-1056,S-1520
C_3IN^+	$ICCCN^+$	E-450
C_3N_2	$C(CN)_2$	V-1017
$C_3N_2O^+$	$CO(CN)_2^+$	E-495
C_3O	CCCO	V-999,S-1447
$C_3O_2^+$	$C_3O_2^+$	E-446
C_4	C_4	S-1446
$C_4Br_2^+$	$Br(CC)_2Br^+$	V-1046,E-496
$C_4Cl_2^+$	$Cl(CC)_2Cl^+$	V-1046,E-496
$C_4F_2^+$	$F(CC)_2F^+$	V-1045,E-495
C_4F_6O	CF_3CCOCF_3	V-1062
C_4F_6O	$(CF_3)_2$(*cyc*-CCO)	V-1062
C_4H	C_4H	V-1016,E-441,S-1471
C_4HBr^+	$H(CC)_2Br^+$	V-1045,E-492
C_4HCl^+	$H(CC)_2Cl^+$	V-1045,E-492
C_4HF^+	$H(CC)_2F^+$	E-491
C_4HI^+	$H(CC)_2I^+$	E-493
$C_4H_2^+$	$C_4H_2^+$	V-1025,E-483,S-1487
C_4H_4	*cyc*-C_4H_4	V-1036,S-1505
C_4H_4	$H_2C{=}$(*cyc*-C_3H_2)	S-1505
$C_4H_4O^+$	*cyc*-$C_4H_4O^+$	S-1532

Formula	*Structure*	*Page Nos.*
C_4H_6S	$(CH_3)_2$(*cyc*-CCS)	V–1062
C_4H_7N	$(CH_3)_2C{=}C{=}NH$	S–1528
C_4H_7N	$CH_3CC{-}NHCH_3$	S–1528
$C_4H_9^+$	*t*-$C_4H_9^+$	V–1038
C_4H_9	*n*-C_4H_9	V–1038
C_4H_9	*i*-C_4H_9	V–1039
C_4H_9	*t*-C_4H_9	V–1039,S–1509
$C_4H_9O_2$	*t*-$C_4H_9O_2$	V–1061,S–1534
$C_4H_{10}Si$	$(CH_3)_2Si{=}CHCH_3$	V–1057
$C_4I_2^+$	$I(CC)_2I^+$	V–1046,E–497
$C_4N_2^+$	$NCCCCN^+$	V–1045,E–494
C_4O	C_4O	S–1475
C_5	C_5	S–1475
$C_5F_4^+$	$CF_3(CC)_2F^+$	V–1047,S–1523
C_5F_6O	$(CF_3)_2$(*cyc*-CCO)	V–1062
C_5F_8O	CF_3(*cyc*-CCO)C_2F_5	V–1062
C_5HN^+	$H(CC)_2CN^+$	V–1045,S–1500
$C_5H_3Br^+$	$CH_3(CC)_2Br^+$	V–1046,S–1522
$C_5H_3Cl^+$	$CH_3(CC)_2Cl^+$	V–1046,S–1522
$C_5H_3F_2N^+$	*cyc*-$C_5H_3F_2N^+$	V–1058
C_5H_3N	*cyc*-C_5H_3N	S–1528
$C_5H_4^+$	$CH_3(CC)_2H^+$	V–1039,S–1509
C_5H_4	*cyc*-C_5H_4	V–1039
C_5H_4O	(*cyc*-C_5H_4)O	S–1532
$C_5H_4O_2$	*cyc*-C_5H_4O-1-O	V–1061
C_5H_5	*cyc*-C_5H_5	V–1040,S–1510
C_5H_6Se	$(CH_2)_3C{=}C{=}Se$	S–1532
$C_5H_6Si^+$	$C_5SiH_6^+$	S–1521
C_5H_6Si	C_5SiH_6	V–1057,S–1521
C_5H_6Si	C_5SiH_6(Dewar)	V–1057,S–1521
C_5H_{11}	*n*-C_5H_{11}	V–1040
C_5H_{11}	$(CH_3)_3CCH_2$	V–1040
C_5O_2	C_5O_2	S–1500
$C_6Br_3F_3^+$	*sym*-$C_6F_3Br_3^+$	V–1051
$C_6ClF_5^+$	$C_6F_5Cl^+$	V–1053
$C_6Cl_3F_3^+$	*sym*-$C_6F_3Cl_3^+$	V–1050
C_6F_5N	$(C_6F_5)N$	S–1529
$C_6F_6^+$	$CF_3(CC)_2CF_3^+$	V–1047,S–1524
$C_6F_6^+$	$C_6F_6^+$	V–1053,S–1524
$C_6HF_5^+$	$C_6HF_5^+$	V–1052
$C_6HF_5O^+$	$C_6F_5OH^+$	V–1053
$C_6H_2^+$	$C_6H_2^+$	V–1037,S–1507
$C_6H_2F_4^+$	1,2,3,4-$C_6H_2F_4^+$	V–1051
$C_6H_2F_4^+$	1,2,3,5-$C_6H_2F_4^+$	V–1051
$C_6H_2F_4^+$	1,2,4,5-$C_6H_2F_4^+$	V–1052
$C_6H_3Cl_2F^+$	1,3,5-$C_6H_3Cl_2F^+$	V–1050
$C_6H_3Cl_3^+$	1,3,5-$C_6H_3Cl_3^+$	V–1050
$C_6H_3F_3^+$	1,2,3-$C_6H_3F_3^+$	V–1048
$C_6H_3F_3^+$	1,2,4-$C_6H_3F_3^+$	V–1048
$C_6H_3F_3^+$	1,3,5-$C_6H_3F_3^+$	V–1049,S–1522
$C_6H_3N^+$	$CH_3(CC)_2CN^+$	V–1047,S–1528
C_6H_4	C_6H_4	V–1040,S–1510
$C_6H_4^-$	$C_6H_4^-$	S–1511
$C_6H_4F_2^+$	1,3-$C_6H_4F_2^+$	V–1048
$C_6H_4F_2O^+$	3,5-$F_2C_6H_3OH^+$	V–1049
$C_6H_4S_2$	*p*-$C_6H_4S_2$	V–1063
$C_6H_5^+$	$C_6H_5^+$	S–1511

Formula	*Structure*	*Page Nos.*
C_6H_5	C_6H_5	V–1040,S–1511
C_6H_5N	3-CH(cyc-C_5H_4N)	V–1059
C_6H_5N	*cyc*-C_6H_5N	V–1058
C_6H_5O	C_6H_5O	S–1532
C_6H_5S	C_6H_5S	S–1533
$C_6H_6^+$	$C_6H_6^+$	S–1512
$C_6H_6^+$	$CH_3(CC)_2CH_3^+$	V–1041,S–1514
C_6H_6F	C_6H_6F	V–1055
C_6H_6Li	LiC_6H_6	S–1521
$C_6H_6O^+$	$C_6H_5OH^+$	S–1533
$C_6H_7N^+$	$C_6H_5NH_2^+$	V–1048
$C_6H_8^+$	*t*-CH2$(CH)_4CH_2^+$	V–1041
C_6H_8Si	1-$CH_3C_5SiH_5$	V–1058
$C_6N_2^+$	$NC(CC)_2CN^+$	V–1046,S–1529
$C_7F_8^+$	$C_6F_5CF_3^+$	V–1053
$C_7H_3F_5^+$	$C_6F_5CH_3^+$	V–1053
C_7H_5Cl	C_6H_5CCl	S–1525
C_7H_5Cl	(2-ClC_6H_4)CH	S–1526
C_7H_5Cl	*cyc*-1-C_7H_5Cl	S–1526
C_7H_5ClO	C_6H_5OCCl	S–1533
C_7H_5F	C_6H_5CF	S–1525
C_7H_5F	*cyc*-1-C_7H_5F	S–1525
$C_7H_5F_3^+$	*sym*-$C_6H_2F_3CH_3^+$	V–1051
$C_7H_5N^+$	$C_2H_5(CC)_2CN^+$	V–1047,S–1529
C_7H_6	C_6H_5CH	V–1041,S–1514
C_7H_6	*cyc*-C_7H_6	V–1042,S–1514
C_7H_6	*cyc*-C_7H_6:	S–1515
$C_7H_7^+$	*cyc*-$C_7H_7^+$	V–1042
$C_7H_7^+$	$C_6H_5CH_2^+$	V–1042
C_7H_7	$C_6H_5CH_2$	V–1042,S–1515
$C_7H_7^-$	$C_6H_5CH_2^-$	S–1516
C_8H_8	*o*-$(CH_2)_2C_6H_4$	V–1043,S–1517
C_8H_8	$C_6H_5CCH_3$	S–1518
C_8H_8	*m*-$CH_3C_6H_4CH$:	S–1517
C_8H_8	*o*-$CH_3C_6H_4CH$:	S–1517
C_8H_8	*p*-$CH_3C_6H_4CH$:	S–1516
C_8H_8	1-CH_3(cyc-C_7H_5)	S–1518
C_8H_8	4-CH_3(cyc-C_7H_5)	S–1519
C_8H_8	5-CH_3(cyc-C_7H_5)	S–1518
CaHO	CaOH	E–288
CaH_2N	$CaNH_2$	E–356,S–1430
CaH_2O	HCaOH	S–1431
CaH_2O_2	$Ca(OH)_2$	S–1467
CaN_3	CaN_3	E–386
Ca_2H_2O	HCaOCaH	S–1465
Ca_2H_2O	HCa_2OH	S–1465
$ClFH^-$	$FHCl^-$	V–961
ClFO	FClO	V–979
$ClFO_2S^+$	$FClSO_2^+$	E–467
$ClFO_3^+$	$FClO_3^+$	E–466
ClFS	FSCl	S–1424
ClFXe	XeClF	V–984
ClF_2	ClF_2	V–980
ClF_2^-	$FClF^-$	V–981
ClF_2^-	$FFCl^-$	V–981
ClF_2P^+	PF_2Cl^+	E–409
ClF_3^+	ClF_3^+	E–414

Formula	*Structure*	*Page Nos.*
ClF_3P^-	$PClF_3^-$	V-1022
ClF_3S	$SClF_3$	S-1481
ClF_3Si^+	SiF_3Cl^+	E-460
ClF_4Si^-	SiF_4Cl^-	V-1029
ClFeH	HFeCl	S-1399
ClGeH	HGeCl	V-958,E-300
$ClGeH_2$	H_2GeCl	V-990
$ClGeH_3^+$	GeH_3Cl^+	E-426
$ClHI^-$	$ClHI^-$	V-962
$ClHO^+$	$HOCl^+$	E-306
ClHSi	HSiCl	V-958,E-299
ClH_2^+	H_2Cl^+	S-1398
ClH_2N^+	H_2NCl^+	E-368
ClH_3Si^+	SiH_3Cl^+	E-425
ClIO	OICl	S-1424
$ClIO_2$	O_2ICl	S-1456
ClKrNe	NeKrCl	E-350
ClKrXe	KrXeCl	E-350
$ClKr_2$	Kr_2Cl	E-350
$ClNO^+$	$ClNO^+$	E-331
$ClNO_2^+$	$ClNO_2^+$	E-405
$ClNO_2$	ClONO	V-1004,S-1453
$ClNO_2$	OClNO	V-1004
$ClNS^+$	$NSCl^+$	E-332
ClN_3^+	ClN_3^+	E-396
ClOP	ClPO	V-975,S-1421
ClO_2^+	ClO_2^+	E-340
ClO_2	ClOO	V-977,E-344
ClO_2^-	$OClO^-$	V-979
ClO_2P	PO_2Cl	S-1453
ClPS	ClPS	V-975
ClS_2	SSCl	V-978,E-345
$ClXe_2$	Xe_2Cl	E-350
Cl_2F	ClClF	V-980
Cl_2F^-	$ClFCl^-$	V-982
Cl_2F^-	$FClCl^-$	V-982
Cl_2F_2	Cl_2F_2	V-1009
Cl_2F_2S	SCl_2F_2	S-1482
$Cl_2F_3Si^-$	$SiF_3Cl_2^-$	V-1029
Cl_2Ga	$GaCl_2$	S-1417
Cl_2Ge^+	$GeCl_2^+$	E-329
Cl_2Ge	$GeCl_2$	E-339,S-1421
$Cl_2GeH_2^+$	$GeH_2Cl_2^+$	E-439
Cl_2H^-	$ClHCl^-$	V-962,S-1406
Cl_2HN^+	$HNCl_2^+$	E-384
$Cl_2H_2Si^+$	$SiH_2Cl_2^+$	E-438
Cl_2N	NCl_2	V-976,E-343
Cl_2O^+	Cl_2O^+	E-345
Cl_2O	ClClO	V-980
Cl_2OP	$OPCl_2$	S-1455
Cl_2OS^+	Cl_2SO^+	E-412
Cl_2OSi	Cl_2SiO	V-1004
Cl_2O_2	ClOOCl	S-1456
$Cl_2O_2S^+$	$Cl_2SO_2^+$	E-467
Cl_2O_2Si	*cyc*-Cl_2SiO_2	S-1477
Cl_2O_3	Cl_2O_3	S-1478
Cl_2O_4	$ClOClO_3$	S-1494
Cl_2P	PCl_2	V-976
Cl_2S^+	SCl_2^+	E-346
$Cl_2S_2^+$	$S_2Cl_2^+$	E-413
Cl_2S_2	$SSCl_2$	V-1009
Cl_2Se^+	$SeCl_2^+$	V-978,E-346
$Cl_2Se_2^+$	$Se_2Cl_2^+$	E-413
Cl_2Si^+	$SiCl_2^+$	E-329
Cl_2Si	$SiCl_2$	V-974,E-338,S-1420
Cl_2Xe	$XeCl_2$	V-984
Cl_3^-	Cl_3^-	V-982,S-1424
Cl_3FS	SCl_3F	S-1482
$Cl_3F_2Si^-$	$SiF_2Cl_3^-$	V-1030
Cl_3Ge	$GeCl_3$	S-1455
Cl_3HSi^+	$HSiCl_3^+$	E-445
Cl_3N^+	NCl_3^+	E-408
Cl_3OP^+	Cl_3PO^+	E-463
Cl_3O_2P	$OPCl_2OCl$	S-1494
Cl_3P^+	PCl_3^+	E-409
Cl_3PS^+	Cl_3PS^+	E-464
Cl_3Sb^+	$SbCl_3^+$	E-411
Cl_3Si^+	$SiCl_3^+$	V-1004
Cl_3Si	$SiCl_3$	V-1008
Cl_4FSi^-	$SiFCl_4^-$	V-1030
Cl_4Ge^+	$GeCl_4^+$	E-462,S-1481
Cl_4Si^+	$SiCl_4^+$	E-461,S-1480
Cl_5P^+	PCl_5^+	E-505
CoH_2	CoH_2	E-278
CoH_2O	HCoOH	S-1432
CrH_2	CrH_2	S-1395
CrH_2O	HCrOH	S-1432
CrH_3O_2	$HCr(OH)_2$	S-1485
CuHO	CuOH	E-290
CuH_2N	$CuNH_2$	S-1430
CuH_2O	HCuOH	S-1433
CuH_3N	$HCuNH_2$	S-1458
Cu_2H_2	Cu_2H_2	S-1428
Cu_3H_2	Cu_3H_2	S-1463
DOSc	ScOD	S-1398
FFeH	HFeF	S-1399
FFe_2H	HFe_2F	S-1440
FGaO	OGaF	V-970
$FGeH_3^+$	GeH_3F^+	E-426
FHI^-	FHI^-	V-961
FHN	HNF	V-960,E-303
FHO^+	HOF^+	E-306
FHSi	HSiF	V-958,E-299
FH_2^+	H_2F^+	V-953,S-1397
FH_2N^+	NH_2F^+	S-1438
FH_2N	NH_2F	S-1438
FH_2P	PH_2F	S-1438
FH_3N_2	NH_2NHF	S-1487
FH_3Si^+	SiH_3F^+	E-424
FI_2	IIF	V-981
FKrXe	KrXeF	E-350
FKr_2	Kr_2F	E-349,S-1425
FNO^+	FNO^+	E-331
FNO	FON	V-975

Formula	*Structure*	*Page Nos.*
FNO_2^+	FNO_2^+	E-405
FNO_2	FONO	V-1004
FNS^+	NSF^+	E-331
FN_3^+	FN_3^+	S-1449
FNeXe	NeXeF	E-350
FNe_2	Ne_2F	E-349
FOP	FPO	S-1421
FOS	FSO	V-978
FO_2	FOO	V-977,E-343,S-1423
FO_2S^-	FSO_2^-	V-1008
FO_3S^+	FSO_3^+	E-453
FO_3S	FSO_3	V-1020,E-465
FPS	FPS	S-1422
F_2Ge^+	GeF_2^+	E-329
$F_2GeH_2^+$	$GeH_2F_2^+$	E-439
F_2GeO	F_2GeO	S-1453
F_2H^-	FHF^-	V-961,S-1405
F_2HN^+	HNF_2^+	E-383
F_2HP^+	HPF_2^+	E-384
$F_2H_2Si^+$	$SiH_2F_2^+$	E-438
F_2H_3P	PH_3F_2	S-1487
F_2I^-	FIF^-	V-982
F_2I^-	FFI^-	V-982
F_2I_2	I_2F_2	V-1009
F_2Kr^+	KrF_2^+	E-347
F_2Kr	KrF_2	V-984,E-348
F_2N^+	NF_2^+	V-975,E-340
F_2N	NF_2	V-976,E-342
$F_2N_2^+$	*t*-$N_2F_2^+$	E-404
F_2O^+	OF_2^+	E-345
F_2OS^+	F_2SO^+	E-411
F_2OSi	F_2SiO	V-1004
$F_2O_2S^+$	$F_2SO_2^+$	E-466
F_2O_2Si	*cyc*-F_2SiO_2	S-1477
F_2O_2Xe	XeO_2F_2	S-1482
F_2O_3Xe	XeO_3F_2	V-1030
F_2P^+	PF_2^+	V-975
F_2P	PF_2	S-1423
F_2S^+	SF_2^+	V-978,E-346
F_2S	SF_2	V-979,S-1424
$F_2S_2^+$	F_2SS^+	E-412
$F_2S_2^+$	$FSSF^+$	E-412
F_2Se^+	SeF_2^+	V-978
F_2Si^+	SiF_2^+	E-329
F_2Si	SiF_2	V-974,E-337
F_2Xe^+	XeF_2^+	E-347
F_2Xe	XeF_2	V-984,E-348
F_3^-	F_3^-	V-981
F_3HSi^+	$HSiF_3^+$	E-445
F_3N^+	NF_3^+	E-407
F_3NO^+	F_3NO^+	E-462
F_3NS^+	F_3NS^+	E-462
F_3OP^+	F_3PO^+	E-463
F_3OS^-	SOF_3^-	V-1022
$F_3O_2S^-$	$SO_2F_3^-$	V-1030
F_3P^+	PF_3^+	E-408
F_3PS^+	F_3PS^+	E-464
F_3S	SF_3	V-1009
F_3Sb^+	SbF_3^+	E-410
F_3Si	SiF_3	V-1007,S-1455
F_4Ge^+	GeF_4^+	E-461,S-1481
F_4OXe^+	$XeOF_4^+$	E-506
F_4P^-	PF_4^-	V-1022
$F_4P_2^+$	$P_2F_4^+$	E-504
F_4P_2	$PF_3{=}PF$	S-1494
F_4Si^+	SiF_4^+	E-459,S-1479
F_4Xe^+	XeF_4^+	E-467
F_5I^+	IF_5^+	E-506
F_5P^+	PF_5^+	E-505
F_5S	SF_5	V-1030
F_5S^-	SF_5^-	V-1030
F_5Si^-	SiF_5^-	V-1029
FeHI	HFeI	S-1399
FeH_2	FeH_2	E-277
FeH_2O	HFeOH	S-1432
FeH_2O_2	$Fe(OH)_2$	S-1468
FeH_3N	$HFeNH_2$	S-1457
Fe_2H_2O	HFeOFeH	S-1465
Fe_2H_2O	HFe_2OH	S-1465
Fe_2H_3N	HFe_2NH_2	S-1483
GaHO	GaOH	E-294
GaH_2O	HGaOH	S-1434
Ga_2H_6	Ga_2H_6	S-1501
GeH_2	GeH_2	V-952
$GeH_2I_2^+$	$GeH_2I_2^+$	E-439
GeH_2O	H_2GeO	S-1436
GeH_2O	HGeOH	S-1436
GeH_2O_3	H_2GeO_3	S-1491
GeH_3^+	GeH_3^+	S-1425
GeH_3	GeH_3	V-986,S-1427
GeH_3I^+	GeH_3I^+	E-426
GeH_4^+	GeH_4^+	E-416
GeH_4O	GeH_3OH	S-1483
GeH_4S^+	GeH_3SH^+	E-472
GeI_2^+	GeI_2^+	E-330
Ge_2H_2O	HGe_2OH	S-1470
Ge_2O_2	Ge_2O_2	S-1448
Ge_3O_3	$(GeO)_3$	S-1493
HIO	HOI	S-1405
HISi	HSiI	V-958,E-300
HI_2^-	IHI^-	V-963
HInO	InOH	E-294
HKO^+	KOH^+	E-288
HKr_2^+	HKr_2^+	V-964
HNO	HNO	V-959,E-301,S-1403
HNO^-	HNO^-	V-959,S-1404
$HNOS^+$	$HNSO^+$	E-379
HNOS	*t*-HONS	E-380
HNOS	*t*-HSNO	V-996,E-381
HNOS	*c*-HSNO	V-995,E-380
HNOS	*c*-HNSO	V-996,E-381
HNOS	*t*-HNSO	V-996,E-382
HNOS	*c*-HOSN	V-997,E-382
HNO_2	*t*-HONO	S-1444

Formula	*Structure*	*Page Nos.*
HNO_2	*c*-HONO	S-1445
HNO_3^+	HNO_3^+	E-442
HNO_4	$HOONO_2$	S-1491
HNSi	HNSi	V-956
HN_2^+	HN_2^+	V-956,S-1401
HN_2O^+	$HONN^+$	S-1443
HN_3^+	HN_3^+	E-376
$HNaO^+$	$NaOH^+$	E-288
HNiO	NiOH	S-1398
HOP	HPO	V-959,E-302
HOS	HSO	V-961,E-305,S-1405
$HOSi^+$	$HOSi^+$	S-1401
HOSr	SrOH	E-289
HOXe	XeOH	E-307
HOZn	ZnOH	S-1398
HO_2^+	HO_2^+	V-959
HO2	HO_2	V-960,E-303,S-1404
HO_2^-	HO_2^-	E-306
HO_2P	*c*-HOPO	S-1446
HO_3P	$HOPO_2$	S-1473
HO_3P	HOOPO	S-1473
HO_3P	$HP(O_2)O$	S-1473
HO_3S	$HOSO_2$	V-1016,S-1474
HO_3Sb	$HSbO_3$	S-1474
HO_3Sb	$HOSbO_2$	S-1474
HS_2	HS_2	E-305
HS_2^-	HS_2^-	S-1405
$H_2I_2Si^+$	$SiH_2I_2^+$	E-438
H_2InO	HInOH	S-1434
H_2Mg	MgH_2	S-1395
H_2MgO	HMgOH	S-1431
H_2Mg_2O	HMgOMgH	S-1464
H_2Mg_2O	HMg_2OH	S-1464
H_2Mn	MnH_2	E-277
H_2MnO	HMnOH	S-1432
H_2Mn_2O	HMn_2OH	S-1465
H_2Mn_2O	HMnOMnH	S-1465
H_2N^+	NH_2^+	V-952,E-281,S-1396
H_2N	NH_2	V-952,E-282,S-1396
H_2N^-	NH_2^-	E-287,S-1397
H_2NSr	$SrNH_2$	E-356
$H_2N_2^+$	*t*-$N_2H_2^+$	V-987,E-362
H_2N_2	*t*-N_2H_2	V-989,E-365
H_2N_2	H_2NN	E-366,S-1436
$H_2N_2O_2$	NH_2NO_2	E-490
H_2NiO	HNiOH	S-1433
H_2NiO_2	$Ni(OH)_2$	S-1468
H_2Ni_2O	HNi_2OH	S-1466
H_2O^+	H_2O^+	V-953,E-285,S-1397
H_2OS	HSOH	V-991
H_2OSc	HScOH	E-358
H_2OSi	HSiOH	V-989,S-1435
H_2OSi	H_2SiO	S-1435
H_2OSn	HSnOH	S-1436
H_2OSn_2	HSn_2OH	S-1470
H_2OSr	HSrOH	S-1431
H_2OTi	HTiOH	E-358
H_2OV	HVOH	E-358
$H_2O_2^+$	$H_2O_2^+$	E-369
H_2O_2	H_2O_2	S-1439
H_2O_2Si	HSiOOH	S-1471
H_2O_3Si	H_2SiO_3	S-1491
H_2OP	H_2PO	S-1437
H_2OP	HPOH	S-1438
H_2P^+	PH_2^+	E-282,S-1396
H_2P	PH_2	V-953,E-283,S-1397
H_2S^+	H_2S^+	E-286
$H_2S_2^+$	$H_2S_2^+$	E-369
H_2Sb	SbH_2	E-285,S-1397
H_2Se^+	H_2Se^+	E-286
H_2Si^+	SiH_2^+	E-279
H_2Si	SiH_2	V-951,E-280,S-1396
H_2Si^-	SiH_2^-	V-952,E-282
H_2Te^+	H_2Te^+	E-287
H_3^+	H_3^+	V-951,S-1393
H_3	H_3	E-276,S-1393
H_3ISi^+	SiH_3I^+	E-425
H_3N^+	NH_3^+	E-354,S-1428
H_3NNi	$HNiNH_2$	S-1458
H_3NO^+	NH_2OH^+	E-426
H_3NSi	$HSiNH_2$	S-1459
H_3O^+	H_3O^+	V-986,S-1428
H_3OP	PH_3O	S-1462
H_3OP	*c*-H_2POH	S-1462
H_3OSb	H_3SbO	S-1463
H_3OSb	H_2SbOH	S-1463
H_3O_3P	$(HO)_2HPO$	S-1500
H_3P^+	PH_3^+	E-354
H_3S^+	H_3S^+	S-1428
H_3Sb^+	SbH_3^+	E-355
H_3Si^+	SiH_3^+	V-985,S-1425
H_3Si	SiH_3	V-986,E-354,S-1426
H_3Si^-	SiH_3^-	E-355
H_4N^+	NH_4^+	V-1010,S-1456
H_4N	NH_4	E-416
$H_4N_2^+$	$N_2H_4^+$	E-472
H_4N_2O	NH_2NHOH	S-1497
H_4OSi	SiH_3OH	S-1483
$H_4P_2^+$	$P_2H_4^+$	E-473
H_4SSi^+	SiH_3SH^+	E-472
H_4Si^+	SiH_4^+	E-415,S-1456
H_5^+	H_5^+	S-1456
$H_5O_2^+$	$H_5O_2^+$	S-1496
H_6OSi	SiH_3SiH_2OH	S-1531
$H_7O_3^+$	$H_7O_3^+$	S-1529
$H_9O_4^+$	$H_9O_4^+$	S-1529
IKrXe	KrXeI	E-351
INO_2	INO_2	V-1005
INS^+	NSI^+	S-1418
INS	NSI	S-1422
I_2S	SI_2	V-979
I_3^-	I_3^-	V-983
Li_3	Li_3	S-1406
Mn_3	Mn_3	S-1407

Formula	*Structure*	*Page Nos.*
NOP	PNO	S-1417
NOS	SNO	V-972
NOS	NSO	V-972
NO_2^+	NO_2^+	E-326
NO_2^-	NO_2^-	V-975,S-1421
NO_3	NO_3	V-1002,E-404,S-1452
N_2O^+	N_2O^+	V-969,E-326,S-1415
$N_2O_2^+$	$(NO)_2^+$	E-396
N_2O_2	*c*-$(NO)_2$	V-1000,S-1450
N_2O_2	*t*-$(NO)_2$	V-1000
N_2O_2S	ON—NSO	S-1477
N_2O_2S	ONSNO	S-1477
N_2O_3	O_2N-NO	V-1017,S-1476
N_2O_3	O=N—O—N=O	V-1018,S-1476
$N_2O_4^+$	$N_2O_4^+$	E-502
N_2O_4	N_2O_4	V-1027,S-1492
N_2O_4	N_2O_4 (V_d)	V-1027
N_2O_4	$ONO-NO_2$ (D)	V-1028,S-1492
N_2O_4	$ONO-NO_2$(D′)	V-1028
N_2O_5	$O_2N-O-NO_2$	V-1035,S-1500
N_2S^+	NNS^+	S-1416
N_2S	NNS	S-1417
$N_2S_2^+$	$N_2S_2^+$	E-396
$N_2S_4^+$	$N_2S_4^+$	E-502
N_2Si	SiNN	V-967,E-315
N_3^+	N_3^+	V-967,E-315
N_3	N_3	E-325,S-1415
N_3^-	N_3^-	E-326,S-1416
N_3P_3	$(PN)_3$	S-1493
$N_3S_3^+$	$S_3N_3^+$	E-498
N_3Sr	SrN_3	E-387
N_4^+	N_4^+	S-1447
Na_3	Na_3	E-307,S-1406
Ni_3	Ni_3	S-1407
OP_2	P_2O	S-1417
OP_4	P_4O	S-1475
OP_4	*br*—P_4O	S-1476
OSSi	OSiS	S-1416
OS_2^+	SSO^+	E-334,S-1418
OS_2	SSO	E-341,S-1422
OS_2^-	SSO^-	E-344
O_2P	PO_2	V-972,E-330,S-1418
O_2P^-	PO_2^-	S-1421
O_2P_2	$(PO)_2$	S-1450
O_2S^+	SO_2^+	V-972,E-333
O_2S^-	SO_2^-	V-977,E-344
O_2Si	SiO_2	V-970
O_2Si_2	Si_2O_2	S-1448
O_3^+	O_3^+	E-332
O_3^-	O_3^-	V-977,E-343,S-1423
O_3P	PO_3	S-1452
O_3S^+	SO_3^+	E-406
O_3S^-	SO_3^-	S-1456
O_3Se	SeO_3	S-1453
O_3Si_3	$(SiO)_3$	S-1493
O_4^+	*t*-O_4^+	S-1452
O_4^-	*t*-O_4^-	V-1008,S-1455
O_4S	SO_4	V-1018
O_5P_2	P_2O_5	S-1501
P_3	P_3	S-1415
P_4^+	P_4^+	E-388,S-1448
Pd_3	Pd_3	S-1408
Pt_3	Pt_3	S-1408
S_2Si	SiS_2	S-1416
S_3	S_3	E-342
S_4	S_4	V-1005,E-406
Sb_3	Sb_3	S-1415
Sb_4	Sb_4	S-1448
Sc_3	Sc_3	S-1407
Se_3	Se_3	S-1422
Te_3	Te_3	S-1423

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9. References

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