Electronic Energy Levels of Small Polyatomic Transient Molecules

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The experimentally determined electronic energy levels of approximately 500 neutral and ionic transient molecules possessing from 3 to 6 atoms are tabulated, together with the associated vibrational structure, the radiative lifetime, the principal rotational constants, and references to the pertinent literature. Vibrational and rotational data for the ground state are also given. Observations in the gas phase, in molecular beams, and in rare-gas and nitrogen matrices are included. The types of measurement surveyed include conventional and laser-based absorption and emission techniques, laser absorption with mass analysis, and ultraviolet photoelectron spectroscopy.

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

Contents

1. Introduction

Most chemical processes—including those characteristic of combustion, atmospheric pollution, industrial chemical syntheses, chemical vapor deposition, and microcircuit etching—consist of a complicated sequence of elementary reactions, many of which involve free radicals, molecular ions, and other short-lived reaction intermediates. In order to test reaction mechanisms and to achieve optimum control of chemical processes, it is necessary to develop techniques to monitor these transient molecules in the gas phase, on catalytic surfaces, and in the condensed phase. Ideally, such monitoring techniques should be non-intrusive and space and time specific. Often, these requirements are most satisfactorily met by electronic spectral measurements. The emission spectra of flames, shock fronts, and electric discharges have long been studied, and a number of simple free radicals have been identified in them. The pioneering flash photolysis studies of Porter[1] and Herzberg[2], in which free radical production in the flash was coupled with absorption studies having a time resolution of a few microseconds, opened a new era in the detection and spectral study of free radicals.

A landmark in the spectroscopic study of free radicals was the publication in 1966 of a volume by Herzberg[3] which provided a detailed summary of the basic principles important in the spectroscopic analysis of the electronic spectra of polyatomic molecules. Although the analysis of free radical spectra has grown in sophistication and has profited greatly from the development of modern computational methods, this remains the basic reference in the field. Included in this volume was a set of tables summarizing critically evaluated electronic spectral data for polyatomic molecules with from 3 to 12

atoms. Even at this early date, many of the species included in the tables were free radicals, and a few were molecular ions.

The twenty years since the publication of the Herzberg tables have seen not only the further application of the techniques then in use for the spectral study of transient molecules, but also the development of several important new techniques. Photoelectron spectroscopy has yielded information on the electronic energy levels of hundreds of small polyatomic molecular cations. The advent of the laser was closely followed by the development of many laser-based techniques which have afforded enhanced sensitivity for the detection of transient molecules and which are amenable to the probing of specific regions of a reaction system with time resolution which now extends to the femtosecond regime. Laser-excited fluorescence studies have made feasible the determination of radiative lifetimes for excited electronic states of free radicals and molecular ions. During the last few years, laser-based techniques have been used in conjunction with molecular beams, providing an even more powerful tool for the study of the spectra of transient molecules. Finally, the development of modern computational techniques has greatly facilitated not only the collection and analysis of spectral data but also the prediction of the spectral properties of as yet undetected free radicals and molecular ions.

Despite these developments, the Herzberg tables remain the prime source of data on the electronic spectra of small polyatomic molecules. While the data presented for stable molecules have since been considerably refined, data for many small transient molecules had not yet been obtained when these tables were published. A few subsequent references have dealt with portions of the literature on transient molecules. Photoelectron spectral data for stable molecules, from which electronic spectral data for the corresponding molecular cation can be derived, have been summarized by several workers, including Turner et al.,[4] Rabalais,[5] and Kimura et al.[6]. Reviews of the photoelectron spectra of transient molecules have also appeared.[7-9] A recent survey of progress in the high resolution electronic spectroscopy of small free radicals since the publication of Herzberg's book has been provided by Ramsay.[10] However, a comprehensive, critically evaluated compilation of the more recent electronic spectral data for small polyatomic transient molecules has not yet appeared. The objective of this paper is to bring together critically evaluated electronic spectral data for transient molecules which possess from three to six atoms, in order partially to fill this gap in the literature.

2. Scope of Review

The definition of a transient molecule as one whose lifetime is less than a few minutes in the pressure range (typically 0.1–1.0 Torr) encountered in its production, suggested by Dyke and co-workers,[7] will be adopted for this review. Because of the great volume of available experimental data, it is necessary to limit the review to species possessing from three to six atoms. Although ground-state vibrational data for many of these species, as well as for somewhat larger transient molecules, formed the subject of a critical compilation[11] only three years ago, already there are many additions to the literature for these species. For this reason and because of the convenience of having all of the data for a given species in one place, the ground-state vibrational energy levels of species for which there are also electronic spectral data are included in this compilation. Estimates of relative intensities, which are specific to infrared absorption measurements, have been omitted. On the other hand, the principal rotational constants, A_0, B_0, and C_0, for the ground-state transient molecule have been added. It is planned also to publish a supplement to the earlier ground-state vibrational data compilation within the coming year. That compilation will include new and revised tables for transient molecules for which no electronic spectral data are available and for transient molecules which possess from 7 to 16 atoms. It will also include a master index to the three compilations.

Because of the importance of the chemistry of the heavier atoms in catalysis, chemical vapor deposition, and microcircuit etching systems, these tables cover a somewhat wider range of elements than did the earlier vibrational tables. The first two full rows of the Periodic Table are included, with partial coverage for species containing heavier atoms such as selenium, bromine, iodine, krypton, and xenon. A number of electron-deficient molecules which are found in high temperature vapors are included. An important class of compounds for which many new data have recently been published and which are included in this compilation are the products of metal-atom addition to water or to other simple molecules. Many of these species possess ionic ground-state structures and were, therefore, not included in the ground-state vibrational data compilation. Because the extent of ionic character varies with the electronic state of the molecule, such species are included in this compilation.

Photoelectron spectra are now available for almost all small stable polyatomic molecules which can be obtained with an adequate vapor pressure for gas-phase observation. The photoelectron spectrum provides a powerful tool for mapping the electronic and vibrational energy levels of the corresponding cation. Unfortunately, except in a few recent studies using molecular beams and very high resolution, the precision is inherently limited, compared to that of typical infrared or ultraviolet spectral observations. Because many electronic transitions cover a rather wide spectral region, compared with the uncertainty of the photoelectron spectral data, and because these data offer a major source of information on the properties of molecular cations, it was decided to include photoelectron spectral data for stable molecules in this compilation.

In recent years, several laboratories have also obtained photoelectron spectra for anions. These have been in-

cluded in this compilation if vibrational structure has been observed for the anion. The threshold for photoelectron detachment, which corresponds to the onset of a dissociative excited electronic state, is also given. Where spectroscopic structure has not been observed, the threshold for electron detachment can be obtained from the recent compilation by Lias and co-workers.[12]

3. Types of Measurement

Much of the spectral data summarized in these tables was obtained using conventional gas-phase ultraviolet absorption or emission spectroscopy, which affords the potential for both a broad spectral survey and very high resolution. The photographic plate provides a cumulative detector for visible and ultraviolet radiation, but not for the infrared region. Therefore, gas-phase studies of the electronic spectra of transient molecules were for many years much more readily conducted than were studies of ground-state vibrational spectra. The concentration of transient molecules in flames, chemiluminescent reactions, or various types of discharge may be sufficiently high for spectroscopic study. However, flash photolysis often yields a relatively high concentration of transient molecules at a short time interval after the flash. Because the products are generally formed with much less internal energy than is typical of systems with detectable emission spectra, the absorption spectra obtained in flash photolysis studies are more readily analyzed. Furthermore, the time-resolved detection used in flash photolysis studies provides information on the rates of formation and disappearance of transient molecules in the system.

Recent years have seen the development of a wide variety of laser-based techniques for the study of the spectra of transient molecules in the gas phase. Since a given laser is tunable over a relatively limited spectral region, laser studies of transient molecules are greatly aided by the availability of survey spectra obtained using other techniques. Although laser studies often are cumbersome for the primary identification of electronic transitions of transient molecules, once the basic spectroscopic identification has been established they afford the important advantages of high sensitivity and of space and time specificity. The combination of molecular beam and laser technology is very effective for studies of transient molecules. If a supersonic molecular beam is used, excited rotational and vibrational energy levels can be very effectively depopulated, and the absorption spectrum of the molecule is greatly simplified. When laser excitation is coupled with photon detection, it has often been possible to obtain information on the radiative lifetimes of individual vibronic levels, greatly enhancing our understanding of the patterns of energy redistribution in electronically excited molecules. Recently, laser excitation combined with mass detection has led to such new modes of study of transient molecules as photofragment spectroscopy and resonance-enhanced multiphoton ionization (REMPI). This latter technique, which is now undergoing rapid development,[13] has several special advantages. Whereas laser-excited fluorescence measurements depend upon the presence of electronic energy levels which decay by photon emission, all molecules possess Rydberg energy levels. REMPI measurements depend on multiphoton excitation into a suitable electronic energy level, most often one of Rydberg character. The selection rules may permit excitation of levels which are not accessible by one-photon excitation from the ground state. The range of tunability of the laser is multiplied by the number of photons required for the excitation of the Rydberg level, significantly broadening the spectral region which can be probed with a given laser. When the parent molecule is a free radical, almost all of the mass signal is generally found to arise from the parent cation, with very little fragmentation. For these reasons, REMPI has already established itself as a powerful tool for mapping the Rydberg transitions of transient molecules.

Selective coverage of the voluminous literature on photoelectron spectroscopy is employed in these tables. An effort has been made to include the best data available for each molecule. Several criteria are important in determining whether a given reference should be included. The first criterion is resolution. In the few instances in which high resolution photoelectron data are available, these are heavily weighted. Where direct spectroscopic observation is possible, the results of such measurements generally are of considerably higher precision than photoelectron data, which are then omitted from the tables. A second criterion is the availability of adiabatic ionization potentials. In order to obtain information on the positions of electronic transitions from photoelectron spectral data, it is necessary to subtract the first ionization potential from the energy of the photoelectron band. Where there is little change in the molecular geometry in the transition, the difference between the vertical ionization potentials gives a reasonable approximation to the position of the electronic transition. However, this is not the general case. Where the first photoelectron transition has a gradual onset, a better value of the first ionization potential may have been obtained from photoionization data or from the extrapolation of Rydberg series in the spectrum of the parent molecule. Supplementary sources of data for the first ionization potential are cited in the tables. However, if the difference between the first adiabatic ionization potential obtained in the photoelectron spectrum and that obtained in other measurements amounts to only 10 or 20 meV, the photoelectron spectroscopic value is used, because of the value of a consistent set of measurements. Where threshold energies differ by one quantum in a vibrational progression, a best value for the ionization potential is chosen which coincides with the most probable position of the vibrationally unexcited transition.

Most photoelectron spectroscopic studies have been conducted at low to moderate resolution. Uncertainties of 10 to 20 meV (80 to 160 cm^{-1}) are typical of these measurements, and the absolute uncertainty is doubled in

the subtraction process. Smaller uncertainties, often on the order of 40 cm^{-1}, are usually cited for vibrational frequencies within a transition. The authors' estimated uncertainties have been given in these tables. However, where several laboratories have reported photoelectron studies on a given system at similar resolution the spread in the vibrational frequencies reported frequently exceeds the estimated error, suggesting that the uncertainty has been underestimated. For typical photoelectron spectroscopic studies, vibrational frequency uncertainties of 80 cm^{-1} seem to be more realistic.

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

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

Matrix isolation studies also provide a valuable source of survey spectra on which a search using high resolution gas-phase absorption or laser-based techniques may be based. All of the absorptions of a species trapped in dilute solid solution in a cryogenic matrix arise from the ground vibrational and electronic state of the molecule, a factor which may aid in the assignment. It is sometimes possible to trap detectable concentrations of reaction intermediates which have a shallow potential minimum but which are formed in gas-phase reaction systems with energy which exceeds their dissociation potential. Rotational energy is effectively quenched by the matrix. Therefore, positive identifications of the electronic spectra of molecules isolated in matrices are difficult. Primary identifications are best made in the infrared, where isotopic shifts and splittings can be resolved and assigned and a detailed vibrational analysis achieved. It is often valuable to classify products in a matrix system according to the spectral range in which they are photolytically stable. The correspondence of the behavior of electronic band systems with those of the infrared absorptions which have been assigned to the species of interest then provides strong support for the assignment of the new band systems to that species. At the same time, it provides information on dissociative electronic transitions and on the photodissociation products of that molecule.

It is necessary to consider the extent of perturbation of the spectrum which results from isolation of the molecule in a matrix. This perturbation is expected to be minimal for rare-gas and small covalent molecule matrices, to which the following discussion and coverage in the tables will be restricted.

As was shown in the compilation of the ground-state vibrational fundamentals of transient molecules[11] and in a comparison of the ground-state vibrational fundamentals of diatomic molecules in the gas phase and in inert solid matrices,[15] shifts tend to be smallest for a neon matrix and to increase with increasing mass of the rare gas atom. Somewhat larger shifts are typical of a nitrogen matrix. Most matrix shifts in ground-state vibrational fundamentals of covalently bonded molecules isolated in solid neon are less than about 1%, and in solid argon less than about 2%. Although larger shifts—usually to lower frequencies (a "red" shift)—occur for vibrations of a diatomic molecule which has a large dipole moment, shifts in the frequencies of intraionic vibrations lie within the range typical of uncharged species.

In contrast to the behavior of ground-state vibrational absorptions of molecules in matrices, at all but extremely low temperatures electronic absorption bands are typically dominated by the relatively broad, prominent phonon wings. As the sample deposit is cooled, the sharp zero phonon lines grow in intensity. For absorption measurements, the absorption maximum of the phonon wing generally lies at a higher frequency than the zero phonon line, whereas for emission measurements the maximum of the phonon wing generally is observed at a lower frequency than the zero phonon line. Because it is necessary to study neon matrices at a temperature near 4 K, this effect is minimal for them. However, the convenience and ready availability of closed-cycle helium refrigeration systems, which can cool the sample to temperatures as low as about 11 K, has led to the more frequent use of an argon matrix. Both because of the increased molecular interaction with the matrix and because of the higher temperature which is often used, electronic absorptions tend to be relatively broad in an argon matrix.

A comparison of the electronic energy levels of diatomic molecules in the gas phase and in inert solid matrices has recently been published.[16] For valence transitions of covalently bonded molecules isolated in solid neon, the distribution of the matrix shifts is quite sharply peaked near zero deviation, with a "tail" extending toward higher frequencies (a "blue" shift). As the mass of the rare-gas atom is increased, an increasing red shift in the electronic band origin tends to occur. The blue shift in

the apparent band origin which results from detection of the phonon maxima rather than of the zero phonon lines in an absorption measurement amounts to approximately 1 to 1.5% in a typical system. A red shift of similar magnitude occurs in emission measurements. For an argon matrix, the reported values of most electronic band origins lie within about 2% of the band origin. Rydberg transitions of molecules in matrices are usually greatly broadened and are shifted by as much as several thousand cm^{-1}. Relatively large matrix shifts may also result from charge transfer interaction between species with highly polar bonds and the heavier rare gases. The sign of this shift depends on whether the molecular bonding is more polar in the excited electronic state (favoring a red shift) or in the ground state (favoring a blue shift). Although there is often a relatively large experimental uncertainty in the measurement of excited-state vibrational band spacings, in solid neon these are usually within about 1% of the gas-phase values and in solid argon within about 3%.

These generalizations appear to remain valid for polyatomic transient molecules isolated in rare-gas matrices. In these tables, there are 25 pairs of observations for which T_0 values are reported for both the gas phase and a neon matrix. Of these, 23 pairs agree within $\pm 2\%$ and 15 within $\pm 1\%$. Similarly, there are 28 pairs of observations of T_0 for both the gas phase and an argon matrix. Of these, 26 correspond within $\pm 2\%$ and 19 within $\pm 1\%$. As for diatomic molecules, argon-matrix values tend to be somewhat red-shifted; 16 of the pairs correspond between 0 and $+1\%$.

These generalizations have been found to apply for certain species with ionic bonds and for many molecular ions (several of which were included in the comparisons of pairs of data in this set of tables), as well as for neutral molecules. As is shown in the tables of Sec. 6.2, because the ionic character of CaOH, SrOH, and BaOH changes relatively little in their low-lying electronic transitions, only small shifts in the band origins of these species occurred when they were isolated in a krypton matrix. The vibronic spectroscopy of covalently bonded molecular ions isolated in rare-gas matrices has been reviewed by Bondybey and Miller.[17] These workers have also recently published a detailed study of matrix effects for $C_6F_6^+$ isolated in solid neon.[18] In order to minimize charge transfer interaction with the matrix, which can lead to large perturbations of excited electronic states, it is highly desirable to study molecular ions in a neon matrix.

Although in the early days of matrix isolation spectroscopy it was believed that extremely rapid quenching of excited vibrational and electronic states should occur in a matrix environment, this assumption has been found not always to be valid. Indeed, matrix isolation measurements have proved useful for determining approximate radiative lifetimes in a number of systems. As has been noted in the review by Bondybey and Miller[17], the matrix may induce nonradiative energy transfer when there is a strong quantum mechanical coupling between the electronic state and lower-lying electronic states or the ground state. Thus, the existence of spectroscopic perturbations may lead to effective quenching of small-molecule fluorescence in a matrix. An interesting example is provided by C_3. As is summarized in the tables of Sec. 6.3, even in a neon matrix the lifetime of the $\tilde{A}\ ^1\Pi_u$ state is greatly shortened, and emission from the $\tilde{a}\ ^3\Pi_u$ state, which has not been detected in the gas phase, is observed. This observation suggests the potential utility of matrix isolation studies for detecting low-lying excited electronic states which are not readily accessible in gas-phase studies. For larger molecules, the density of states in the electronic spectral region is sufficiently great to provide a unimolecular mechanism for nonradiative energy transfer in the gas phase. Bondybey and Miller have observed fluorescence from electronically excited states of a large number of substituted benzene cations isolated in rare-gas matrices. The radiative lifetime typical of a neon matrix is generally about 85% of the gas-phase value. Experiment and theory suggest that in the absence of matrix-induced nonradiative processes the matrix shift in the radiative lifetime is approximately related to the square of the index of refraction of the matrix.

4. Guide to the Compilation

The goal of this compilation is to summarize the experimentally determined electronic energy levels for approximately 500 transient molecules which possess from three to six atoms, in order to aid in spectral identification and to provide energy level data needed for other types of research. The literature has been surveyed through January 1988; only limited addition of more recent data has been possible. Attempts have been made to provide a critically evaluated compilation. Often only a single set of observations has been reported. As additional data become available, it is hoped that later versions of this compilation can be more definitive. Data have been omitted when later data dictate a reassignment or when there has been a substantial refinement, as when high resolution spectroscopic studies have supplanted photoelectron spectroscopic observations. Of course, there are also inadvertent omissions. The author invites communication of additions and revisions for inclusion in later editions of or supplements to this compilation.

As for the ground-state vibrational energy levels, isotopic substitution studies provide the most definitive identification of the carrier of a set of spectral features. However, often such data are not available. The extent to which chemical evidence can establish a positive identification varies widely. There are many examples in the literature where characteristic impurities have led to the appearance of a band system, resulting in a misassignment. Where chemical evidence has presented a reasonable argument for the identification of a transient molecule, the data have been included in this compila-

tion, in the hope that, with the recognition that the identification has yet to be finally established, further study will be encouraged.

The order of appearance of molecules in this compilation is similar to that adopted by Herzberg[3] and by the earlier vibrational data compilation.[11] Species are ordered first by the number of atoms in the molecule, then by the number of hydrogen atoms, and finally by the number of valence electrons. When all three of these criteria match, the order of appearance is determined first by the number of valence electrons on the central atom and then by its row in the Periodic Table. For a few molecules with a chain of heavy atoms, the sequence is somewhat arbitrary. Data are given for both the normal and the fully deuterium-substituted molecule. However, only the hydrogen-containing species is listed in the index.

The heading for each electronic state gives its symmetry, the point group to which the molecule belongs in that electronic state, and, where available, references to a quantitative molecular structure. For a discussion of the molecular point groups and the symmetry species of the molecular electronic and vibrational transitions, see standard texts on spectroscopy. 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,[19] 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 state of the molecule when all of the vibrational and rotational quantum numbers in both electronic states equal zero, is given. However, where only low resolution data or photoelectron data are available, it is often possible only to give the position of the absorption maximum. 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. It is more likely that the first adiabatic ionization potential can be determined than that higher adiabatic ionization potentials are accessible. The footnote phrase "from vertical ionization potential" implies that the first adiabatic ionization potential is known but 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. Above about 18 eV, there are often relatively large uncertainties in the positions and assignments of photoelectron bands. Since transitions which correspond to these higher bands generally lie well into the vacuum ultraviolet spectral region, the coverage of higher energy photoelectron data has been truncated. Except where otherwise indicated, the units of all quantities in these tables are cm^{-1}. As in the tables of Herzberg,[3] T_0 values are given to the center of multiplet structure. Thus, 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 range in which various electronic transitions involving the state of interest occurs is also tabulated. This range is a composite of the values typical of absorption and emission measurements. Laser-excited fluorescence measurements may 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 compilation of ground-state vibrational energy levels,[11] except that relative intensities have been omitted and error estimates are incorporated into the tables. 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. 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) $\equiv$ 1234.56 $\pm$ 0.78). Where the error includes a decimal point, the decimal point has been included. 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. If the bending vibration 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[3] 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 structure due to inversion splitting. For these, the specific component for which the vibrational frequency is reported is designated in a footnote.

Where radiative lifetimes have been measured, they are given following the vibrational table. τ_0, the radiative lifetime of the vibrationless transition, is given wherever possible. Where the lifetime is accessible only for excited vibrational states, the subscripts give the vibrational quantum numbers of the observed band.

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

Finally, in order to 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, more precise values of these constants and a far more detailed set of molecular constants, have been derived from the analysis of high resolution spectra. The references to the experimental literature should facilitate the location of such data.

5. Abbreviations

AB	near infrared-visible-ultraviolet absorption
CC	color-center laser
CL	Chemiluminescence
DL	diode laser
ED	electron diffraction
EF	electron-excited fluorescence
EM	near infrared-visible-ultraviolet emission
ESR	electron spin resonance
HFD	high frequency deflection
ID	ion drift
IR	infrared absorption (conventional or Fourier transform)
LD	laser difference frequency
LF	laser-excited fluorescence (excitation and resolved emission)
LMR	laser magnetic resonance
LS	laser Stark spectroscopy
MO	molecular orbital calculations
MODR	microwave-optical double resonance
MPI	multiphoton ionization
MW	microwave and millimeter wave
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
TPE	threshold photoelectron spectroscopy
UV	near infrared-visible-ultraviolet absorption and emission

6.1. H_3 and Triatomic Dihydrides

H_3

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

T_o[a] = 18511 gas EM[8] 3d-2p$^2A_2''$ 568-615 nm

EM[8] 3d-3p$^2E'$ 3891-4456 cm^{-1}

B_o = 42.99; C_o = 22.735 EM[8]

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

T_o[a] = 18409 gas EM[8] 3d-2p$^2A_2''$ 568-615 nm

EM[8] 3d-3p$^2E'$ 3891-4456 cm^{-1}

B_o = 42.99; C_o = 22.735 EM[8]

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

T_o[a] = 18037 gas EM[8] 3d-2p$^2A_2''$ 568-615 nm

EM[8] 3d-3p$^2E'$ 3891-4456 cm^{-1}

B_o = 42.99; C_o = 22.735 EM[8]

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

T_o[a] = 17789 gas EM[2,3,8] 3p$^2A_2''$-2s$^2A_1'$ 556-574 nm

τ = 37(4) ns gas EM[10]

B_o = 47.45; C_o = 23.495 EM[8]

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

T_o[a] = 17600 gas EM[3] 3s$^2A_1'$-2p$^2A_2''$ 592-615 nm

EM[6] 3s$^2A_1'$-3p$^2E'$ 3178-3847 cm^{-1}

B_o = 44.19; C_o = 22.676 EM[6]

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

T_o[a] = 13961 gas EM[2,4] 3p$^2E'$-2s$^2A_1'$ 708-736 nm

EM[6] 3s$^2A_1'$-3p$^2E'$ 3178-3847 cm^{-1}

EM[8] 3d-3p$^2E'$ 3891-4456 cm^{-1}

B_o = 42.15; C_o = 21.505 EM[6]

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

T_o[a] = 993 gas EM[3,6] 3s$^2A_1'$-2p$^2A_2''$ 592-615 nm

EM[8] 3d-2p$^2A_2''$ 568-615 nm

B_o = 44.58; C_o = 22.288 EM[6]

2s $^2A_1'$[b] 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_o = 46.82; C_o = 23.41 EM[3]

D_3

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

T_o[a] = 18530 gas EM[8] 3d-2p$^2A_2''$ 569-601 nm

EM[8] 3d-3p$^2E'$ 3772-4517 cm^{-1}

τ = 13(1) ns gas EM[9]

B_o = 21.72(2); C_o = 10.91(2) EM[8]

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

T_o[a] = 18433 gas EM[8] 3d-2p$^2A_2''$ 569-601 nm

EM[8] 3d-3p$^2E'$ 3772-4517 cm^{-1}

τ = 13(1) ns gas EM[9]

B_o = 21.72(2); C_o = 10.91(2) EM[8]

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

T_o[a] = 18098 gas EM[8] 3d-2p$^2A_2''$ 569-601 nm

EM[8] 3d-3p$^2E'$ 3772-4517 cm^{-1}

τ = 13(1) ns gas EM[9]

B_o = 21.72(2); C_o = 10.91(2) EM[8]

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

T_o[a] = 17872 gas EM[2,3,8]LF[7] 3p$^2A_2''$-2s$^2A_1'$ 553-569 nm

τ = 29(1) ns gas EM[9]

B_o = 22.73(6); C_o = 10.68(2) EM[8]

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

T_o[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}

B_o = 21.98; C_o = 12.41 EM[6]

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

T_o[a] = 14092 gas EM[2,4]LF[7] 3p$^2E'$-2s$^2A_1'$ 703-735 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.
e'	2	Deformation	~1750[c]	gas	EM	4

τ = 18.5(1.0) ns gas EM[9]

B_o = 21.15; C_o = 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

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

gas $EM^{2,3}LF^7$ $3p^2A_2''$-$2s^2A_1'$ 553-569 nm

EM^4 $3p^2E'$-$2s^2A_1'$ 703-735 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Ring breathing	~2400[c]	gas	EM	4
e'	2	Deformation	~1990[c]	gas	EM	4

B_0 = 22.99; C_0 = 11.495 EM^3

[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. In the absence of vibrational and rotational excitation, this process is exothermic by 5.52 eV. Unstructured emission observed[11] between 190 and 280 nm, with a maximum near 230 nm, upon charge transfer between K and H_3^+ or D_3^+ has been attributed to transitions originating in bound Rydberg states of H_3 or D_3 and terminating in the dissociative ground state continuum.

[b] 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]

[c] Tentative assignment.

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MnH_2

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

X $^6A_1$ C_{2v}

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

MnD_2

X $^6A_1$ C_{2v}

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

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FeH_2

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

X

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

FeD_2

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

$\tilde{X}$

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

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CoH_2

Photodissociation into Co + H_2 was observed[1] on irradiation at 22000.

$\tilde{X}$

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

CoD_2

$\tilde{X}$

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

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BH_2 [a]

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

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

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

B_0 = 6.13 AB[1]

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

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

BD_2 [a]

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

$B_0 \sim 3.2$ AB[1]

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

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

a ^{11}B.
b The $\tilde{A}\ ^2B_1$ and $\tilde{X}\ ^2A_1$ states are perturbed by strong Renner-Teller interaction. While molecular orbital arguments indicate that the $\tilde{A}$ state should be linear, lower members of the bending progression could not be observed, and there may be a small barrier to linearity in the $\tilde{A}$ state.
c Assumed value.

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AlH_2

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

$T_0 < 15200$ 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]

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

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SiH_2^+

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

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

Predissociation into $Si^+ + H_2$ and into $SiH^+ + H$ was observed.

B = 3.956(1) PF[1]

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

B = 5.094(2); C = 3.772(4) PF[1]

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CH_2

$\tilde{D}$

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

$\tilde{C}$

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

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

T_0 = 70634 gas AB[1] $3d^3A_2$-$\tilde{X}$ 141.5 nm

Diffuse. First member of Rydberg series converging to 83851. Higher members observed (AB^2) at 76553, 79241, and 80688.

B_0 = 6.89[a] AB[1]

$\tilde{c}\ ^1A_1$

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

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

T_0 = 10255(20) gas AB[1,3,27]LMR[21] $\tilde{b}$-$\tilde{a}$ 490-920 nm

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

τ = 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 = 1193 [14]

$\bar{a}\ ^1A_1{}^b$ C_{2v} Structure: AB[3]

T_0 = 3156(5) gas AB[1,3,27,28]LMR[21,26]PE[23,24] $\tilde{b}$-$\bar{a}$ 490-920 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH s-stretch	2805.9(1)	gas	LF,LD	10,20
	2	Bend	1352.6	gas	AB	3,27,28
b_2	3	CH a-stretch	2864.5(3)	gas	LD	20

$\tau \sim 18$ s[c]

A_0 = 20.118(2); B_0 = 11.205(2); C_0 = 7.069(2) AB[3,27,28]

Barrier to linearity = 9451 [14]

$\tilde{X}\ ^3B_1$ 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

A_0 = 73.811; B_0 = 8.450; C_0 = 7.184 IR[25]

Barrier to linearity = 1931(30) [26]

CD_2

$\tilde{D}$

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

$\tilde{C}$

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

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

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

B_0 = 3.595 AB[1]

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

$\tau(0,16,0)$ = 6.0(7) μs LF[13]

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

T_o = 3140(50) PE[23]

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

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

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

A_o = 37.787; $\frac{1}{2}(B+C)_o$ = 3.962;

$\frac{1}{2}(B-C)_o$ = 0.267 LMR[18,22]

[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] They are also strongly perturbed by interaction with the $\tilde{X}\ ^3B_1$ state.[27,28]
[c] Calculated value.[21]

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SiH_2

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

T_o = 15533 gas AB[1,2] $\tilde{A}$-$\tilde{X}$ 480-650 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	860	gas	AB	1

τ[b] = 0.6 μs gas LF[6]

A_o = 17.75[c]; B_o = 4.9[c]; $C_o \sim 2.8$[c] AB[2]

Barrier to linearity ~ 8000 [3]

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

T_o = 7340(240)[d] gas PI[8]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1964[e]	Ar	IR	5
	2	Bend	~1004	gas	AB	2
			990(20)	gas	LF	4
			995	Ar	IR	5
b_2	3	Asym. stretch	1973	Ar	IR	5

A_o = 8.096(1); B_o = 7.021(1); C_o = 3.700(1) AB[2]

SiD_2

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

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

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

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

[a] The $\tilde{A}\ ^1B_1$ and $\tilde{X}\ ^1A_1$ states are perturbed by strong Renner-Teller interaction.[3]
[b] Preliminary studies[7] at higher resolution indicate that the collision-free lifetime varies from ∿ 10 to > 500 ns, depending on the rotational transition.
[c] Extrapolated values.[2]
[d] Possibly 6290(240).[8]
[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^+

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

$T_o \leq 20490(160)$[a] gas PE[1]

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

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

T_o = 10530(80) gas PI[2]

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

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	840(50)	gas	PE	1
b_2	3	Asym. stretch	3359.94	gas	LD	3

Barrier to linearity ∿ 330 LD[3]

ND_2^+

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

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

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

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

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

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

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PH_2^+

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

$T_o \geq 5730$ gas PI[1]

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

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CH_2^-

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

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

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

CD_2^-

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

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

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

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SiH_2^-

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

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

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

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NH_2

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

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

T_o = 11122.6 gas AB[1,8]LF[6] $\tilde{A}$-$\tilde{X}$ 430-950 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 associated with levels which are substantially perturbed.

B_o = 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
			3220[c]	N_2	IR	5
	2	Bend	1497.32	gas	UV,LF LMR,IR	1,6,8-10 13,20
			1499	N_2	IR	5
b_2	3	Asym. stretch	3301.11	gas	LD	16

A_o = 23.693; B_o = 12.952; C_o = 8.173 AB[1,8]LMR[13]IR[20]

Barrier to linearity = 12024 [14]

ND_2

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

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

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

B_0 = 4.41 AB[1]

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

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

A_0 = 13.343; B_0 = 6.488; C_0 = 4.290 AB[1,18] LMR[11]

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

[b] Origin not observed. Typically, bands appear in argon at frequencies approximately 25 cm^{-1} higher than in the gas phase and in krypton and xenon[3] at frequencies approximately 5 and 35 cm^{-1}, respectively, lower than in the gas phase. In all three matrices the bands associated with large quantum numbers of v_2 are shifted to lower frequencies. Rotational structure is resolved. 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

18188(10) Ar AB[13]

Evidence for predissociation above 22000. LF[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	949.12	gas	UV	2,6
			962(25)	Ar	AB	13

τ = 4(1) μs gas LF[11] EM[12]

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

Barrier to linearity = 6840 [7]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	2270(80)	gas	PE	10
	2	Bend	1101.91	gas	UV,LMR	2,4,14
			1103	Ar	IR	13

A_0 = 9.132; B_0 = 8.084; C_0 = 4.214

AB[4,16] LMR[8,14,15] MW[17,18]

Barrier to linearity = 25100 [7]

PD_2

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

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

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

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

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

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

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

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AsH_2

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

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

Predissociated above 23300 [1]

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

τ = 130(20) ns gas EM^2

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

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

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

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

AsD_2

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

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

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

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

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SbH_2

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

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

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

τ = 70(20) ns gas EM^2

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H_2O^+

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

T_o = 36757(12) gas PE^9

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

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

T_{050} = 13409.3 gas $EM^{1,5}$ $\tilde{A}$-$\tilde{X}$ 400-750 nm

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

τ = 10.5(1.0) μs gas EF^6

B_{050} = 8.57 EM^5

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

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
	2	Bend	1408.4	gas	EM,PE	1,5,9
b_2	3	Asym. stretch	3253.03	gas	LD	11

A_o = 29.037(3); B_o = 12.423(2); C_o = 8.469(2) LMR^8LD^{11}

Barrier to linearity = 9187 [7]

D_2O^+

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

T_o = 37430(50) gas $PE^{2,4}$

38498(12) gas PE^9

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

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

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

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

τ is ∿12% greater than for H_2O^+.[3]

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

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

A_o = 16.03; B_o = 6.240(3); C_o = 4.407(3) EM^{10}

[a] Best fit of simulated photoelectron spectrum.
[b] The $\tilde{A}\ ^2A_1(\Pi_u)$ and $\tilde{X}\ ^2B_1$ states are perturbed by strong Renner-Teller interaction.

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H_2S^+

B $^2B_2$ C_{2v}

T_o = 34770(160) gas PE[2]

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

Ã $^2A_1$[a] C_{2v} Structure: EF[3]

T_o = 18518 gas EF[1,3] PE[2,5] Ã-X̃ 400-500 nm

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

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

τ = 4.2(4) μs gas EF[4]

B_{020} = 5.03 EF[3]

Barrier to linearity ∿ 4600 [1]

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

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

A_o = 10.18(2); B_o = 8.63(1); C_o = 4.60(6) EF[3]

D_2S^+

Ã $^2A_1$ C_{2v}

T_o = 18574 gas EF[3] Ã-X̃ 400-500 nm

B_{030} = 2.46 EF[3]

X̃ $^2B_1$ C_{2v}

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

A_o = 5.37(2); B_o = 4.32(1); C_o = 2.34(2) EF[3]

[a] The Ã $^2A_1$ and X̃ $^2B_1$ states are perturbed by strong Renner-Teller interaction.

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H_2Se^+

B $^2B_2$ C_{2v}

T_o = 34060(40) gas PE[1,2]

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

Ã $^2A_1$ C_{2v}

T_o = 20270(70) gas PE[1,2]

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

Barrier to linearity ∿ 6450 [2]

X̃ $^2B_1$ C_{2v}

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

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H_2Te^+

B $^2B_2$ C_{2v}

T_0 = 31470(160) gas PE[1]

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

Ã $^2A_1$ C_{2v}

T_0 = 20090(160) gas PE[1]

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

X̃ $^2B_1$ C_{2v}

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

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NH_2^-

Threshold for electron detachment from ground-state NH_2^- is 0.77(5).[1-3]

X̃ $^1A_1$ 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
b_2	3	Asym. stretch	3190.29	gas	CC	5

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

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6.2. Triatomic Monohydrides

$NaOH^+$

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

T_0 = 28400(1200) gas PE[1]

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

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KOH^+

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

T_0 = 31000(1200) gas PE[1]

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

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CaOH

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

T_0 = 18022.268(1) gas $CL^2LF^{4,6}$ $\tilde{B}$-$\tilde{X}$ 555 nm

Absorption maximum at 18236(15) in a krypton matrix.[5]

B_0 = 0.339 $LF^{4,6}$

$\tilde{A}\ ^2\Pi$ $C_{\infty v}$ Structure: LF^3

T_0 = 15998.128(1) gas $CL^2LF^{3,6}$ $\tilde{A}$-$\tilde{X}$ 600-650 nm

Absorption maximum at 16096(15) in a krypton matrix.[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	∿345	gas	LF	3
Σ^+	3	CaO stretch	635(2)[a]	gas	LF	3

A = 66.795(1) gas $LF^{3,6}$

B_0 = 0.341 $LF^{3,6}$

$\tilde{X}\ ^2\Sigma^+$ $C_{\infty v}$ Structure: LF^3

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	339(1)	gas	LF	3
Σ^+	3	CaO stretch	606(1)	gas	LF	3

B_0 = 0.334 $LF^{3,4,6}$

CaOD

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	∿243	gas	LF	3
Σ^+	3	CaO stretch	623(2)[a]	gas	LF	3

B_0 = 0.308 LF^3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	240[a]	gas	LF	3
Σ^+	3	CaO stretch	603(1)	gas	LF	3

B_0 = 0.304 LF^3

[a] $\omega_1 + \frac{1}{2}x_{13}$.

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SrOH

$\tilde{B}\ ^2\Sigma^+$ $C_{\infty v}$ Structure: LF[3]

T_0 = 16377.505(1) gas CL^{2}LF[3] $\tilde{B}$-$\tilde{X}$ 605-611 nm

Absorption maximum at 16553(15) in a krypton matrix.[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	397(3)	gas	LF	3
Σ^+	3	SrO stretch	582(3)	gas	LF	3

B_0 = 0.252 LF[3]

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

T_0 = 14674.332(2) gas CL^{2}LF[6] $\tilde{A}$-$\tilde{X}$ 645-695 nm

Absorption maximum at 14598(15) in a krypton matrix.[4] An incompletely resolved absorption at 14598(15) may be contributed either by SrOH trapped in another matrix site or by the excitation of bending vibration in the $\tilde{A}$ state.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	SrO stretch	544(1)	gas	LF	6

A = 260 gas LF[6]

B_0 = 0.254 gas LF[6]

$\tilde{X}\ ^2\Sigma^+$ $C_{\infty v}$ Structure: LF[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	361(1)	gas	LF	3,6
Σ^+	3	SrO stretch	528(1)	gas	LF	3,6
			479.3	Ar	IR	5

B_0 = 0.249 LF[3,6]

SrOD

$\tilde{B}\ ^2\Sigma^+$ $C_{\infty v}$ Structure: LF[3]

T_0 = 16366.107(1) gas LF[3] $\tilde{B}$-$\tilde{X}$ 607-611 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	311(10)	gas	LF	3
Σ^+	3	SrO stretch	516(10)	gas	LF	3
			470.6	Ar	IR	5

B_0 = 0.228 LF[3]

$\tilde{X}\ ^2\Sigma^+$ $C_{\infty v}$ Structure: LF[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	282(10)	gas	LF	3
Σ^+	3	SrO stretch	510(10)	gas	LF	3

B_0 = 0.225 LF[3]

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BaOH

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

T_0 = 13205.777(3) gas LF[4] $\tilde{B}$-$\tilde{X}$ 710-757 nm

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

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

B_0 = 0.213 LF[4]

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

T_o = 11572(1) gas LF[4] $\tilde{A}$-$\tilde{X}$ 860-880 nm

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

A = 635(1) LF[4]

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

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

B_o = 0.217 LF[4]

BaOD

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

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

B_o = 0.19 gas LF[4]

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

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

B_o = 0.196 LF[4]

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CuOH [a]

$^1A''$ C_s Structure: LF[1]

T^b = 18433.0 gas CL[1]LF[1] 500-560 nm

A_o = 25.85(3); B_o = 0.382; C_o = 0.376 LF[1]

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

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

A_o = 22.95(3); B_o = 0.392; C_o = 0.385 LF[1]

CuOD [a]

$^1A''$ C_s

T^b = 18436.9 gas LF[1] 500-560 nm

A_o = 14.12(3); B_o = 0.354; C_o = 0.344 LF[1]

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

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

A_o = 12.40(3); B_o = 0.366; C_o = 0.354 LF[1]

a ^{63}Cu.
b Position of R(0) line of (1,0) sub-band of $\tilde{A}$(000) - $\tilde{X}$(000).

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HBS^+ [a]

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

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

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

Ã $^2\Sigma^+$ $C_{\infty v}$

T_0 = 19827 gas EF[3] Ã-X̃ 479-635 nm

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

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

X̃ $^2\Pi_{3/2}$ $C_{\infty v}$

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

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

DBS$^+$ [a]

Ã $^2\Sigma^+$ $C_{\infty v}$

T_0 = 19913 gas EF[3] Ã-X̃ 462-646 nm

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

X̃ $^2\Pi_{3/2}$ $C_{\infty v}$

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

[a] ^{11}B.
[b] 975.9(4) in X̃ $^2\Pi_{1/2}$ state.
[c] 937.4(4) in X̃ $^2\Pi_{1/2}$ state.

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HCC

T_0 = 51387(25)[a] Ar AB[8] 195-160 nm

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

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

An absorption band system between 340 and 246 nm, with band spacings of approximately 2700, 1300 and 840 cm^{-1}, which has been observed on vacuum UV photolysis of C_2H_2 in an argon matrix is tentatively attributed to HC_2.

Ã $^2\Pi$ $C_{\infty v}$

$T_0 < 3800$ Ar AB[21]

In an argon matrix, a complicated absorption band system of HC_2 extends from approximately 3800 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] and by high resolution emission spectroscopy.[24] 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] 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.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch[c]	3610	Ar	IR	3,20,21
Π	2	Bend	370.15	gas	DL	25
Σ^+	3	CC stretch	1840.57	gas	DL	23
			1846.2	Ar	IR	1,3,20, 21

A = ~ 10 IR[14]

B_0 = 1.457 MW[4,6,7,9] LMR[12]

DCC

T_0 = 51493(25)[a] Ar AB[8] 194-170 nm

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

Ã $^2\Pi$

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 have been studied in the gas phase using color-center laser absorption.[22]

X $^2\Sigma^+$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2798.5	Ar	IR	3,20,21
	3	CC stretch	1746.3	Ar	IR	1,3,20, 21

B_0 = 1.203 MW[16]

[a] Tentatively assigned to HCC (DCC).
[b] Observed band spacing; $2\nu_2$ if upper state is linear.
[c] Assignment to the CH stretch is based on assignment of $H^{13}CC$ absorptions at 3541 and 3581 to Fermi resonance between ν_1 and $2\nu_3$ (Σ^+) and on position relative to the DCC absorption at 2798, which has C-13 shifts appropriate for the CD-stretching fundamental. However, a $\Pi - \Sigma^+$ transition arising from X(000) of HCC has been observed[22] at 3600, calling into question the assignment to ν_1.

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HCN^+

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

$T_0 \leq$ 42380(40) gas PE[1]

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

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

T_0 = 3260(30) gas PE[1]

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

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	2985(30)	gas	PE	1
Π	2	Bend	298(30)[a]	gas	PE	1
Σ^+	3	CN stretch	1800(30)	gas	PE	1

DCN^+

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

$T_0 \leq$ 41986(40) gas PE[1]

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

T_0 = 3114(30) gas PE[1]

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

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2412(40)	gas	PE	1
Π	2	Bend	234(30)[a]	gas	PE	1
Σ^+	3	CN stretch	1686(30)	gas	PE	1

[a] Large quartic anharmonicity; $2\nu_2 \sim 839$ for HCN^+ and 662 for DCN^+.
[b] $\frac{1}{2}(2\nu_2)$.

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HCP^+

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

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

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

$\tau \geq$ 1.2(1) μs gas EF[2]

B_0 = 0.669(2) EF[3]

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

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

A = -146.97(3) EF^3, $\varepsilon\omega_2$ = -26.4(6) EF^4

B_0 = 0.622(2) EF^3

DCP^+

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

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

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

B_0 = 0.568 EF^3

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

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

A = -146.71(1) EF^3, $\varepsilon\omega_2$ = -18.7(6) EF^4

B_0 = 0.528 EF^3

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

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AlOH

A

Kr $AB^{2,3}$ A-X 245-252 nm

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

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

AlOD

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

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

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GaOH

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

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

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

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

GaOD

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

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

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InOH

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

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

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

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

InOD

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

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

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HNC

$\tilde{A}^a$

T_o = 32850 gas AB^7 $\tilde{A}$-$\tilde{X}$ 250-305 nm

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

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NH stretch	3652.66	gas	IR	3,6,8
			3620	Ar	IR	2
			3583	Ar^b	IR	1,2
			3567	N_2	IR	2
Π	2	Bend	464.24	gas	IR	8
			477	Ar	IR	2
			535	Ar^b	IR	1
			559	N_2	IR	2

$\tilde{X}$---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	NC stretch	2023.86	gas	IR	8
			2029	Ar	IR	2
			2032	Ar^b	IR	1
			2035	N_2	IR	2

$B_o = 1.512\ MW^4IR^8$

DNC

$\tilde{X}$

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

$B_o = 1.273\ MW^4$

[a] Tentative identification.
[b] N_2 trapped in adjacent site.

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HCO

$3p^2\Pi(A'')$ $C_{\infty v}$

T_o = 45568(2) gas MPI[19,20] $3p^2\Pi$-$\tilde{X}$ 187-210 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	822.1(7)	gas	MPI	20
Σ^+	3	CO stretch	2177(3)	gas	MPI	20

B = 1.500(3) MPI[19,20]

$3s^2\Sigma^+$?

Several strong bands between 44400 and 48000 in the REMPI spectrum of HCO have been tentatively assigned to the $3s^2\Sigma^+$ - $\tilde{X}\ ^2A'$ transition.[19,20]

$\tilde{C}$ C_s

T_o = 41270(3) gas EM[6] $\tilde{C}$-$\tilde{X}$ 280-242 nm

41280(45) Ar AB[11] $\tilde{C}$-$\tilde{X}$ 242-212 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2		1200(45)	Ar	UV	11
	3		960(45)	Ar	UV	11

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

T_o = 38691 gas EM[6] $\tilde{B}$-$\tilde{X}$ 280-410 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'	2		1375(35)	Ar	UV	5,11
			1375(35)	CO	UV	5
	3		1035(35)	Ar	UV	5,11
			1035(35)	CO	UV	5

A^a = 16.7(1.0) UV[6]; B^a = 1.149(21) UV[6]

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

T_o = 9297(3) gas AB[1,3,8] $\tilde{A}$-$\tilde{X}$ 460-860 nm

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^c = 46(4) ns LF[15]

B_o = 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 DL,LD	17,18 22
			2483	Ar	IR	5
			2488	CO	IR	4
	2	Bend	1080.76	gas	UV LS LMR	1,3,8 9 10
			1087	Ar	IR	5
			1090	CO	IR	2,4
	3	CO stretch	1868.17	gas	IR LMR	12 13
			1863	Ar	IR	5
			1861	CO	IR	2,4

A_o = 24.329; B_o = 1.494; C_o = 1.399 UV[1,3,8] MW[16]

DCO

$3p^2\Pi(A'')$ $C_{\infty v}$

T_o = 45485(15) gas MPI[20] $3p^2\Pi$-$\tilde{X}$ 187-230 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	657(2)	gas	MPI	20
Σ^+	3	CO stretch	1900(5)	gas	MPI	20

B̃ $^2A'$ C_s

T_o = 38568(70) Ar AB^5 B̃-X̃ 200-260 nm

38569(35) CO AB^5 B̃-X̃ 204-260 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	1150(35)	Ar	UV	5
			1150(35)	CO	UV	5
	3	CO stretch	925(35)	Ar	UV	5
			925(35)	CO	UV	5

Ã $^2A''$(II) $C_{\infty v}$

T_o = 9162(3) gas $UV^{1,3,8}$ Ã-X̃ 460-860 nm

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

B_o = 1.10 $UV^{1,3,8}$

X̃ $^2A'$ C_s

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

A_o = 14.734; B_o = 1.281; C_o = 1.171 $UV^{1,3,8}MW^{21}$

[a] Rotational constants for 338 nm band.
[b] Measured for 090-000 band.
[c] Bands with K' > 0 are diffuse.

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HCF

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

T_o = 17277.47 gas $AB^1CL^3LF^{5,10}$ Ã-X̃ 430-635 nm

17320(15) Ar AB^2 Ã-X̃ 469-546 nm

Evidence has been obtained[8,9] for perturbation of the Ã state by high vibrational levels of the ground state and by the low-lying triplet state. However, molecular parameters of the triplet state have not been determined.

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_o = 25.69; B_o = 1.162; C_o = 1.107 AB^1LF^5

τ_o = 2.45(10) μs gas LF^4

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

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a' 2	Bend	1406.87	gas	AB,LF	1,7
		1406	Ar	IR	2
3	CF stretch	1181.5	Ar	IR	2

A_o = 15.563; B_o = 1.223; C_o = 1.130 AB^1LF^5

DCF

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

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

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

A_o = 15.10; B_o = 1.014; C_o = 0.945 LF^6

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

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a' 2	Bend	1046	Ar	IR	2
3	CF stretch	1183	Ar	IR	2

A_o = 8.828; B_o = 1.120; C_o = 0.990 LF^6

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HCCl

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

T_o = 12274 gas AB^1LF^4 $\tilde{A}$-$\tilde{X}$ 550-820 nm

Ar AB^2 $\tilde{A}$-$\tilde{X}$ 570-750 nm

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a' 2	Bend	∿865	gas	AB	1
		855(50)	Ar	AB	2

Barrier to linearity = 2250 [1]

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

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a' 2	Bend	1201	Ar	IR	2
3	CCl stretch	815	Ar	IR	2

A_o = 15.759; B_o = 0.605; C_o = 0.581 AB^1LF^3

DCCl

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

T_o = 12274 gas AB^1 $\tilde{A}$-$\tilde{X}$ 550-820 nm

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

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

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

A_o = 8.75; B_o = 0.557; C_o = 0.525 AB^1

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HSiF

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

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	∿560	gas	LF	2

τ_0 = 185(10) ns gas LF[2]

A_0 = 9.319; B_0 = 0.549; C_0 = 0.516 LF[3,4]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SiH stretch	1913	Ar	IR	1
	2	Bend	∿860	gas	LF	2
			859	Ar	IR	1
	3	SiF stretch	834	Ar	IR	1

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

DSiF

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

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

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HSiCl

$\tilde{A}\ ^1A''$ [a] C_s Structure: UV[1]

T_0 = 20717.65 gas UV[1] $\tilde{A}$-$\tilde{X}$ 410-600 nm

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

τ ∿ 250 ns gas LF[4]

A_0 = 9.857; B_0 ∿ 0.246; C_0 ∿ 0.240 UV[1]

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

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

A_0 = 7.587; B_0 ∿ 0.246; C_0 ∿ 0.238 UV[1]

DSiCl

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

T_0 = 20718 gas UV[1] $\tilde{A}$-$\tilde{X}$ 410-600 nm

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

A_0 ∿ 3.99; B_0 ∿ 0.238; C_0 ∿ 0.155 UV[1]

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

A_0 ∿ 5.26; B_0 ∿ 0.235; C_0 ∿ 0.225 UV[1]

[a] See Ref. 2.
[b] Alternate assignment[1] giving ν_1 = 1756 is supported by analysis given in Ref. 3.

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HSiBr

$\tilde{A}\ ^1A''$ [a] C_s Structure: UV[1]

T_o = 19903.0 gas UV[1] $\tilde{A}$-$\tilde{X}$ 430-620 nm

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

A_o = 9.906; $B_o \sim 0.159$; $C_o \sim 0.156$ UV[1]

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

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

A_o = 7.580; $B_o \sim 0.158$; $C_o \sim 0.155$ UV[1]

[a] See Ref. 2.
[b] Alternate assignment[1] giving ν_1 = 1785 is supported by analysis given in Ref. 3.

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HSiI

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

T_o = 18259.01 gas AB[1] $\tilde{A}$-$\tilde{X}$ 460-560 nm

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

A_o = 9.795; B_o = 0.118; C_o = 0.117 AB[1]

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

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

A_o = 7.557; B_o = 0.118; C_o = 0.116 AB[1]

DSiI

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

T_o = 18671.1 gas AB[1] $\tilde{A}$-$\tilde{X}$ 460-560 nm

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

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HGeCl

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

T_o = 21540 gas CL[2] $\tilde{A}$-$\tilde{X}$ 445-520 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	431	gas	CL	2
	3	GeCl stretch	386.4	gas	CL	2

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

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

DGeCl

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	~360	gas	CL	2

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

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

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HNO

T_o = 48240 gas AB^5 198-208 nm. Diffuse bands.

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

T_o = 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

τ = 25(4) μs $LF^{12,14}$

A_o = 22.156; B_o = 1.325; C_o = 1.242 $AB^{1,4}MODR^{11,17}$

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

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

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

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH stretch	2683.95	gas	IR,EM	9,16,21
			2716.3[a]	Ar	IR	8
			2756	N_2	IR	8
	2	Bend	1500.82	gas	LS	10
			1505	Ar	IR	8
			1511	N_2	IR	8
	3	NO stretch	1565.34	gas	LS	10
			1563.2[a]	Ar	IR	8
			1568.5	N_2	IR	8

A_o = 18.476; B_o = 1.411; C_o = 1.306 $AB^1MW^7IR^{10,16,21}$

DNO

T_o = 48400 gas AB^5 196-206 nm. Diffuse bands.

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

T_o = 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

A_o = 12.630; B_o = 1.199; C_o = 1.088 $AB^{1,4}$

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

T_o = 6330(160) gas PE^{15}

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

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

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

A_o = 10.524; B_o = 1.292; C_o = 1.146 $AB^1MW^6IR^{10,16}$

[a] Refined value from unpublished Fourier transform spectra.

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HPO

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

T_o = 19032.778(7) gas $EM^{1-4,6}$ $\tilde{A}$-$\tilde{X}$ 460-680 nm

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

A_o = 8.269; B_o = 0.643; C_o = 0.594 $EM^{3,6}$

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

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

A_o = 8.850; B_o = 0.703; C_o = 0.649 $EM^{3,6}MW^7$

DPO

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

T_o = 19116 gas EM^{2-4} $\tilde{A}$-$\tilde{X}$ 460-680 nm

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

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	PD stretch	1530	Ar	IR	5
	2	Bend	745	gas	EM	2
			750	Ar	IR	5
	3	PO stretch	1177	gas	EM	2
			1186	Ar	IR	5

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

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HNF

$\tilde{A}\ ^2A'$ C_s Structure: AB^3

T_o = 20141.26(1) gas $AB^{1,3}CL^4$ $\tilde{A}$-$\tilde{X}$ 380-650 nm

20140(20) Ar AB^2 $\tilde{A}$-$\tilde{X}$ 395-497 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	1074	gas	AB	3
			1033[a]	Ar	AB	2
	3	NF stretch	1121(5)	gas	AB	3

A_o = 27.570(5); B_o = 1.033; C_o = 0.992 AB^3

$\tilde{X}\ ^2A''$ C_s Structure: AB^3

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	1419	gas	CL	4
			1432	Ar	IR	2
	3	NF stretch	1000	Ar	IR	2

A_o = 17.688(8); B_o = 1.039; C_o = 0.978 AB^3

DNF

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

T_o = 20220 Ar AB^2 $\tilde{A}$-$\tilde{X}$ 413-495 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	798[a]	Ar	AB	2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	1069[b]	Ar	IR	2
	3	NF stretch	1000	Ar	IR	2

[a] Average value.
[b] Overlapped by NF_2 absorption.

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HO_2

Broad, unstructured gas-phase absorption between 200 and 280 nm, with maximum near 205 nm.[2,3,5,6]

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

T_o = 7029.684(2) gas $AB^{9,15}EM^{10,16,19,20,35}$

$\tilde{A}$-$\tilde{X}$ 1.13-2.12 μm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3268.5	gas	EM	35
	2	Bend	1285	gas	EM	35
	3	OO stretch	929.068	gas	AB,EM	15,19,28 35

A_o = 20.486; B_o = 1.021; C_o = 0.968 $EM^{16,20,35}$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3436.20	gas	LD	26
			3412.5[a]	Ar	IR	1,4,7
			3400	O_2	IR	32
	2	Bend	1391.75	gas	DL	24
			1388.5[a]	Ar	IR	1,4,7
			1392	O_2	IR	32

$\tilde{X}\ ^2A''$---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	3	OO stretch	1097.63	gas	LMR DL	18 29,30
			1101.1[a]	Ar	IR	1,4,7
			1109	O_2	IR	32

A_o = 20.356; B_o = 1.118; C_o = 1.056 LMR[8,11,12,18] MW[13,17,25] EM[16]

DO_2

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

T_o = 7041.1(1) gas AB[9] EM[10,19,21] $\tilde{A}$-$\tilde{X}$ 1.13-2.12 μm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	OO stretch	940(28)	gas	AB,EM	8,19

A_o = 11.147(7); B_o = 0.970; C_o = 0.887 EM[21]

$\tilde{X}\ ^2A''$ 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
			2529.5[a]	Ar	IR	1,4,7
			2521	O_2	IR	32
	2	Bend	1020.16	gas	LMR,DL	22,33
			1019.9[a]	Ar	IR	1,4,7
			1024	O_2	IR	32
	3	OO stretch	1121.47	gas	LMR,DL	22,33
			1122.9[a]	Ar	IR	7

A_o = 11.194; B_o = 1.056; C_o = 0.961 MW[14,27,34] EM[21] LMR[22,23,34] ESR[23]

[a] Refined value from unpublished Fourier transform spectra.

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HSO

Ã $^2A'$ C_s Structure: LF[2,3]

T_o = 14367 gas CL[1] Ã-X̃ 520-960 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	SO stretch	702(5)	gas	CL	1

τ_{001} = 74(1) μs gas LF[6]

Values decrease steadily as v_3' increases.

A_{003} = 9.735; B_{003} = 0.565; C_{003} = 0.527 LF[2]

X̃ $^2A''$ C_s Structure: LF[2,3]MW[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	1063(5)	gas	CL	1
	3	SO stretch	1009.36	gas	LMR	5

A_o = 9.990; B_o = 0.684; C_o = 0.638 LF^2MW^4

DSO

Ã $^2A'$ C_s

T_o = 14371 gas CL[1] Ã-X̃ 520-960 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	575(10)	gas	LF	7
	3	SO stretch	702(10)	gas	CL	1

τ^a = 76 μs gas LF[6]

A_{021} = 5.162; B_{021} = 0.567; C_{021} = 0.499 LF[7]

X̃ $^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	770(10)	gas	CL	1
	3	SO stretch	1030(15)	gas	CL	1

A_o = 5.295; B_o = 0.662; C_o = 0.586 LF^3MW^4

[a] Measured at 606.0 nm.

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HS_2

gas AB[1-3] 307-380 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SH stretch	∿2500	gas	AB	3
	2	Bend	∿900	gas	AB	3
	3	SS stretch	∿600	gas	AB	3

Ã $^2A'$ C_s

T_o = 7255(7) gas CL[4] Ã-X̃ 950-2100 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	SS stretch	504(4)	gas	CL	4

A_o = 9.7(5) CL[4]

X̃ $^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	904(8)	gas	CL	4
	3	SS stretch	595(4)	gas	CL	4

A_o = 9.7(5) CL[4]

DS_2

Ã $^2A'$ C_s

T_o = 7264(15) gas CL[4] Ã-X̃ 950-2100 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	SS stretch	502(15)	gas	CL	4

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	696(20)	gas	CL	4
	3	SS stretch	591(10)	gas	CL	4

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HOF^+

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

T_0 = 25740(500) gas PE[1]

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

T_0 = 14440(320) gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	OF stretch	946[a]	gas	PE	1

[a] Average value.

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$HOCl^+$

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

T^a = 36150(900) gas PE[1]

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

T^a = 28080(900) gas PE[1]

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

T_0 = 7830(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	1250(80)	gas	PE	1
	3	OCl stretch	700(50)	gas	PE	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	OCl stretch	830(50)	gas	PE	1

[a] From vertical ionization potential.

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HO_2^-

Threshold for electron detachment from ground-state HO_2^- is 8700(140) [1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	OO stretch	775(250)	gas	PE	1

DO_2^-

Threshold for electron detachment from ground-state DO_2^- is 8790(140) [1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	OO stretch	900(250)	gas	PE	1

References

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XeOH

Unstructured gas-phase emission[1] between 225 and 240 nm, with maximum near 234 nm.

$\tau \leq 4$ ns gas EM[1]

References

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6.3. Triatomic Nonhydrides

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]

T_0 = 20813 gas MPI[2,4,6] $\tilde{C}$-$\tilde{X}$ 472-481 nm

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

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

Vibronic pseudorotation accompanied by fractional quantization occurs.[3]

$^2E''$ 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

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	139	gas	MPI	4,6
	2	Bend	49.5	gas	MPI	4,6
	3	Asym. stretch	87	gas	MPI	6

[a] Distorted by Jahn-Teller interaction.

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CaCN

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

Unstructured absorption gas LF[1] $\tilde{C}$-$\tilde{X}$ 385-418 nm

τ = 165(38) ns gas LF[1]

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

Unstructured band gas LF[1,3] CL[2] $\tilde{A},\tilde{B}$-$\tilde{X}$ 572-670 nm

τ(607 nm) = 40.8(1.5) ns gas LF[1]

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

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SrCN

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

Unassigned structure gas LF[1] $\tilde{C}$-$\tilde{X}$ 395-455 nm

τ = 104.4(6.3) ns gas LF[1]

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

Unstructured absorption gas LF[1] $\tilde{A},\tilde{B}$-$\tilde{X}$ 645-663 nm

τ = 51.2(6.2) ns gas LF[1]

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

References

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BaCN

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

Unstructured absorption gas LF[1] $\tilde{C}$-$\tilde{X}$ ~500-629 nm

τ = 229(13) ns gas LF[1]

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

References

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C_3

$1^1\Sigma_u^+$ $D_{\infty h}$

T_o = 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

$\tilde{A}\ ^1\Pi_u$ $D_{\infty h}$ Structure: UV[6]

T_o = 24675.5	gas	EM[1,2,6] AB[3,6,9]	$\tilde{A}$-$\tilde{X}$ 340-410 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_o = 200(10) ns gas LF[12,13]

In a neon or argon matrix,[11] efficient intersystem crossing into the $\tilde{a}\ ^3\Pi_u$ state occurs, and $\tau \leq 10$ ns.

B_o = 0.430 UV[6]

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

T_0 = 17080 Ne EM^5LF^{11} $\tilde{a}$-$\tilde{X}$ 585-631 nm

16930 Ar EM^5

$\tau \sim 0.02$ s Ne EM^5

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1224.5	gas	AB	9
			1226	Ne	EM	5
Π_u	2	Bend	63.7	gas	UV	6
			~70[e]	Ne,Ar	AB	5
Σ_u^+	3	Asym. stretch	2042	Ne	IR	4
			2038	Ar	IR	4,10

B_0 = 0.412 UV^6

[a] $\frac{1}{2}(2\nu_1)$.
[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] 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

T_0 = 20069.7 gas $EM^1AB^3LF^4$ $\tilde{A}$-$\tilde{X}$ 402-507 nm

20142 Ne AB^2LF^4 $\tilde{A}$-$\tilde{X}$ 409-611 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CC stretch	1464	gas	EM,AB LF	1,3,4
			1462	Ne	AB,LF	2,4
	2	CSi s-stretch	979	gas	AB,LF	3,4
			1011	Ne	AB,LF	2,4
b_2	3	CSi a-stretch	228[a]	gas	EM,AB LF	1,3,4
			231[a]	Ne	AB,LF	2,4

τ_0 = 370 ns gas LF^4

310 ns Ne LF^4

A_0 = 1.652(3); B_0 = 0.419(2); C_0 = 0.335(2) PI^5

$\tilde{X}\ ^1A_1$ C_{2v} Structure: $PI^5MW^{6,7}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CC stretch	1742	gas	EM	1
			1746	Ne	IR,LF	2,4
			1741	Ar	IR	8
	2	CSi s-stretch	837	gas	EM	1,9
			836	Ne	IR,LF	2,4
			824	Ar	IR	8
b_2	3	CSi a-stretch	177[a]	gas	LF	4
			172[a]	Ne	LF	4

A_0 = 1.75; B_0 = 0.439; C_0 = 0.348 $MW^{6,7}$

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

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Al_2O

Absorption bands observed at 210 and 212 nm in an argon matrix, between 202 and 217 nm in a krypton matrix, and between 207 and 225 nm in a xenon matrix when Al is vaporized from a Knudsen cell coated with Al_2O_3 have been attributed[9] to Al_2O.

C̃

T_0 = 37121(15) Ar AB[7] C̃-X̃ 263-270 nm

36444(15)[a] Kr AB[5-7]LF[7] C̃-X̃ 267-283 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	451(15)	Ar	AB	7
			454(15)	Kr	AB	5-7
	2	Bend	156(15)	Ar	AB	7
			186(15)	Kr	AB	5-7

B̃

T_0 = 34331(15) Kr LF[7] B̃-X̃ 291 nm

Ã

T_0 = 23286(15) Kr AB[7] Ã-X̃ 415-430 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	482(15)	Kr	AB	7
	2	Bend	133(15)	Kr	AB	7

X̃ $D_{\infty h}$?

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	472	Ar	Ra	10
			471(15)	Kr	LF	7

X̃---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	3	Asym. stretch	993	Ar	IR	1-4
			989.4	Kr	IR	1,2
			992	N_2	IR	8

[a] From absorption measurements.

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CCN

C̃ $^2\Sigma^+$ $C_{\infty v}$

T_0 = 26661.73 gas AB[1] C̃-X̃ 350-375 nm

Evidence for predissociation above 29100.[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Sym. stretch	1859.20	gas	AB	1
Π	2	Bend	~465	gas	AB	1

B_0 = 0.413 AB[1]

B̃ $^2\Sigma^-$ $C_{\infty v}$

T_0 = 22413.25 gas AB[1] B̃-X̃ 442-446 nm

22180 Ar AB[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	∿445	gas	AB	1

B_0 = 0.405 AB[1]

Ã $^2\Delta$ $C_{\infty v}$

T_0 = 21259.203 gas AB[1]LF[4] Ã-X̃ 376-471 nm

21377 Ar LF[2]AB[3] Ã-X̃ 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

τ = 170 ns Ar LF[2]

A_{eff} = -0.807 gas AB[1]LF[4,6]

B_0 = 0.414 AB[1]LF[4,6]MODR[7]

X̃ $^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Sym. stretch	1064.9	gas	LF	5,8
			1066	Ar	LF	2
Π	2	Bend	324	gas	AB,LF	1,8
Σ^+	3	Asym. stretch	1915.77	gas	LF	5,8
			1717	Ar	LF	2

A = 41.76, $\varepsilon\omega_2$ = 132.8 gas LF[8]

B_0 = 0.398 AB[1]LF[4,6]

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CNC

B̃ $^2\Sigma_u^-$ $D_{\infty h}$ Structure: AB[1]

T_0 = 34802.33 gas AB[1] B̃-X̃ 283-288 nm

34602(20) Ar[a] AB[2] B̃-X̃ 276-292 nm
34305(20)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	398	gas	AB	1
			385(20)[b]	Ar	AB	2

B_0 = 0.443 AB[1]

Ã $^2\Delta_u$ $D_{\infty h}$ Structure: AB[1]

T_0 = 30338.53 gas AB[1] Ã-X̃ 325-332 nm

30048(20) Ar AB[2] Ã-X̃ 324-333 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	440	gas	AB	1

A = 0.33 gas AB[1]

B_0 = 0.450 AB[1]

X̃ $^2\Pi_g$ $D_{\infty h}$ Structure: AB[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	321[c]	gas	AB	1
Σ_u^+	3	Asym. stretch	1453	Ar	IR	2

A = 26.41; ε = 0.549 AB[1]

B_0 = 0.454 AB[1]

[a] Two prominent sites in argon matrix.
[b] $\frac{1}{2}(2\nu_2)$.
[c] Calculated position of lowest frequency component ($^2\Sigma_u^-$) is 144 cm^{-1}. Moderately intense absorption at 134 cm^{-1} in an argon matrix is tentatively assigned to this transition.

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CCO

In an argon matrix,[1] a broad, unstructured absorption is observed near 500 nm, and CCO photodissociates on exposure of the sample to visible light.

Ã $^3\Pi$ $C_{\infty v}$ Structure: AB^3

T_0 = 11650.80(3) gas $AB^{2,3}LF^6$ Ã-X̃ 500-860 nm

≅ 11860 Ar AB^5 Ã-X̃ 600-850 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	2045.7	gas	AB	3
Π	2	Bend	607.8	gas	AB	3
Σ^+	3	CC stretch	∿1270[a]	gas	AB	3

The fluorescence decay pattern[7] of CCO Ã(101) and of higher vibronic levels is complex. There is a short-lived (∿ 15 μs) component and a long-lived (333 +105/-64 μs) component which is, in turn, nonexponential, suggesting perturbation by the heretofore unobserved $\tilde{b}\ ^1\Sigma^+$ and $\tilde{a}\ ^1\Delta$ states, as well as by high ground-state vibrational levels.

A = -35.36(4); ε = -0.172 gas AB^3

B_0 = 0.407 AB^3

X̃ $^3\Sigma^-$ $C_{\infty v}$ Structure: AB^3

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1970.86	gas	LF,DL	6,9
			1969	Ar	IR	1,4
			1978	Ar[b]	IR	1
			1987	N_2	IR	1
Π	2	Bend	379.4	gas	AB	3
			381	Ar	IR	1

X̃ $^3\Sigma^-$---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	CC stretch	1063	gas	LF	6
			1064	Ar	IR	1
			1074	Ar[b]	IR	1
			1077	N_2	IR	1

B_0 = 0.385 AB^3MW^8

[a] In Fermi resonance with $2\nu_2$.
[b] N_2 trapped in adjacent site.

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SiCO

Ã $^3\Pi$? $C_{\infty v}$

T_0 = 24056(10) Ar AB^1 Ã-X̃ 365-416 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1857(10)	Ar	AB	1
	3	SiC stretch	750(10)	Ar	AB	1

X̃ $^3\Sigma^-$?

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1899	Ar	IR	1

References

[1]R. R. Lembke, R. F. Ferrante, and W. Weltner, Jr., J. Am. Chem. Soc. 99, 416 (1977).

NCN

$^1\Delta_u$ $D_{\infty h}$

gas AB[6] 250-290 nm

$\tilde{B}\ ^3\Sigma_u^-$ $D_{\infty h}$

$T_0 \leq 33512$ gas AB[6] $\tilde{B}$-$\tilde{X}$ 258-300 nm

33100 Ar AB[2] $\tilde{B}$-$\tilde{X}$ 240-302 nm

33215 N_2 AB[2] $\tilde{B}$-$\tilde{X}$ 240-301 nm

In the gas phase, bands are diffuse. Threshold for photodecomposition into C + N_2 observed in argon and nitrogen matrices[2,4] near 280 nm.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1100(10)	gas	AB	6
			1050(10)	Ar,N_2	AB	2

$\tilde{b}\ ^1\Pi_u$ $D_{\infty h}$ Structure: AB[5]

$T_0 = x + 30045.76$ gas AB[5] $\tilde{b}$-$\tilde{a}$ 330-334 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1160[a]	gas	AB	6

$\varepsilon\omega_2 = -84.2$ gas AB[5]

$B_0 = 0.395$ AB[5]

$\tilde{A}\ ^3\Pi_u$ $D_{\infty h}$ Structure: AB[1]

$T_0 = 30383.74$ gas AB[1] $\tilde{A}$-$\tilde{X}$ 326-329 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1154[a]	gas	AB	6
Π_u	2	Bend	460(50)	gas	AB	1

$A = -37.56$; $\varepsilon\omega_2 = -85.7$[b] gas AB[1]

$\tau_0 = 183(6)$ ns gas LF[8]

$B_0 = 0.396$ AB[1]

$\tilde{a}\ ^1\Delta_g$ $D_{\infty h}$ Structure: AB[5]

$T_0 = x$ gas AB[5] $\tilde{b}$-$\tilde{a}$ 330-334 nm

$B_0 = 0.399$ AB[5]

$\tilde{X}\ ^3\Sigma_g^-$ $D_{\infty h}$ Structure: AB[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1197[c]	Ar	IR	4
Π_u	2	Bend	370(50)	gas	AB	1
			423	Ar	IR	2,4
Σ_u^+	3	Asym. stretch	1475	Ar	IR	2,4
			1478	N_2	IR	2-4

$B_0 = 0.397$ AB[1]

[a] Tentative assignment.
[b] An alternate assignment[7] gives $\varepsilon\omega_2 = -90.95$. [c] Frequency deduced from weak combination with ν_3 which appears at 2672.

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[1]G. Herzberg and D. N. Travis, Can. J. Phys. 42, 1658 (1964).
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PCN

$\tilde{A}\ ^3\Pi$ [a]

$T_0 = 33165$ gas AB[1] $\tilde{A}$-$\tilde{X}$ 280-306 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			~1830	gas	AB	1

$A \sim 104$ gas AB[1]

$\tilde{X}\ ^3\Sigma^-$ [a]

[a] Tentative assignment, by analogy with NCN.

References

[1]N. Basco and K. K. Yee, Chem. Commun. 152 (1968).

AsCN

$\tilde{A}\ ^3\Pi$ [a]

$T_0 \sim 34900$ gas AB[1] $\tilde{A}$-$\tilde{X}$ 280-295 nm

$A \sim 550$ gas AB[1]

$\tilde{X}\ ^3\Sigma^-$ [a]

[a] Tentative assignment, by analogy with NCN.

References

[1]N. Basco and K. K. Yee, Chem. Commun. 153 (1968).

NCO^+

1Π[a]

$T_0 = 57280(160)$ gas PE[1]

3Π[a]

$T_0 = 56960(160)$ gas PE[1]

1Π[a]

$T_0 = 55910(160)$ gas PE[1]

$\tilde{A}\ ^3\Pi$ $C_{\infty v}$

$T_0 = 23960(160)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	"Sym." stretch	1320(30)	gas	PE	1

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

$T_0 = 14520(160)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	"Sym." stretch	1150(30)	gas	PE	1

$\tilde{a}\ ^1\Delta$ $C_{\infty v}$

$T_0 = 9360(160)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Stretch	2020(30)	gas	PE	1
	3	Stretch	1110(30)	gas	PE	1

$\tilde{X}\ ^3\Sigma^-$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	"Sym." stretch	1000(30)	gas	PE	1

[a] Tentative assignment.

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[1]J. M. Dyke, N. Jonathan, A. E. Lewis, J. D. Mills, and A. Morris, Mol. Phys. 50, 77 (1983).

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.[9]

$\tilde{C}\ ^3\Pi$? $C_{\infty v}$

$T_0 = 48540(50)$ Ar AB[9] $\tilde{C}$-$\tilde{X}$ 206 nm

49100(50) N_2 AB[9] $\tilde{C}$-$\tilde{X}$ 203.7 nm

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

$T_0 \leq 39950$ Ar AB[9] $\tilde{B}$-$\tilde{X}$ 210-251 nm

39850 N_2 AB[9] $\tilde{B}$-$\tilde{X}$ 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	9
		Stretch	990(40)	Ar,N_2	AB	9

$\tilde{A}\ ^3\Pi$ $C_{\infty v}$

$T_0 = 23750$ Ne AB[5] $\tilde{A}$-$\tilde{X}$ 397-420 nm
23830

23597 Ar $AB^{2,3}LF^{7,8}$ $\tilde{A}$-$\tilde{X}$ 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	2,3,7,8
			1335(10)	N_2	AB	2,3
Π	2	Bend	525(2)	Ar	LF	7
Σ^+	3	"Asym."stretch	1807(2)	Ar	LF	7

τ_o = 250(30) ns Ar LF[7,8]

A = 9; ε = -0.07 Ar LF[7]

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	7
			2847	Ar[b]	IR	3
			2856	N_2	IR	3,4,6
Π	2	Bend	394	Ar	LF	7
			393	Ar[b]	IR	3
			394	N_2	IR	4,6
Σ^+	3	NN stretch	1235	Ne	EM	5
			1235	Ar	LF	7
			1241	Ar[b]	IR	3
			1252	N_2	IR	3,4,6

[a] Possibly 2440(40).[9]
[b] N_2 trapped in adjacent site.

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SiNN

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

T_o = 32162(10) Ar AB[1] B̄-X̄ 295-311 nm

31892(25) Kr AB[2] B̄-X̄ 297-314 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NN stretch	1672(10)	Ar	AB	1
			1671(25)	Kr	AB	2

A $^3\Pi$? $C_{\infty v}$

$T_o \leq$ 27170(20) Ar AB[1] Ā-X̄ 331-368 nm

Kr AB[2] Ā-X̄ 333-360 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	SiN stretch	∿450	Ar	AB	1
			∿450	Kr	AB	2

X $^3\Sigma^-$? $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NN stretch	1731	Ar	IR	1
	3	SiN stretch	485	Ar	IR	1

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N_3^+

b $^1\Sigma^+$

T_o = 14520(160) gas PE[1]

ā $^1\Delta$

T_o = 9120(160) gas PE[1]

$\tilde{X}\ ^3\Sigma^-$ $C_{\infty v}$ Structure: PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Sym. stretch	1170(30)	gas	PE	1
Σ^+	3	Asym. stretch	2565(30)[a]	gas	PE	1

[a] Assigned by analogy with the isoelectronic species CNN. Alternate assignment of ν_3 = 1395 cm^{-1}, with the observed band separation of 2565 cm^{-1} corresponding to $\nu_1 + \nu_3$, would be consistent with assignments of ν_3 for such related species as NCN and CO_2^+ and cannot be excluded.

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CCO^-

Threshold for electron detachment from ground-state CCO^- is 14910(220).[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1625(350)	gas	PE	1

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BO_2 [a]

$\tilde{B}\ ^2\Sigma_u^+$ $D_{\infty h}$ Structure: AB[1]

T_o = 24508.0 gas AB[1] $\tilde{B}$-$\tilde{X}$ 405-410 nm

24481 Ar AB[2] $\tilde{B}$-$\tilde{X}$ 408-412 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	505	gas	AB	1
Σ_u^+	3	Asym. stretch	1410[b]	gas	AB	1

B_o = 0.325 AB[1]

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

T_o = 18291.6 gas UV^1LF^{3-5} $\tilde{A}$-$\tilde{X}$ 396-700 nm

17915[d] 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	484	gas	UV	1
Σ_u^+	3	Asym. stretch	2357[c]	gas	UV	1

τ_o = 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 = -101.3; $\varepsilon\omega_2$ = -13.1 gas UV^1

B_o = 0.311 UV^1

$\tilde{X}\ ^2\Pi_g$ $D_{\infty h}$ 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	447.4[e]	gas	UV,LF	1,3-5
Σ_u^+	3	Asym. stretch	1278.26	gas	DL	8
			1276	Ar	IR	2

A = -148.6; $\varepsilon\omega_2$ = -92.2 gas UV^1LF^3

B_o = 0.329 $UV^1LF^{3,7}DL^8$

[a] ^{11}B.
[b] Estimated from isotopic shifts.
[c] $\frac{1}{2}(2\nu_2)$.
[d] 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.
[e] Band origin of $(010)\kappa^2\Sigma$-$(000)^2\Pi_{3/2}$ vibration-rotation transition observed[11] at 633.8049(9) using diode laser spectroscopy.

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BS_2 [a]

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

T_o = 24072(5) Ne AB^2 $\tilde{B}$-$\tilde{X}$ 395-412 nm

gas $AB^{1,3}$ $\tilde{B}$-$\tilde{X}$ 409-418 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	509	Ne	AB	2

$\tilde{A}\ ^2\Pi_u$ $D_{\infty h}$

T_o = 13766(2) Ne AB^2 $\tilde{A}$-$\tilde{X}$ 514-721 nm

gas $AB^{1,3}$ $\tilde{A}$-$\tilde{X}$ 592-800 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	504(2)	Ne	AB	2
Π_u	2	Bend	311[b]	Ne	AB	2
Σ_u^+	3	Asym. stretch	1535[b]	Ne	AB	2

A = -263(2) Ne AB^2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	510	Ne	AB	2
Π_u	2	Bend	~120[c]	Ne	AB	2
Σ_u^+	3	Asym. stretch	1014.6(5)	Ne	IR	2

A = -440 gas $AB^{1,2}$

a $^1\Pi_g$.
b $\frac{1}{2}(2\nu_i)$.
c Estimated from isotope shift in origin of $\tilde{A}$ - $\tilde{X}$ transition.

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FBS^+ [a]

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

T_o = 70360(240) gas PE[1]

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

T_o = 50800(900) gas PE[1]

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

T_o = 26687.9(8) gas PE^1EF^2 $\tilde{A}$-$\tilde{X}$ 350-425 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BS stretch	1718(2)	gas	PE,EF	1,2
	3	BF stretch	691(2)	gas	EF	2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BS stretch	1721(2)	gas	EF	2
Π	2	Bend	339(2)	gas	EF	2
Σ^+	3	BF stretch	637(2)	gas	EF	2

A = -370(2) gas EF^2

a $^1\Pi_g$.

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$ClBS^+$ [a]

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

T^b = 50500(1000) gas PE[1]

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

T_o = 26019 gas EF^2 $\tilde{B}$-$\tilde{X}$ 405-516 nm

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

T_o = 24961.5(4) gas EF^2 $\tilde{A}$-$\tilde{X}$ 392-440 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BS stretch	1390.6(8)	gas	EF	2
	3	BCl stretch	516.0(8)	gas	EF	2

τ = 240(13) ns gas EF^2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BS stretch	1347.8(8)	gas	EF	2
	3	BCl stretch	508.9(8)	gas	EF	2

A = -383 gas EF^2

a ^{11}B.
b From vertical ionization potential.

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NCO

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

T_o = 31751.1(5) gas UV^2LF^{18} $\tilde{B}$-$\tilde{X}$ 265-320 nm
31616(25) Ne UV^3 $\tilde{B}$-$\tilde{X}$ 260-320 nm
31437(25) Ar UV^3 $\tilde{B}$-$\tilde{X}$ 232-315 nm
31339(25) N_2 UV^3 $\tilde{B}$-$\tilde{X}$ 256-315 nm

Diffuse bands above 33700.[2] Large change in radiative lifetime between 000 and 100 vibrational levels indicates that onset of predissociation lies somewhat below 32800.[13]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Stretch	2303	gas	UV	2
			2295(50)	Ne	UV	3
			2303(50)	Ar	UV	3

$\tilde{B}\ ^2\Pi$---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	3	Stretch	1047	gas	UV	2
			1033(50)	Ne	UV	3
			1053(50)	Ar	UV	3
			1025(50)	N_2	UV	3

τ_o = 63(3) ns gas LF^{13}

A = -76.6 gas LF^{18}

B_o = 0.356 LF^{18}

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

T_o = 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_o = 435(10) ns gas $LF^{9,13}$
350(30) ns gas $LF^{11,12}$
170 ns Ar LF^8

B_o = 0.402 UV^1

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$ Structure: $UV^{1,7}MW^{4-6}$

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
			1275	Ar	IR,LF	3,8

$\tilde{X}\ ^2\Pi$---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	535.4	gas	UV,LF	1,7,15
			529.5[c]	Ar	LF	8
Σ^+	3	Asym. stretch	1920.61	gas	LMR LF	10 14,15
			1923	Ar	IR,LF	3,8
			1935	N_2	IR	3

$A_{010} = -94.19$, $\varepsilon\omega_2 = -76.9$ gas UV[7]

$B_0 = 0.389$ UV[1]MW[16]

[a] in Fermi resonance with $2\nu_2$, at 1385.3.
[b] $\nu_1 - 1/2\alpha_A$. For $^2\Pi_{3/2}$. Value for $^2\Pi_{1/2}$ is 1364.05(20) gas LF[14,15,19].
[c] Lowest frequency component ($^2\Sigma^+$) contributes a strong infrared absorption at 487.[3] Four components ($^2\Sigma^+$, $^2\Delta_{5/2}$, $^2\Delta_{3/2}$, $^2\Sigma^-$) observed at 484, 531, 626, and 672 in LF experiments.[8] Components of (020) have also been assigned from LF studies.[19]

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NCS

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

$T_0 = 26843.96(10)$ gas EM^1AB^2 $\tilde{B}$-$\tilde{X}$ 353-485 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	343(10)	gas	AB	2

$B_0 = 0.197$ AB^2

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

$T_0 = 26053.71(5)$ gas EM^1AB^2 $\tilde{A}$-$\tilde{X}$ 337-394 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

$\tau_0 = 164(10)$ ns gas LF[3]

$A = -125(20)$[a]; $-89.16(20)$[b]; $|\varepsilon\omega_2| = 103(5)$ gas AB^2

$B_0 = 0.191$ AB^2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CN stretch	1930	gas	LF	3
Π	2	Bend	387(10)	gas	AB	2
Σ^+	3	CS stretch	~715	gas	AB	2

$A = -356(20)$[a]; $-319.92(20)$[b]; $|\varepsilon\omega_2| = 55(15)$ gas AB^2

$B_0 = 0.204$ AB^2

[a] From 0-0 band of $\tilde{A}$-$\tilde{X}$ system.
[b] Also using data for 0-0 band of $\tilde{B}$-$\tilde{X}$ system.

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CO_2^+

$\tilde{C}\ ^2\Sigma_g^+$ $D_{\infty h}$

T_0 = 45250(20) gas TPE[20]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1400(20)	gas	TPE	20
Π_u	2	Bend	625(20)	gas	TPE	20
Σ_u^+	3	Asym. stretch	1530(20)	gas	TPE	20

$\tilde{B}\ ^2\Sigma_u^+$ $D_{\infty h}$ 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	1270(20)	gas	TPE	20
Π_u	2	Bend	558(10)	gas	EM	9
Σ_u^+	3	Asym. stretch	1820(20)	gas	TPE	20

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
Π	2	Bend	461	gas	EM	11
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; $\varepsilon\omega_2$ = -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	511.35(30)	gas	EM,DL	11,19,21
Σ_u^+	3	Asym. stretch	1423.08	gas	DL	18

A = -161.02(6) $\varepsilon\omega_2$ = -98.8(3) gas EM[1,9,11]DL[19,21]

B_0 = 0.380 EM[1,3,9,11]

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OCS^+

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

T_0 = 54580(20) gas PI[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	2128(20)	gas	PI	4
Π	2	Bend	379(20)	gas	PI	4
Σ^+	3	CS stretch	929(20)	gas	PI	4

B̄ $^2\Sigma^+$ $C_{\infty v}$

T_o = 39171 gas PI[4]PF[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	495	gas	PF	9
Σ^+	3	CS stretch	829	gas	PF	9

Ā $^2\Pi_{3/2}$ $C_{\infty v}$

T_o = 31404.099(7) gas EF[1]LF[8]PF[9] Ā-X̄ 318-432 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	2121(20)	gas	PI	4
	3	CS stretch	803.8[a]	gas	PF	9

τ_o = 93(9) ns[c] gas PEFCO[5]

τ_o (Ω = 3/2) = 105(3) ns; τ_o (Ω = 1/2) = 77(3) ns gas HFD[6]EF[7]

A = -111.8 gas EF[1]PF[9]

B_o = 0.187 LF[8]

X̄ $^2\Pi_{3/2}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CS stretch	695.7[b]	gas	PF	9
Π	2	Bend	417(20)	gas	PI	4
Σ^+	3	CO stretch	2069	gas	EF	1

A = -367.2 gas EF[1]PF[9]

B_o = 0.195 LF[8]

[a] 816.9 for Ω = 1/2.[9]
[b] 699.7 for Ω = 1/2.[9]
[c] Absence of emission from states above the Ā $^2\Pi$ 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.

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CS_2^+

C̄ $^2\Sigma_g^+$ $D_{\infty h}$

T_o = 49120(20) gas PI[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	651(20)	gas	PI,PE	5,9,11
Π_u	2	Bend	400(20)	gas	PE	11

B̄ $^2\Sigma_u^+$ $D_{\infty h}$ Structure: EM[1]

T_o = 35238.01 gas EM[1] B̄-X̄ 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	gas	EM	3
Π_u	2	Bend	400(20)	gas	PE	11

τ_o = 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_o = 0.108 EM[1]

$\tilde{A}\ ^2\Pi_u$ $D_{\infty h}$ Structure: EM^3

T_o = 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[b]	gas	EM	3
			280[b]	Ne	LF	6,7
Σ_u^+	3	Asym. stretch	1644[b]	Ne	LF	7

τ = 4.09(19) μs gas $PIFCO^4ID^{10}UV^{12}$

2.3(1) μs Ne $LF^{6,7}$

A = -176 gas EM^3

B_o = 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[b]	gas	EM	3
			349[b]	Ne	LF	6,7
Σ_u^+	3	Asym. stretch	1203[b]	gas	EM	3
			1224[b]	Ne	LF	6,7

A = -440.39(3) gas $EM^{1,2}$

B_o = 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] $\frac{1}{2}(2\nu_i)$.

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FCN^+

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

T^a = 74700(1000) gas PE^1

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

T^a = 48100(1000) gas PE^1

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

T_o = 9200(500) gas PE^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	CF stretch	1230(160)	gas	PE	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CN stretch	2100(160)	gas	PE	1

[a] From vertical ionization potential.

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$ClCN^+$

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

T_o = 54000(300) gas $PE^{1,2}$

B̃ $^2\Pi_{3/2}$ $C_{\infty v}$

T_0 = 22515.54 gas EF[8] LF[10,11] B̃-X̃ 365-569 nm

22598(5) Ne AB[6] B̃-X̃ 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]

Ã $^2\Sigma^+$ $C_{\infty v}$

T_0 = 11690(1) gas EF[3,8] Ã-X̃ 843-881 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	CCl stretch	774(2)	gas	EF	8

τ = 4.4(1.0) μs gas EF[3]

X̃ $^2\Pi_{1/2}$ $C_{\infty v}$

T_0 = 276(2) gas EF[3,8,9] Ã-X̃ 843-881 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡N stretch	1914(2)	gas	EF	8
	3	CCl stretch	827(2)	gas	EF	8

X̃ $^2\Pi_{3/2}$ $C_{\infty v}$ Structure: UV,PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡N stretch	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.

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$BrCN^+$

C̃ $^2\Sigma^+$ $C_{\infty v}$

T_0 = 50200(200) gas PE[1,2]

B̃ $^2\Pi_{3/2}$ $C_{\infty v}$

T_0 = 19234(1)[a] gas EF[7] B̃-X̃ 460-620 nm

18586(14) Ne AB[5] B̃-X̃ 418-538 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡N stretch	1939(2)[a]	gas	EF	7
			1830(10)	Ne	AB	5
Π	2	Bend	394(2)[ab]	gas	EF	7
			377(10)	Ne	AB	5
Σ^+	3	CBr stretch	471(2)[a]	gas	EF	7
			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]

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

T_0 = 13699(1)[a] gas EF[7] $\tilde{A}$-$\tilde{X}$ 708-853 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CN stretch	1930(2)[a]	gas	EF	7
Π	2	Bend	421(2)[a]	gas	EF	7
Σ^+	3	CBr stretch	584(2)[a]	gas	EF	7

τ = 2750(100) ns gas T-PEFCO[8]

$\tilde{X}\ ^2\Pi_{3/2}$ $C_{\infty v}$ Structure: UV,PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡N stretch	1906(2)	gas	EF	7
Π	2	Bend	288(2)[b]	gas	EF	7
Σ^+	3	CBr stretch	650(2)[a]	gas	EF	7

A = -1477(2) gas EF[3]PIFCO[4]

a $^{79}BrCN^+$.
b $\frac{1}{2}(2\nu_2)$.

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ICN^+

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

T_0 = 46600(200) gas PE[1,2]

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

T_0 = 19630(160) gas EF[6] $\tilde{B}$-$\tilde{X}$ 568-644[a] nm

20023(16) Ne AB[4] $\tilde{B}$-$\tilde{X}$ 446-522 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CN stretch	2100(40)	gas	PE	7
Π	2	Bend	300(40)	gas	PE	7
Σ^+	3	CI stretch	473(2)[b]	gas	EF	6
			400(20)	Ne	AB	4

τ = 300(60) ns EF[3], 300(30) ns PIFCO[4] for overlapping $\tilde{A}$ and $\tilde{B}$ states. Triexponential fit of PIFCO data[5] gives $\tau_1 \cong 270$ ns and $\tau_2 \cong 2.3$ μs.

A = -890(160) gas EF[6]; -1130(40) gas PE[7]

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

T_0 = 18262(1) gas EF[3,6] $\tilde{A}$-$\tilde{X}$ 537-758 nm

19135(15) Ne AB[4] $\tilde{A}$-$\tilde{X}$ 499 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	274(2)	gas	EF	6

τ = 1.2(2) μs EF[3]; ∿900 ns from triexponential fit to PIFCO data.[5]

$\tilde{X}\ ^2\Pi_{1/2}$ $C_{\infty v}$

T_0 = 4343(2) gas EF[3,6] $\tilde{A}$,$\tilde{B}$-$\tilde{X}$ 537-758 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	253(2)	gas	EF	6
Σ^+	3	CI stretch	559(2)	gas	EF	6

$\tilde{X}\ ^2\Pi_{3/2}$ $C_{\infty v}$ Structure: UV,PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡N stretch	2082(2)	gas	EF	6
Π	2	Bend	239(2)	gas	EF	6
Σ^+	3	CI stretch	535(2)	gas	EF	6

[a] $\tilde{B}\ ^2\Pi_{1/2}$ - $\tilde{X}\ ^2\Pi_{1/2}$ transition observed.
[b] $\Omega = 1/2$.

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FCP$^+$

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

T_o = 56960(320) gas PE[1]

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

T_o = 24077.7(6) gas PE[1]EF[2] $\tilde{A}$-$\tilde{X}$ 395-485 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CP stretch	1866(2)	gas	EF	2
	3	CF stretch	817(2)	gas	EF	2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡P stretch	1729(2)	gas	PE,EF	1,2
Σ^+	3	CF stretch	765(1)	gas	PE,EF	1,2

A = -190.2(6) gas EF[2]

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CNO

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

T_o = 12611.8 gas UV[2] $\tilde{A}$-$\tilde{X}$ 789-804 nm

12541 Ne UV[1] $\tilde{A}$-$\tilde{X}$ 581-797 nm

Threshold for photoisomerization to NCO at wavelength longer than 700 nm.[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CN stretch	2239	Ne	UV	1
Π	2	Bend	605	Ne	UV	1
Σ^+	3	NO stretch	1247	Ne	UV	1

B_o = 0.398 UV[2]

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

A = -110.6 UV[2]

B_o = 0.38 UV[2]

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N_3

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

T_o = 36739.1 gas AB[1,2]LF[3] $\tilde{B}$-$\tilde{X}$ 260-273 nm

All bands above 37000 are diffuse.

$\tau \leq 20$ ns gas LF[3]

B_o = 0.432 gas AB[2]

$\tilde{X}\ ^2\Pi_g$ $D_{\infty h}$ Structure: AB^2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	∿1320	gas	LF	3
Π_u	2	Bend	∿457[a]	gas	LF	3

A_{eff} = -71.3; $\varepsilon\omega_2$ = -94.38 gas AB[2]

B_o = 0.431 AB[2]

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N_2O^+

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

T_0 = 58245(32) gas PE[1]PI[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Sym. stretch	1280(50)	gas	PE	1
	3	Asym. stretch	2300(50)	gas	PE	1

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

T_0 = 38440(100)[a] gas PE[1]

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[3]

T_0 = 28162.33 gas EM[3,14]PF[6,10,11] $\tilde{A}$-$\tilde{X}$ 317-421 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Sym. stretch	1345.52	gas	EM,PF	3,10
Π	2	Bend	614.45	gas	EM	3,14
Σ^+	3	Asym. stretch	2451.7	gas	EM	3

τ = 230(10) ns gas EF[2,9]PIFCO[4]PEFCO[7]ID[8]EM[12]HFD[13]

B_0 = 0.433 EM[3,14]PF[10,11]

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$ Structure: EM[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Sym. stretch	1126.51	gas	EM	3
Π	2	Bend	452.42	gas	EM,PF	3,11,14
Σ^+	3	Asym. stretch	1737.6	gas	EM	3

A = -133.40, ε_2 = -0.176 gas EM[3,14]PF[11]

B_0 = 0.412 EM[3]PF[10,11]

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

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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]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1986.47	gas	DL	2

B_0 = 0.426 DL[2]

References

[1] E. Ilenberger, P. B. Comita, J. I. Brauman, H. P. Fenzlatt, M. Heni, N. Heinrich, W. Koch, and G. Frenking, Ber. Bunsenges. Phys. Chem. 89, 1026 (1985).
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NO_2^+

$^3B_2$ C_{2v}

T_0[a] = 74580(100) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1113(20)	gas	PE	1,2
	2	Bend	686(20)	gas	PE	1,2

$\tilde{d}\ ^3A_1$ C_{2v}

$T^{ab} \sim 67600$ gas PE[2]

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

$T_o^a = 60670(100)$ gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1017(20)	gas	PE	1,2

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

$T_o^a = 60100(100)$ gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1041(20)	gas	PE	1,2

$\tilde{B}\ ^1B_2$ C_{2v}

$T_o^a = 38940(100)$ gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1025(20)	gas	PE	2
	2	Bend	573(20)	gas	PE	1,2

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

$T_o^a = 35900(100)$ gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	984(20)	gas	PE	1,2
	2	Bend	694(20)	gas	PE	1,2

$\tilde{b}\ ^3A_2$ C_{2v}

$T_o^a = 32110(100)$ gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	662(20)	gas	PE	1,2

$\tilde{a}\ ^3B_2$ C_{2v}

$T_o^a = 26170(100)$ gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	654(20)	gas	PE	1,2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	650(80)	gas	PE	1

[a] The band origins given here have been calculated using a first ionization potential of 9.62(1) eV for NO_2, as found in the photoionization study of Ref. 3.

References

[1] C. R. Brundle, D. P. Neumann, W. C. Price, D. Evans, A. W. Potts, and D. G. Streets, J. Chem. Phys. 53, 705 (1970).
[2] O. Edqvist, E. Lindholm, L. E. Selin, and L. Åsbrink, Phys. Scripta 1, 127 (1970).
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FCO

$\tilde{C}$

$T_o \leq 35741$	gas	AB[2]	$\tilde{C}$-$\tilde{X}$ 232-280 nm	
≤ 35587	Ar	AB[3]	$\tilde{C}$-$\tilde{X}$ 234-281 nm	
≤ 35211	CO	AB[1,3]	$\tilde{C}$-$\tilde{X}$ 217-284 nm	

In the gas phase,[2] bands are diffuse. In an argon matrix,[3] the threshold for photodissociation into F + CO was observed near 280 nm.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			~650	gas	AB	2
			~650	Ar	AB	3
			~650	CO	AB	1,3

$\tilde{B}$

$T_o \geq 27586$	gas	CL^5LF^6	$\tilde{B}$-$\tilde{X}$ 362-455 nm	
≤ 29586	Ar	AB[3]	$\tilde{B}$-$\tilde{X}$ 284-338 nm	
≤ 29516	CO	AB[1,3]	$\tilde{B}$-$\tilde{X}$ 289-339 nm	

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			∿700[a]	Ar	AB	3
			∿700[a]	CO	AB	1,3

τ = 40(3) ns gas LF[6]

X C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CO stretch	1861.64	gas	DL	4
			1857	Ar	IR	3
			1855	CO	IR	1
	2	Bend	627.5	Ar	IR	3
			626	CO	IR	1
	3	CF stretch	1026.13	gas	DL	4
			1023	Ar	IR	3
			1018	CO	IR	1

A_o = 6.38; B_o = 0.382; C_o = 0.360 DL[4]

[a] A second progression, offset by ∿350, may be contributed by excitation of a CF-stretching mode near 1050; in the gas-phase chemiluminescence,[5] the major progression is in the ground-state bending mode, but structure associated with the CF-stretching mode is also observed.

References

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FCS

T_o = 18500(1200) gas CL[1,2] 550-860 nm

Chemiluminescence in the reaction of F_2 with CS_2 has been tentatively assigned to FCS.[1,2]

X ? C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	356(5)	gas	CL	1
	3	CS stretch	831(8)	gas	CL	1

References

[1] R. J. Glinski, Chem. Phys. Lett. 129, 342 (1986).
[2] R. J. Glinski, E. A. Mishalanie, and J. W. Birks, J. Photochem. 37, 217 (1987).

CF_2^+

F $^2A_1$

T_o = 101500(1000)[a] gas PE[1]

E $^2B_2$

T_o = 87000(1000)[a] gas PE[1]

D $^2B_1$

T_o = 75920(160)[a] gas PE[1]

C $^2A_1$

T_o = 62800(1000)[a] gas PE[1]

B $^2A_2$

T_o = 48200(1000)[a] gas PE[1]

Calculations[3] indicate that this state should dissociate into $CF^+ + F$.

A $^2B_2$

T_o = 40180(240)[a] gas PE[1]

X $^2A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	650(40)	gas	PE	1
b_2	3	Asym. stretch	1588[b]	Ar	IR	2

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

References

[1]J. M. Dyke, L. Golob, N. Jonathan, A. Morris, and M. Okuda, J. Chem. Soc., Faraday Trans. 2 70, 1828 (1974).
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[3]D. A. Hrovat and W. T. Borden, J. Am. Chem. Soc. 107, 8034 (1985).

SiF_2^+

E $^2B_2$

T_o = 56600(1600) gas PE[2]

D $^2B_1$

T_o = 50700(800)[a] gas PE[1,2]

C $^2A_1$

T_o = 48600(1200)[a] gas PE[2]

B $^2A_2$

T_o = 40500(1200)[a] gas PE[2]

A $^2B_2$

T_o = 32400(1200) gas PE[1,2]

X $^2A_1$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	350(100)	gas	PE	2

[a] From vertical ionization potential.

References

[1]T. P. Fehlner and D. W. Turner, Inorg. Chem. 13, 754 (1974).
[2]N. P. C. Westwood, Chem. Phys. Lett. 25, 558 (1974).

$SiCl_2^+$

F C_{2v}

T^a = 52850(1000) gas PE[1]

E $^2B_2$ C_{2v}

T^a = 30260(1000) gas PE[1]

C,D $^2B_1$,$^2A_1$ C_{2v}

T^a = 23800(1000) gas PE[1]

A,B $^2B_2$,$^2A_2$ C_{2v}

T^a = 14120(400) gas PE[1]

X $^2A_1$ C_{2v}

[a] From vertical ionization potentials.

References

[1]H. Bock, B. Solouki, and G. Maier, Angew. Chem. 97, 205 (1985); Angew. Chem. Int. Ed. Engl. 24, 205 (1985).

GeF_2^+

F $^2A_1$ C_{2v}

T_o = 54220(480) gas PE[1]

E $^2B_2$ C_{2v}

T_o = 34050(1860) gas PE[1]

D $^2B_1$ C_{2v}

T_o = 31630(1860) gas PE[1]

C $^2A_1$ C_{2v}

T_o = 28800(640) gas PE[1]

A,B $^2B_2$,$^2A_2$ C_{2v}

T_o = 19530(1860) gas PE[1]

X $^2A_1$ C_{2v}

References

[1]G. Jonkers, S. M. van der Kerk, R. Mooyman, and C. A. de Lange, Chem. Phys. Lett. 90, 252 (1982).

$GeCl_2^+$

F $^2A_1$ C_{2v}

T_o = 49860(560) gas PE[1]

E $^2B_2$ C_{2v}

T_o = 23080(480) gas PE[1]

D $^2A_1$ C_{2v}

T_o = 17270(640) gas PE[1]

C $^2B_1$ C_{2v}

T_o = 16380(640) gas PE[1]

B $^2A_2$ C_{2v}

T_o = 9280(560) gas PE[1]

A $^2B_2$ C_{2v}

T_o = 7180(560) gas PE[1]

X $^2A_1$ C_{2v}

References

[1]G. Jonkers, S. M. van der Kerk, and C. A. de Lange, Chem. Phys. 70, 69 (1982).

$GeBr_2^+$

F $^2A_1$ C_{2v}

T_o = 51640(640) gas PE[1]

E $^2B_2$ C_{2v}

T_o = 20900(480) gas PE[1]

D $^2A_1$ C_{2v}

T_o = 14520(640) gas PE[1]

C $^2B_1$ C_{2v}

T_o = 13310(640) gas PE[1]

B $^2A_2$ C_{2v}

T_o = 6780(480) gas PE[1]

A $^2B_2$ C_{2v}

T_o = 4200(560) gas PE[1]

X $^2A_1$ C_{2v}

References

[1]G. Jonkers, S. M. van der Kerk, and C. A. de Lange, Chem. Phys. 70, 69 (1982).

GeI_2^+

E $^2B_2$ C_{2v}

T_o = 20090(480) gas PE[1]

C,D $^2B_1$,$^2A_1$ C_{2v}

T_o = 12430(480) gas PE[1]

B $^2A_2$ C_{2v}

T_o = 6050(480) gas PE[1]

A $^2B_2$ C_{2v}

T_o = 3390(480) gas PE[1]

X $^2A_1$ C_{2v}

References

[1]G. Jonkers, S. M. van der Kerk, R. Mooyman, C. A. de Lange, and J. G. Snijders, Chem. Phys. Lett. 94, 585 (1983).

PO_2

$^2B_1$? C_{2v}

T_o = 30378(3) gas AB[1]LF[3] $^2B_1$-X 268-600 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
	2	Bend	396	gas	AB	1

$\tau \sim 500$ ns gas LF[3]

$\tau_{cont} \sim 4.5$ μs gas LF[3]

X $^2A_1$ C_{2v} Structure: AB[1]MW,LMR[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PO s-stretch	1117(20)	gas	MW,LMR LF	2,3
	2	Bend	387(20)	gas	MW,LMR LF	2,3
b_2	3	PO a-stretch	1278[a]	gas	MW,LMR	2

A_o = 3.486; B_o = 0.287; C_o = 0.264 MW,LMR[2]

[a] Average of values of 1059, 1371, and 1405 cm^{-1}, obtained from centrifugal distortion constants.

References

[1]R. D. Verma and C. F. McCarthy, Can. J. Phys. 61, 1149 (1983).
[2]K. Kawaguchi, S. Saito, E. Hirota, and N. Ohashi, J. Chem. Phys. 82, 4893 (1985).
[3]P. A. Hamilton, J. Chem. Phys. 86, 33 (1987).

FNO^+

T_o = 41870(160) gas PE[1,2]

T^a = 14800(1000) gas PE[1,2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	590(25)	gas	PE	2

[a] From vertical ionization potential. Onset near 6780.

References

[1] D. C. Frost, S. T. Lee, C. A. McDowell, and N. P. C. Westwood, J. Electron Spectrosc. Relat. Phenom. 7, 331 (1975).
[2] R. S. Alderdice and R. N. Dixon, J. Chem. Soc., Faraday Trans. 73, 245 (1977).

$ClNO^+$

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

T_o = 61800(240) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO stretch	910[a]	gas	PE	2
	3	NCl stretch	520(30)	gas	PE	2

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

T_o = 46800(160) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO stretch	1250(30)	gas	PE	1,2
	3	NCl stretch	~580	gas	PE	2

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

T_o = 36550(160) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO stretch	1560(30)[b]	gas	PE	2
	3	NCl stretch	520(30)[b]	gas	PE	2

$\tilde{X}\ ^2A'$[c] C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	NCl stretch	540(30)	gas	PE	2

[a] Gradually increases to 1160.
[b] Average value.
[c] Overlapped by very low-lying transitions to the $\tilde{A}$ and $\tilde{B}$ states.[1-3] A band separation of approximately 1200 has been tentatively attributed to a spin-orbit splitting.[3]

References

[1] D. C. Frost, S. T. Lee, C. A. McDowell, and N. P. C. Westwood, J. Electron Spectrosc. Relat. Phenom. 7, 331 (1975).
[2] M. I. Abbas, J. M. Dyke, and A. Morris, J. Chem. Soc., Faraday Trans. 2 814 (1976).
[3] R. S. Alderdice and R. N. Dixon, J. Chem. Soc., Faraday Trans. 73, 245 (1977).

$BrNO^+$

$\tilde{F}$

T_o = 63200(1000) gas PE[1]

$\tilde{E}$

T_o = 53500(1000) gas PE[1]

$\tilde{D}$

T_o = 45400(1000) gas PE[1]

$\tilde{C}$

T_o = 36500(1000) gas PE[1]

$\tilde{X}\ ^2A'$[a] C_s

[a] Overlapped by very low-lying transitions to the $\tilde{A}$ and $\tilde{B}$ states.[1,2] A band separation of approximately 3200 has been tentatively attributed to a spin-orbit splitting.[2]

References

[1] D. C. Frost, S. T. Lee, C. A. McDowell, and N. P. C. Westwood, J. Electron Spectrosc. Relat. Phenom. 7, 331 (1975).
[2] R. S. Alderdice and R. N. Dixon, J. Chem. Soc., Faraday Trans. 73, 245 (1977).

NSF^+

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

T^a = 46000(800) gas PE[3]

D $^2A''$ C_s

T^a = 40500(320) gas PE[1-3]

C $^2A'$ C_s

T_o = 27350(160) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NS stretch	895(30)	gas	PE	1-3

B $^2A''$ C_s

T_o = 18030(120) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NS stretch	1060(40)	gas	PE	1-3
	2	Bend	365(40)	gas	PE	1-3
	3	SF stretch	695(40)	gas	PE	1-3

A $^2A'$ C_s

T_o = 14860(120) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	460(50)	gas	PE	1-3
	3	SF stretch	820(40)	gas	PE	1-3

X $^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	300(50)	gas	PE	3

[a] From vertical ionization potential.

References

[1] D. O. Cowan, R. Gleiter, O. Glemser, E. Heilbronner, and J. Scharblin, Helv. Chim. Acta 54, 1559 (1971).
[2] R. N. Dixon, G. Duxbury, G. R. Fleming, and J. M. V. Hugo, Chem. Phys. Lett. 14, 60 (1972).
[3] R. L. DeKock, D. R. Lloyd, A. Breeze, G. A. D. Collins, D. W. J. Cruickshank, and H. J. Lempka, Chem. Phys. Lett. 14, 525 (1972).

$NSCl^+$

F $^2A'$ C_s

T_o = 47500(1000) gas PE[2]

E $^2A''$ C_s

T^a = 35400(1000) gas PE[2]

D $^2A'$ C_s

T_o = 29610(240) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NS stretch	970(40)	gas	PE	2

C $^2A'$ C_s

T_o = 25170(240) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	250(30)	gas	PE	2

A,B $^2A'$,$^2A''$ C_s

T_o = 6210(240) gas PE[1,2]

X $^2A'$ C_s

[a] From vertical ionization potential.

References

[1] D. O. Cowan, R. Gleiter, O. Glemser, and E. Heilbronner, Helv. Chim. Acta 55, 2418 (1972).
[2] R. L. DeKock, M. A. Sheheth, D. R. Lloyd, and P. J. Roberts, J. Chem. Soc., Faraday Trans. 2 72, 807 (1976).

O_3^+

E,F $^2A_1$,$^2B_2$ C_{2v}

T_o^b = 37680(160) gas PE[2,3,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1000(40)	gas	PE	5

D $^2B_1$ C_{2v}

T_o[b] = 29530(160) gas PE[3,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	850(40)	gas	PE	5

C $^2B_2$ C_{2v}

T^{ab} = 25580(160) gas PE[3,5]

B $^2A_2$ C_{2v}

T^{ab} = 8960(160) gas PE[1-3,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	∿900	gas	PE	2,5

A $^2B_2$ C_{2v}

T^{ab} = 4600(160) gas PE[1-3,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1380(40)	gas	PE	2,5

X $^2A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1050(80)	gas	PI	4
	2	Bend	∿640[c]	gas	PE,PI	1-5

[a] From vertical ionization potential.
[b] The band origins given here have been calculated using a first ionization potential of 12.43 eV for O_3, as found by Refs. 3 and 5. If instead the value of 12.519(4) eV obtained in the photoionization study of Ref. 4 and in the photoelectron spectroscopy studies of Refs. 1 and 2 is chosen, the positions of the band origins are decreased by approximately 700.
[c] Average value.

References

[1]D. C. Frost, S. T. Lee, and C. A. McDowell, Chem. Phys. Lett. 24, 149 (1974).
[2]C. R. Brundle, Chem. Phys. Lett. 26, 25 (1974).
[3]J. M. Dyke, L. Golob, N. Jonathan, A. Morris, and M. Okuda, J. Chem. Soc., Faraday Trans. 2 70, 1828 (1974).
[4]M. J. Weiss, J. Berkowitz, and E. H. Appelman, J. Chem. Phys. 66, 2049 (1977).
[5]S. Katsumada, H. Shiromaru, and T. Kimura, Bull. Chem. Soc. Japan 57, 1784 (1984).

SO_2^+

F $^2A_1$ C_{2v}

T_o = 62200(500) gas PE[2]

E $^2B_1$ C_{2v}

T_o = 33550(50) gas PE[2,6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	706(4)	gas	PE	2,6

D $^2A_1$ C_{2v}

T_o = 32190(50) gas PE[1,2,6]PF[5] D̃-X̃ 300-317 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	912(1)	gas	PE,PF	1,2,5,6
	2	Bend	411(60)	gas	PF	5

C $^2B_2$ C_{2v}

T_o = 28670(50) gas PE[1,2,6]PF[5] C̃-B̃ 511-437 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	800(4)	gas	PE	6
	2	Bend	371(10)	gas	PF,PE	4-6

B $^2B_2$ C_{2v}

T_o = 7980(60) gas PE[1,6]PF[4,5] C̃-B̃ 437-511 nm[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	465(9)	gas	PE,PF	1,4-6
b_2	3	Asym. stretch	612(7)[b]	gas	PE	6

$\tau \sim 25$ μs gas PF^5

Ã $^2A_2$ C_{2v}

T_o = 5156(65) gas $PE^{1,6}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	981(60)	gas	PE	6
	2	Bend	353(7)	gas	PE	6
b_2	3	Asym. stretch	202(13)	gas	PE	6

X̃ $^2A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	404.2(5)	gas	PE	1,6

Barrier to linearity ∿ 3400 PE^6

[a] Attributed by Ref. 5 to the C̃-Ã transition.
[b] $\frac{1}{2}(2\nu_3)$.

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SSO^+

F $^2A'$ C_s

T^b = 64400(1000) gas $PE^{2,3}$

E $^2A'^a$ C_s

T^b = 42600(320) gas PE^{1-3}

D̃ $^2A''^a$ C_s

T^b = 34700(320) gas PE^{1-3}

C̃ $^2A'^a$ C_s

T^b = 33080(320) gas PE^{1-3}

B̃ $^2A''^a$ C_s

T^b = 6620(320) gas PE^{1-3}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			480(40)	gas	PE	3

Ã $^2A'^a$ C_s

T^b = 5650(320) gas PE^{1-3}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			570(40)	gas	PE	3

X̃ $^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	370(40)	gas	PE	3

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

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CF_2

B̃ [a]

$T_o \sim 72740$ gas AB[10] B̃-X̃ 131-138 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	Bend	625	gas	AB	10

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

T_o = 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 LF	4,6,16 17
			496(2)	N_2	LF	17

τ_o = 61(3) ns gas LF[20,21]

31 ns Ne LF[17]

27 ns Ar LF[17]

23 ns Kr LF[17]

A_o = 4.577; B_o = 0.334; C_o = 0.311 AB[10]

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

T_o = 19828 gas CL[18,19,22,24,28] $\tilde{a}$-$\tilde{X}$ 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, 24,28

$\tau \sim 1s$ 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	23,29
			1220	Ne	IR,LF	12,17
			1222	Ar	IR,LF	6,11,17
	2	Bend	667	gas	UV	1,10
			668	Ar	IR,LF	6,11,17
b_2	3	Asym. stretch	1114.44	gas	IR,DL	7,13 27,29
			1104	Ne	IR	12
			1102	Ar	IR	6,11

A_o = 2.947; B_o = 0.417; C_o = 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.

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CFCl

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

T_o = 25283(5)	gas	LF[6]	$\tilde{A}$-$\tilde{X}$ 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'	2	Bend	394(3)	gas	LF	6
			392(1)	Ar	LF	3
	3	CCl stretch	726(6)[a]	gas	LF	6
			712(2)[a]	Ar	LF	3

τ_0 = 700(10) ns gas LF[4-6]

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
			1146	Ar	IR	1
	2	Bend	448(6)	gas	LF	6
			442	Ar	LF	2,3
	3	CCl stretch	750(6)	gas	LF	6
			742s	Ar	IR	1

[a] $T_{001} - T_{000}$.

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CFBr

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

$T_0 \leq$ 22255 gas LF[3] $\tilde{A}$-$\tilde{X}$ 420-450 nm

23300 Ar LF[1] $\tilde{A}$-$\tilde{X}$ 442-535 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	240(40)	Ar	LF	1

τ = 1150(50) ns gas LF[3]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CF stretch	1157	Ar	IR	2
	2	Bend	∿325	gas	LF	3
			340(5)	Ar	LF	1
	3	CBr stretch	656	Ar	IR	2

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CCl_2

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

T_0 = 16920(4) gas CL[8]LF[7,9,10]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	636(2)	gas	LF	10
			624	Ar	LF	6
	2	Bend	305.4(8)	gas	LF	9,10
			304	Ar	AB,LF	1,3,6

τ = 3.81(30) μs gas LF[7];

τ_1 = 2.17(26) μs, τ_2 = 4.21(12) μs gas EM[11]

τ = 3.6 μs Ar LF[6]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	721	Ar	IR,LF	1-3,5,6
	2	Bend	333	Ar	LF	4-6
b_2	3	Asym. stretch	748	Ar	IR	1-3

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CClBr

Ã C_s

T_0 = 16044 Ar LF[3,4] Ã-X̃ 540-776 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CCl stretch	684[a]	Ar	LF	4
	2	Bend	246	Ar	LF	4
	3	CBr stretch	526	Ar	LF	4

τ = 5.6(6) μs Ar LF[4]

X̃ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CCl stretch	744	Ar	IR	1,2
	2	Bend	260	Ar	LF	3,4
	3	CBr stretch	611	Ar	IR	1,2

[a] Tentative; an alternate assignment gives ν_1 = 944.

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CBr_2

Ã C_{2v}

T_0 = 14962 Ar LF[3,4] Ã-X̃ 600-857 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	468	Ar	LF	4
	2	Bend	186	Ar	LF	4

τ = 14.5(1.5) μs Ar LF[4]

X̃ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	595	Ar	IR	1,2
	2	Bend	196	Ar	LF	3,4
b_2	3	Asym. stretch	641	Ar	IR	1,2

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SiF_2

b̃ $^3B_2$ [a] C_{2v}

T_0 = 62214 gas UV[11]MPI[15] b̃-X̃ 158-165 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	∿790	gas	AB	11
	2	Bend	∿320	gas	AB	11

Ã $^1B_1$ C_{2v} Structure: AB[9]

T_0 = 44113.9 gas EM[1,2]AB[5,9]LF[14] Ã-X̃ 213-276 nm
∿ 43964 Ne AB[7] Ã-X̃ 216-225 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	250.1(3)	gas	AB	5,9
			~253	Ne	AB	7

A_o = 1.446; B_o = 0.241; C_o = 0.206 AB[9]

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

T_o = 26310 gas EM[10] $\tilde{a}$-$\tilde{X}$ 364-420 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	277	gas	EM	10

$\tilde{X}\ ^1A_1$ C_{2v} Structure: MW[3,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	855.01	gas	IR	6,13
			851	Ne	IR	8
			843	Ar	IR	7,8
	2	Bend	345	gas	MW,UV	4,5
			343	Ar	IR	7
b_2	3	Asym. stretch	870.40	gas	IR	6,13
			864.6	Ne	IR	8
			855	Ar	IR	7,8

A_o = 1.021; B_o = 0.294; C_o = 0.228 MW[3,4]

[a] See Ref. 12.

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$SiCl_2$

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

T_o = 30003.6(5) gas AB[4]EM[5-7]LF[8] $\tilde{A}$-$\tilde{X}$ 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^a = 77(3) ns gas LF[8]

$\tilde{X}\ ^1A_1$ C_{2v} Structure: ED[4]MW[b]

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
			512.5	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
			502	Ar	IR	1,2

A_o = 0.493; B_o = 0.094; C_o = 0.079 MW[b]

[a] $v_2'' = 7$.
[b] M. Tanimoto, H. Takeo, and C. Matsumura, Proc. 49th Spring Conference of the Chemical Society of Japan, No. 1, p. 6 (1984), cited in Ref. 8.

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$SiBr_2$

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

An unstructured absorption between 340 and 400 nm, with a maximum near 362 nm (27600) has been attributed[2] to the $\tilde{A}\ ^1B_1 - \tilde{X}\ ^1A_1$ transition of $SiBr_2$, by analogy with the electronic spectra of related compounds.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	402.6	Ar	IR	1
b_2	3	Asym. stretch	399.5	Ar	IR	1

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GeF_2

The high-temperature vapor of GeF_2 shows unstructured absorption between 136 and 156 nm, with a maximum near 146.3 nm.[5]

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

T_0 = 43843(10) gas AB[1] $\tilde{A}$-$\tilde{X}$ 222-243 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	164(3)	gas	AB	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	663	gas	IR	2
			655	Ne	IR	2
			648	Ar	IR,Ra	2,6
			653	N_2	Ra	6
	2	Bend	263(5)	gas	AB	1
b_2	3	Asym. stretch	692	gas	IR	2
			685	Ne	IR	2
			676	Ar	IR	2

A_o = 0.513; B_o = 0.262; C_o = 0.173 MW[3,4]

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$GeCl_2$

$T_0 \sim$ 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

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

$^3B_1$?

T_o = 17461 gas CL[3] 560-666 nm[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	353(4)	gas	CL	3
	2	Bend	130(4)	gas	CL	3

X $^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	399	gas	CL,Ra	1,3,5
			398.6[b]	Ar	IR	4,6,8,9
			390	N_2	Ra	7
	2	Bend	160(4)	gas	CL,AB Ra	1-3 5
			163	N_2	Ra	7
b_2	3	Asym. stretch	373.5[b]	Ar	IR	4,6,8,9
			362	N_2	Ra	7

[a] Lower state is ground state of the molecule.
[b] $^{74}Ge^{35}Cl_2$.

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NF_2^+

Ã $^1B_1$? C_{2v}

$T_o \sim 38400$[a] gas PE[1,2]

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

T_o = 19610(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			520(20)	gas	PE	1,2

X̃ $^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NF stretch	1250(20)	gas	PE	1,2

[a] From vertical ionization potential.

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ClO_2^+

X̃

T_o = 59140(320) gas PE[1]

Ẽ $^3A_2$ C_{2v}

T_o = 47520(320) gas PE[1,2]

B̃ $^1B_2$ C_{2v}

T_o = 39620(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ClO s-stretch	661(20)	gas	PE	2
	2	Bend	440(20)	gas	PE	2

C̃[ab] C_{2v}

$T \sim 24500$ gas PE[1,2]

B[ac] C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	482(20)	gas	PE	2

Ã[a] C_{2v}

T_o = 15810(160) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	395(20)	gas	PE	2

X̃ $^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ClO s-stretch	1014(20)	gas	PE	2
	2	Bend	520(20)	gas	PE	2

[a] $^3B_1$, $^1B_1$, and $^3B_2$ states are expected to lie in this spectral region.
[b] Shoulder.
[c] Overlaps Ã state.

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SSO

An absorption band system between 190 and 230 nm has been attributed[7] to SSO. However, an alternate assignment to the C̃-X̃ band system of SO_2 has been proposed.[15]

Ã $^1A'$ C_s Structure: AB[11]

T_o = 29696 gas AB[1,7,11] LF[12,13] 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	1030	gas	AB,LF	11,13
	2	Bend	252	gas	AB,LF	11,13
	3	SS stretch	405	gas	AB,LF	7,11,13
			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]

ã $^3A'$ C_s

T_o = 13943 gas AB[10,15] LF[13] ã-X̃ 430-670 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SO stretch	1089	gas	AB	10,15
	2	Bend	332	gas	AB	10,15
	3	SS stretch	505	gas	AB	10,15

X̃ $^1A'$ 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	370(30)	gas	MW	2
			382	Ar	IR,Ra	8,9
	3	SS stretch	679	gas	IR,LF	1,3,13
			672.2	Ar	IR,Ra	8,9

A_o = 1.398; B_o = 0.169; C_o = 0.150 MW[2,5,6] DL[14]

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S_3

T_o = 23465(15) gas AB[1,2] 360-500 nm
Ar AB[4] 368-413 nm
Kr AB[1,2] 310-420 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	420	gas	AB	2
			∿420	Ar	AB	4
			420	Kr	AB	2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	590	gas	AB	2
			583	Ar	Ra	3

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NF_2

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

gas AB[1,4,5] $\tilde{A}$-$\tilde{X}$ 237-278 nm
Ar AB[9] $\tilde{A}$-$\tilde{X}$ 247-265 nm

In an argon matrix,[6,9] evidence has been obtained for predissociation into NF + F.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	390[a]	gas	AB	4,5
			408[a]	Ar	AB	9

$\tilde{X}$ $^2B_1$ C_{2v} Structure: IR[2]MW[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1074.99	gas	IR,DL LMR	2,10, 11,12
			1069	Ar	IR	7,9
			1070	N_2	IR	2,3
	2	Bend	573	N_2	IR	3
b_2	3	Asym. stretch	942.48	gas	IR,DL LMR	2,10, 13,14
			932	Ar	IR	7,9
			931	N_2	IR	2,3

A_o = 2.351; B_o = 0.396; C_o = 0.338 MW[8]DL[12]

[a] Average value.

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NCl_2

$\tilde{A}$

gas AB[1-3] $\tilde{A}$-$\tilde{X}$ 275-314 nm

Photodissociation threshold near 310 nm.[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	557[a]	gas	AB	1

$\tilde{X}$ C_{2v} Structure: IR[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	679	Ar	IR	4

[a] Average value.

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O_3^-

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

T_o = 21420(40) gas PF[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	760(20)	gas	PF	8
	2	Bend	190(20)	gas	PF	8

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

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

T_o = 16508(16) gas PF[6,8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	815(10)	gas	PF	6,8
	2	Bend	275(10)	gas	PF	6,8

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

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
			600[a]	Ar	IR	4
b_2	3	Asym. stretch	789[a] 802	Ar	IR	2,4
			802[b]	Ar	IR	1,2,4

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

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FOO

An absorption maximum of gas-phase FOO has been reported[4] at 205 nm.

Unstructured absorption of FOO with a maximum near 420 nm has been observed in liquid CF_4.[2] In liquid O_2 and Ar:O_2 mixtures,[5] the corresponding absorption maximum lies near 445 nm. In all of these systems, photodissociation of FOO occurs in this spectral region. In an argon matrix, the onset of photodissociation has been observed[6] near 490 nm.

$\tilde{X}$ C_s Structure: DL[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OO stretch	1486.93	gas	IR	8,9
			1490	Ar	IR	1,6
			1500	N_2	IR	3

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	376	N_2	IR	3
	3	OF stretch	579.32	gas	DL,IR	7,9
			584	Ar	IR	1,6
			586	N_2	IR	3

A_o = 2.613; B_o = 0.332; C_o = 0.295 DL[7]IR[9]

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ClOO

An unstructured absorption between 225 and 270 nm, with a maximum near 248 nm, in gas-phase modulation experiments has been assigned[3,4] to ClOO.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OO stretch	1443[a]	gas	IR	4
			1441[b]	Ar	IR	2
			1438 1428	N_2	IR	1
	2	Bend	373	Ar	IR	2
	3	ClO stretch	407[b]	Ar	IR	2

[a] Absorption maximum; spectral slit width 13 cm^{-1}.
[b] Peaks at 1415 and 435 cm^{-1}, attributed in Ref. 2 to a structural isomer of ClOO, were attributed in Ref. 5 to the vibrationally unrelaxed molecule.

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SO_2^-

Threshold for electron detachment from ground-state SO_2^- = 8930(65) gas PE[2,3]

$\tilde{X}$ $^2B_1$ C_{2v} Structure: PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	944(48)	gas	PE	3
			985[a]	Ar	IR	1
			990[b]	Ar	IR	1
	2	Bend	435(100)	gas	PE	3
			495[a]	Ar	IR	1
			495[b]	Ar	IR	1
b_2	3	Asym. stretch	1042[a]	Ar	IR	1
			1041[b]	Ar	IR	1

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

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SSO^-

Threshold for electron detachment from ground-state SSO^- = 15140(65) gas PE[1]

$\tilde{X}$ $^2A''$ C_s Structure: PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	SS stretch	620(150)	gas	PE	1

References

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SSCl

T_o = 21650 gas[a] AB[1,2,5] 378-481 nm

≤ 21925 Ar AB[3] 389-456 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	Stretch	480	gas	AB	5
			491(20)	Ar	AB	3
	3	Stretch	407	gas	AB	5

X $^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SS stretch	659	gas	AB	5
		SS stretch	665	Ar	IR	4
	2	Bend	336	gas	AB	5
	3	SCl stretch	404	Ar	IR	4

[a] Diffuse band system. Ref. 3 also reported two very weak bands approximately 600 cm^{-1} below the principal progression which they attributed to ground-state vibrational excitation.

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OF_2^+

E C_{2v}

T^a = 51560(400) gas PE[1,2]

D C_{2v}

$T_o \sim$ 38650 gas PE[1,2]

C $^2A_2$[b] C_{2v}

T^a = 26870(240) gas PE[1,2]

Ã,B̃ $^2B_2$,$^2A_1$[b] C_{2v}

T_o = 21220(240) gas PE[1,2]

X̃ $^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	OF s-stretch	1020(40)	gas	PE	1,2

[a] From vertical ionization potential. The first ionization potential is taken as 13.11(1) eV, from the photoionization study of Ref. 3.
[b] For assignment, see Ref. 4.

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ClO^+

F $^2B_1$ C_{2v}

T^b = 54380(320) gas PE[1]

E $^2A_1$ C_{2v}

T^b = 46070(320) gas PE[1]

D $^2B_2$ C_{2v}

T^b = 40020(320) gas PE[1]

C̃ $^2A_2$[a] C_{2v}

T^b = 14930(320) gas PE[1]

B̃ $^2A_1$[a] C_{2v}

T^b = 13800(320) gas PE[1]

Ã $^2B_2$[a] C_{2v}

T^b = 11540(320) gas PE[1]

X̃ $^2B_1$[a] C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ClO s-stretch	670(40)	gas	PE	1
	2	Bend	300(40)	gas	PE	1

[a] For assignment, see Ref. 2.
[b] From vertical ionization potential.

References

[1]A. B. Cornford, D. C. Frost, F. G. Herring, and C. A. McDowell, J. Chem. Phys. 55, 2820 (1971).
[2]D. Colbourne, D. C. Frost, C. A. McDowell, and N. P. C. Westwood, J. Chem. Phys. 68, 3574 (1978).

SF_2^+

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

T_o = 74400(1000) gas PE[1]

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

T_o = 66300(1000) gas PE[1]

$\tilde{B},\tilde{C}\ ^2B_2,^2A_2$ C_{2v}

T_o = 49400(1000) gas PE[1]

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

T_o = 42900(1000) gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SF stretch	935(40)	gas	PE	1

References

[1]D. M. de Leeuw, R. Mooyman, and C. A. de Lange, Chem. Phys. 34, 287 (1978).

SCl_2^+

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

T^a = 51230(1100) gas PE[1,2]

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

T^a = 42760(400) gas PE[1,2]

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

T^a = 37110(400) gas PE[1,2]

$\tilde{B},\tilde{C}\ ^2A_1,^2A_2$ C_{2v}

T^a = 24290(400) gas PE[1,2]

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

T^a = 22510(400) gas PE[1,2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SCl s-stretch	530(40)	gas	PE	1,2

[a] From vertical ionization potential. The first ionization potential was taken to equal 9.45(3) eV, from the appearance potential measurements of Ref. 3.

References

[1]B. Solouki, P. Rosmus, and H. Bock, Chem. Phys. Lett. 26, 20 (1974).
[2]R. J. Colton and J. W. Rabalais, J. Electron Spectrosc. Relat. Phenom. 3, 345 (1974).
[3]R. Kaufel, G. Vahl, R. Minkwitz, and H. Baumgartel, Z. Anorg. Allg. Chem. 481, 207 (1981).

SBr_2^+

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

$T_o \sim 16000$ gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SBr stretch	400(50)	gas	PE	1

References

[1]D. M. de Leeuw, R. Mooyman, and C. A. de Lange, Chem. Phys. Lett. 61, 191 (1979).

$SeCl_2^+$

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

T_o = 44620(160) gas PE[1]

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

T_o = 37840(160) gas PE[1]

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

T_o = 31390(160) gas PE[1]

$\tilde{B},\tilde{C}\ ^2A_2,^2A_1$ C_{2v}

T_o = 22430(160) gas PE[1]

Ã $^2B_2$ C_{2v}

T_o = 20170(160) gas PE[1]

X̃ $^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	450(50)	gas	PE	1

References

[1]D. M. de Leeuw, R. Mooyman, and C. A. de Lange, Chem. Phys. 38, 21 (1979).

$SeBr_2^+$

F̃ $^2B_2$ C_{2v}

T_o = 41470(160) gas PE[1]

Ẽ $^2A_1$ C_{2v}

T_o = 33890(160) gas PE[1]

D̃ $^2B_1$ C_{2v}

T_o = 27350(160) gas PE[1]

C̃ $^2A_2$ C_{2v}

T_o = 18800(160) gas PE[1]

B̃ $^2A_1$ C_{2v}

T_o = 18070(160) gas PE[1]

Ã $^2B_2$ C_{2v}

T_o = 14850(160) gas PE[1]

X̃ $^2B_1$ C_{2v}

References

[1]D. M. de Leeuw, R. Mooyman, and C. A. de Lange, Chem. Phys. 38, 21 (1979).

KrF_2^+

D̃ $^2\Sigma_u$ $D_{\infty h}$

T^{ab} = 36600(1000) gas PE[1]

C̃ $^2\Pi_u$ $D_{\infty h}$

T_o[a] = 30340(160) gas PE[1]

B̃ $^2\Pi_g$ $D_{\infty h}$

T_o[a] = 9760(160) gas PE[1]

Ã $^2\Sigma_g$ $D_{\infty h}$

T_o[a] = 5970(160) gas PE[1]

X̃ $^2\Pi_u$ $D_{\infty h}$

A = -1050(160) gas PE[1]

[a] Calculated using the upper bound of 13.16 eV for the first adiabatic ionization potential. Value may be increased by as much as 800, corresponding to the lower bound of 13.06 eV for this ionization potential.[1]

[b] From vertical ionization potential.

References

[1]C. R. Brundle and G. R. Jones, J. Chem. Soc., Faraday Trans. 2 68, 959 (1972).

XeF_2^+

D̃ $^2\Sigma_u$ $D_{\infty h}$

T_o = 35900(500) gas PE[1-3]

C̃ $^2\Pi_u$ $D_{\infty h}$

T_o[a] = 23400(500) gas PE[1-3]

Spin-orbit splitting = 3230(800) gas PE[1]

B̃ $^2\Pi_g$ $D_{\infty h}$

T_o = 13310(500) gas PE[1-3]

Ã $^2\Sigma_g$ $D_{\infty h}$

T_o = 9920(500) gas PE[1-3]

X̃ $^2\Pi_{u,3/2}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	XeF_2 stretch	520(30)	gas	PE	1

Spin-orbit splitting = 3790(160) gas PE[1,2]

[a] Onset of transition given.

References

[1]C. R. Brundle, M. B. Robin, and G. R. Jones, J. Chem. Phys. 52, 3383 (1970).
[2]B. Brehm, M. Menzinger, and C. Zorn, Can. J. Chem. 48, 3193 (1970).

[3]B. W. Yates, K. H. Tan, G. M. Bancroft, L. L. Coatsworth, J. S. Tse, and G. J. Schrobilgen, J. Chem. Phys. 84, 3603 (1986).

KrF_2

Continuous absorption in the gas phase between 210 and 320 nm, most intense at 210 nm.[5]

$\tilde{X}$ $D_{\infty h}$ Structure: IR[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	449	gas	Ra	2
			452	Kr	Ra	4
Π_u	2	Bend	233	gas	IR	2
			236	Ar	IR	1
Σ_u^+	3	Asym. stretch	589.9(5)	gas	IR	2,3
			580	Ar	IR	1

B_o = 0.126 IR[3]

References

[1]J. J. Turner and G. C. Pimentel, Science 180, 974 (1963).
[2]H. H. Claassen, G. L. Goodman, J. G. Malm, and F. Schreiner, J. Chem. Phys. 42, 1229 (1965).
[3]C. Murchison, S. Reichman, D. Anderson, J. Overend, and F. Schreiner, J. Am. Chem. Soc. 90, 5690 (1968).
[4]W. F. Howard, Jr., and L. Andrews, J. Am. Chem. Soc. 96, 7864 (1974).
[5]G. N. Makeev, V. F. Sinyanskii, and B. M. Smirnov, Dokl. Akad. Nauk SSSR 222, 151 (1975).

XeF_2

6p $^1\Sigma_g$ $D_{\infty h}$

T_o = 87400 gas AB[11] $6p^1\Sigma_g$-$\tilde{X}$ 114 nm

A higher member of this Rydberg series has also been reported.[11]

5d $^1\Pi_{u,1/2}$ $D_{\infty h}$

T_o = 86000 gas AB[3,4,11] $5d^1\Pi_{u,1/2}$-$\tilde{X}$ 116 nm

Higher members of this Rydberg series have also been reported.[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	484(24)	gas	AB	11
Π_u	2	Bend	∿200	gas	AB	11

5d $^1\Pi_{u,3/2}$ $D_{\infty h}$

T_o = 80800 gas AB[3,4,11] $5d^1\Pi_{u,3/2}$-$\tilde{X}$ 124 nm

Higher members of this Rydberg series have also been reported.[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	524(8)	gas	AB	11
Π_u	2	Bend	∿200	gas	AB	11

6s $^1\Pi_{u,1/2}$ $D_{\infty h}$

T_o = 73870 gas AB[3,4,8,11] $6s^1\Pi_{u,1/2}$-$\tilde{X}$ 135 nm

Higher members of this Rydberg series have also been reported.[3,4,11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	500(16)	gas	AB	11

6s $^1\Pi_{u,3/2}$ $D_{\infty h}$

T_o = 69300 gas AB[3,4,8,11] $6s^1\Pi_{u,3/2}$-$\tilde{X}$ 144 nm

Higher members of this Rydberg series have also been reported.[3,4,11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	532(8)	gas	AB	11
Π_u	2	Bend	73(8)	gas	AB	11

$\tilde{B}$ $^1\Sigma_u$ $D_{\infty h}$

T^a = 63300 gas AB[3,4,11] $\tilde{B}$-$\tilde{X}$ 158 nm

$\tilde{A}$ $^1\Pi_g$ $D_{\infty h}$

T^a = 43500 gas AB[3,4,6,11] $\tilde{A}$-$\tilde{X}$ 230 nm

$\tilde{X}$ $^1\Sigma_g$ $D_{\infty h}$ Structure: IR[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	516.5(5)	gas	Ra	9,13
			512	Ar	Ra	10
			512	Xe	Ra	10

X $^1\Sigma_g$---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	213.2	gas	IR	5
			215	Ar	IR	12
Σ_u^+	3	Asym. stretch	560.10	gas	IR	1,5,7
			547	Ar	IR	2

B_o = 0.114 IR[7]

[a] Absorption maximum.

References

[1]D. F. Smith, J. Chem. Phys. 38, 270 (1963).
[2]J. J. Turner and G. C. Pimentel, in "Noble-Gas Compounds," H. H. Hyman, Ed., University of Chicago Press, Chicago, Ill., 1963, p. 101.
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[10]W. F. Howard, Jr., and L. Andrews, J. Am. Chem. Soc. 96, 7864 (1974).
[11]U. Nielsen and W. H. E. Schwarz, Chem. Phys. 13, 195 (1976).
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[13]N. J. Brassington and H. G. M. Edwards, J. Mol. Struct. 162, 69 (1987).

Ne_2F

Unstructured gas-phase emission[1] between 117 and 125 nm has been attributed[2] to Ne_2F.

References

[1]J. K. Rice, A. K. Hays, and J. R. Woodworth, Appl. Phys. Lett. 31, 31 (1977).
[2]I. N. Konovalov, V. F. Losev, V. V. Ryzhov, V. F. Tarasenko, and A. G. Tastremskii, Opt. Spektrosk. 47, 239 (1979); Opt. Spectrosc. 47, 137 (1979).

Ar_2F

Unstructured gas-phase emission[1-3] between 250 and 340 nm, with maximum near 292 nm.

τ = 185(46) ns gas EM[4]

References

[1]J. A. Mangano, J. H. Jacob, M. Rokni, and A. Hawryluk, Appl. Phys. Lett. 31, 26 (1977).
[2]N. G. Basov, V. A. Danilychev, V. A. Dolgikh, O. M. Kerimov, V. S. Lebedev, and A. G. Molchanov, Pis'ma Zh. Eksp. Teor. Fiz. 26, 20 (1977); J. Exp. Theor. Phys. Lett. 26, 16 (1977).
[3]D. C. Lorents, D. L. Huestis, M. V. McCusker, H. H. Nakano, and R. M. Hill, J. Chem. Phys. 68, 4657 (1978).
[4]C. H. Chen, M. G. Payne, and J. P. Judish, J. Chem. Phys. 69, 1626 (1978).

ArKrF

Unstructured gas-phase emission[1,2] between 240 and 370 nm, with maximum near 305 nm.

References

[1]J. A. Mangano, J. H. Jacob, M. Rokni, and A. Hawryluk, Appl. Phys. Lett. 31, 26 (1977).
[2]H. C. Brashears, Jr., D. W. Setser, and Y.-C. Yu, J. Chem. Phys. 74, 10 (1981).

Kr_2F

9 $^2\Gamma$ C_{2v}

gas AB[6,8] $9^2\Gamma$-$4^2\Gamma$

Broad absorption, with maximum near 335 nm.

8 $^2\Gamma$ C_{2v}

gas AB[8] $8^2\Gamma$-$4^2\Gamma$ ~472 nm

4 $^2\Gamma$ C_{2v}

Unstructured gas-phase emission[1-4] between 340 and 480 nm, with maximum near 410 nm.

τ = 200(28) ns gas LF[5]EF[7]

References

[1]J. A. Mangano, J. H. Jacob, M. Rokni, and A. Hawryluk, Appl. Phys. Lett. 31, 26 (1977).
[2]N. G. Basov, V. A. Danilychev, V. A. Dolgikh, O. M. Kerimov, V. S. Lebedev, and A. G. Molchanov, Pis'ma Zh. Eksp. Teor. Fiz. 26, 20 (1977); J. Exp. Theor. Phys. Lett. 26, 16 (1977).
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[8]D. B. Geohegan and J. G. Eden, Chem. Phys. Lett. 139, 519 (1987).

NeXeF

Unstructured gas-phase emission[1] between 370 and 550 nm.

References

[1]M. Rokni, J. H. Jacob, J. C. Hsia, and D. W. Trainor, Appl. Phys. Lett. 35, 729 (1979).

ArXeF

Unstructured gas-phase emission[1,2] between 380 and 500 nm, with maximum near 460 nm.

References

[1]R. O. Hunter, J. Oldenettel, C. Hawton, and M. V. Cusker, J. Appl. Phys. 49, 549 (1978).
[2]M. Rokni, J. H. Jacob, J. C. Hsia, and D. W. Trainor, Appl. Phys. Lett. 35, 729 (1979).

KrXeF

Unstructured gas-phase emission[1] between 380 and 570 nm.

References

[1]N. G. Basov, V. A. Danilychev, V. A. Dolgikh, O. M. Kerimov, V. S. Lebedev, and A. G. Molchanov, Pis'ma Zh. Eksp. Teor. Fiz. 26, 20 (1977); J. Exp. Theor. Phys. Lett. 26, 16 (1977).

Ar_2Cl

Unstructured gas-phase emission maximum[1,2] at 245(5) nm, with bandwidth (FWHM) of 35 nm.

τ = 240(40) ns gas EF^2

References

[1]D. C. Lorents, D. L. Huestis, M. V. McCusker, H. H. Nakano, and R. M. Hill, J. Chem. Phys. 68, 4657 (1978).
[2]J. Liegel, H. Spiegel, R. Sauerbrey, and H. Langhoff, J. Chem. Phys. 79, 247 (1983).

NeKrCl

Unstructured gas-phase emission[1,2] between 235 and 330 nm.

References

[1]I. N. Konovalov, V. F. Losev, V. V. Ryzhov, V. F. Tarasenko, and A. G. Tastremskii, Opt. Spektrosk. 47, 137 (1979).
[2]V. S. Skakun and V. F. Tarasenko, Opt. Spektrosk. 58, 293 (1985); Opt. Spectrosc. 58, 175 (1985).

ArKrCl

Unstructured gas-phase emission[1] between 224 and 316 nm, with maximum near 270 nm.

References

[1]H. C. Brashears, Jr., D. W. Setser, and Y.-C. Yu, J. Chem. Phys. 74, 10 (1981).

Kr_2Cl

Unstructured gas-phase emission[1,2] between 290 and 380 nm, with maximum near 325 nm.

τ = 470(20) ns gas EF^3

References

[1]D. C. Lorents, D. L. Huestis, M. V. McCusker, H. H. Nakano, and R. M. Hill, J. Chem. Phys. 68, 4657 (1978).
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[3]A. Luches, A. Perrone, and A. Giannattasio, Opt. Commun. 48, 253 (1983).

KrXeCl

Unstructured gas-phase emission[1] between 290 and 450 nm, with maximum near 370 nm.

References

[1]H. C. Brashears, Jr., D. W. Setser, and Y.-C. Yu, J. Chem. Phys. 74, 10 (1981).

Xe_2Cl

9 $^2\Gamma$ C_{2v}

gas $AB^{4,6}$ $9^2\Gamma$-$4^2\Gamma$

Absorption maximum near 335 nm, absorption extending to wavelengths less than 193 nm.

8 $^2\Gamma$ C_{2v}

gas AB^6 $8^2\Gamma$-$4^2\Gamma$ ~435 nm

4 $^2\Gamma$ C_{2v}

gas $EM^{1-4,6}$ $4^2\Gamma$-$1,2^2\Gamma$

Unstructured emission maximum at 485 nm, with bandwidth (FWHM) of 4500 cm^{-1}.

Ar,Kr,Xe EM^5 $4^2\Gamma$-$1,2^2\Gamma$

Unstructured emission maximum at 573 nm, with bandwidth (FWHM) of 2000 cm^{-1}.

τ = 245(10) ns gas EM^4

250(10) ns Ar EM^5

210(10) ns Kr EM^5

225(5) ns Xe EM^5

References

[1]J. A. Mangano, J. H. Jacob, M. Rokni, and A. Hawryluk, Appl. Phys. Lett. 31, 26 (1977).
[2]D. C. Lorents, D. L. Huestis, M. V. McCusker, H. H. Nakano, and R. M. Hill, J. Chem. Phys. 68, 4657 (1978).
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[6]D. B. Geohegan and J. G. Eden, Chem. Phys. Lett. 139, 519 (1987).

ArKrBr

Unstructured gas-phase emission[1] between 227 and 290 nm.

References

[1]V. S. Skakun and V. F. Tarasenko, Opt. Spektrosk. 58, 293 (1985); Opt. Spectrosc. 58, 175 (1985).

Kr_2Br

Unstructured gas-phase emission[1] between 265 and 370 nm.

References

[1]I. N. Konovalov, V. F. Losev, V. V. Ryzhov, V. F. Tarasenko, and A. G. Tastremskii, Opt. Spektrosk. 47, 137 (1979).

NeXeBr

Unstructured gas-phase emission[1] between 255 and 350 nm.

References

[1]I. N. Konovalov and V. F. Tarasenko, Zh. Prikl. Spektrosk. 34, 177 (1981).

ArXeBr

Unstructured gas-phase emission[1] between 270 and 380 nm.

References

[1]V. S. Skakun and V. F. Tarasenko, Opt. Spektrosk. 58, 293 (1985); Opt. Spectrosc. 58, 175 (1985).

KrXeBr

Unstructured gas-phase emission[1] between 285 and 375 nm, with maximum near 330 nm.

References

[1]H. C. Brashears, Jr., D. W. Setser, and Y.-C. Yu, J. Chem. Phys. 74, 10 (1981).

Xe_2Br

Unstructured gas-phase emission[1] between 380 and 460 nm.

References

[1]I. N. Konovalov, V. F. Losev, V. V. Ryzhov, V. F. Tarasenko, and A. G. Tastremskii, Opt. Spektrosk. 47, 137 (1979).

KrXeI

Unstructured gas-phase emission[1] between 260 and 420 nm, with maximum near 290 nm.

References

[1]H. C. Brashears, Jr., D. W. Setser, and Y.-C. Yu, J. Chem. Phys. 74, 10 (1981).

6.4. Four-Atomic Trihydrides

CH_3^+

$\tilde{A}\ ^1E'$ D_{3h}

T_0 = 50510(280) gas PE[2]

$\tilde{a}\ ^3E'$ D_{3h}

T_0 = 39700(280) gas PE[2]

$\tilde{X}\ ^1A_1'$ D_{3h} Structure: LD[3,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	1380(20)	gas	PE	1,2
e'	3	CH stretch	3108.38	gas	LD	3,4

B_0 = 9.362 LD[3,4]

CD_3^+

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	1070(30)	gas	PE	2

References

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CH_3

4f $^2E'^a$ D_{3h}

T_0 = 72508 gas MPI[12]

Higher member of Rydberg series observed (MPI[12]) at 74961.

3d $^2A_1'$ D_{3h} Structure: AB^2

T_0 = 66805 gas $AB^{1,2}$ $3d^2A_1'$-$\tilde{X}$ 147-150 nm

Ar AB^3 $3d^2A_1'$-$\tilde{X}$ ~150.3 nm

First member of Rydberg series converging to 79392(5). Higher members observed (AB^2) at 72326, 74851, 76256, 77090, and 77643.

B_0 = 10.72(8) AB^2

3d $^2E''$ D_{3h} Structure: AB^2

T_0 = 66536 gas $AB^{1,2}$MPI[10] $3d^2E''$-$\tilde{X}$ 144-150 nm

Ar AB^3 $3d^2E''$-$\tilde{X}$ ~150.3 nm

Diffuse. First member of Rydberg series converging to 79392(5). Higher members observed (AB^2) at 72165, 74851, 76256, 77090, and 77643.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	1372[b]	gas	AB,MPI	2,10

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

T_0 = 59972 gas MPI[12]

Higher member of Rydberg series observed (MPI[12]) at 69837.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	CH stretch	2914	gas	MPI	12
a_2''	2	OPLA	1334	gas	MPI	12

3s $^2A_1'$ D_{3h} Structure: AB^2

T_0 = 46205 gas $AB^{1,2,7}$ $3s^2A_1'$-$\tilde{X}$ 216 nm

Diffuse. First member of Rydberg series converging to 79392(5). Next member observed (AB^2) at 71042.

$\tilde{X}\ ^2A_2''$ D_{3h} Structure: AB^2IR^9

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	CH stretch	3004.8	gas	CARS	13
a_2''	2	OPLA	606.453	gas	IR,DL	5,9
			617	Ne	IR	4
			603[c]	Ar	IR	3,8
			611	N_2	IR	3
e'	3	CH stretch	3160.821	gas	LD	11
			3162	Ne	IR	4
			3150	Ar	IR	6
e'	4	Deformation	1396	Ne	IR	4
			1398[d]	Ar	IR	8

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

CD_3

4f $^2E'$[a] D_{3h}

T_0 = 72431 gas MPI[12]

Higher member of Rydberg series observed (MPI[12]) at 74885.

3d $^2A_1'$ D_{3h} Structure: AB^2

T_0 = 66715 gas AB[1,2] $3d^2A_1'$-$\tilde{X}$ 145-150 nm

Ar AB[3] $3d^2A_1'$-$\tilde{X}$ ~150.3 nm

First member of Rydberg series converging to 79315(5). Higher members observed (AB^2) at 72296, 74781, 76181, 77023, 77562, and 77933.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	1040[b]	gas	AB	2

B_0 = 5.14 AB^2

3d $^2E''$ D_{3h} Structure: AB^2

T_0 = 66465 gas AB[1,2] MPI[10] $3d^2E''$-$\tilde{X}$ 146-150 nm

Ar AB[3] $3d^2E''$-$\tilde{X}$ ~150.3 nm

Diffuse. First member of Rydberg series converging to 79315(5). Higher members observed (AB^2) at 72180, 74753, 76166, 77023, 77562, and 77933.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	1031[b]	gas	AB,MPI	2,10

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

T_0 = 59886 gas MPI[12]

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
a_2''	2	OPLA	1032	gas	MPI	12

B_0 = 4.76(2) MPI[12]

3s $^2A_1'$ D_{3h} Structure: AB^2

T_0 = 46629 gas AB[1,2,7] $3s^2A_1'$-$\tilde{X}$ 204-225 nm

First member of Rydberg series converging to 79315(5). Higher members observed (AB^2) at 70910, 74246, 75869, and 76830.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	CD stretch	1684[e]	gas	AB	7
a_2''	2	OPLA	1090[b]	gas	AB	7

B_0 = 4.42 AB^2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	CD stretch	2136	gas	UV	7
a_2''	2	OPLA	457.81	gas	DL	14
			463	Ne	IR	4
			453[c]	Ar	IR	3,8
			463	N_2	IR	3
e'	3	CD stretch	2381	Ne	IR	4
			2369	Ar	IR	6
	4	Deformation	1026	Ne	IR	4
			1029	Ar	IR	6

B_0 = 4.802 AB^2 DL[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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SiH_3

$T_0 \leq 49229$ gas MPI[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	OPLA	∿800	gas	MPI	5

$\tilde{X}$ C_{3v} Structure: ESR[1,2] DL[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	"Umbrella"	727.94[a]	gas	DL	3
			721.05[b]	gas	DL	3

Barrier to inversion = 1900 ± 300 cm^{-1} gas PE[4]

B_0 = 4.763 DL[3]

SiD_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	"Umbrella"	560(100)	gas	PE	4

[a] $1^- - 0^+$ transition.
[b] $1^+ - 0^-$ transition.

References

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[5]R. D. Johnson, III, and J. W. Hudgens, Chem. Phys. Lett. 141, 163 (1987).

NH_3^+

$\tilde{A}\ ^2E$ D_{3h}

T_0 = 36590(100) gas PE[3,4]

Broad, partially resolved vibrational structure has been discussed[3] in terms of the expected Jahn-Teller distortion. Continuous background absorption may be associated with the formation of NH_2^+, for which the threshold is ∿44700,[1,3] or NH^+.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	NH stretch	∿2740	gas	PE	3
a_2''	2	OPLA	896(16)[a]	gas	PE	3
e'	3	NH stretch	3388.01[b]	gas	LD	5

B_0 = 10.645; $C'(1-\zeta_{33}) + 3\eta_k/2$ = 4.679 LD[5]

ND_3^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	725(25)	gas	PE	2

[a] Large negative anharmonicity.
[b] $\nu_3 - C'\zeta_{33} + 7\eta_k/4$.

References

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PH_3^+

$\tilde{A}\ ^2E$

$T_0 \leq$ 21800(120) gas PE[1]

As for NH_3^+, this band shows complicated, poorly resolved vibrational structure, expected to be associated with Jahn-Teller distortion of the molecule.

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2	2	"Umbrella"	694(80)[a]	gas	PE	1

Inversion barrier ~ 1290 [1]

[a] Higher levels are above the inversion barrier, ar have typical spacings near 500.[1] There is also some evidence for a weak $\nu_1 + 2\nu_2$ progression in the photoelectron spectrum.

References

[1]R. Maripuu, I. Reineck, H. Ågren, Wu Nian-Zu, Ji Ming Rong, H. Veenhuizen, S. H. Al-Shamma, L. Karlsson, and K. Siegbahn, Mol. Phys. 48, 1255 (1983).

AsH_3^+

$\tilde{A}\ ^2E$

T_o = 18000(300) gas PE[1]

As for NH_3^+, this band shows complicated, poorly resolved vibrational structure, expected to be associated with Jahn-Teller distortion of the molecule.

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2	2	OPLA[a]	452(25)	gas	PE	1

[a] Low inversion barrier. Observed vibrational structure is above this barrier.

References

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

SbH_3^+

$\tilde{A}\ ^2E$

T_o = 15170(240) gas PE_1

As for NH_3^+, this band shows complicated, poorly resolved vibrational structure, expected to be associated with Jahn-Teller distortion of the molecule.

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2	2	OPLA[a]	387(25)	gas	PE	1

[a] Low inversion barrier. Observed vibrational structure is above this barrier.

References

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

CH_3^-

Threshold for electron detachment from ground-state CH_3^- is 645(240).[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	"Umbrella"	460(40)	gas	PE	1

References

[1]G. B. Ellison, P. C. Engelking, and W. C. Lineberger, J. Amer. Chem. Soc. 100, 2556 (1978).

SiH_3^-

Threshold for electron detachment from ground-state SiH_3^- = 11340(110) gas PE[1]

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	"Umbrella"	880(120)	gas	PE	1

Barrier to inversion = 9000(2000) gas PE[1]

SiD_3^-

Threshold for electron detachment from ground-state SiD_3^- = 11180(180) gas PE[1]

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1 2	"Umbrella"	580(160)	gas	PE	1

References

[1]M. R. Nimlos and G. B. Ellison, J. Am. Chem. Soc. 108, 6522 (1986).

6.5. Four-Atomic Dihydrides

$CaNH_2$

$\tilde{C}\ ^2A_1$ C_{2v} Structure: LF^2

T_o[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_o = 15802(10) gas CL^1LF^3 $\tilde{B}$-$\tilde{X}$ 620-650 nm

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

T_o = 15605(10) gas CL^1LF^3 $\tilde{A}$-$\tilde{X}$ 620-650 nm

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

$\tilde{X}\ ^2A_1$ C_{2v} Structure: LF^2

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1 3	CaN stretch	524(10)	gas	LF	3

B^a = 0.301; C^a = 0.293 LF^2

[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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[3]A. M. R. P. Bopegedera, C. R. Brazier, and P. F. Bernath, J. Phys. Chem. 91, 2779 (1987).

$SrNH_2$

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

T_o = 15862(10) gas CL^1LF^2 $\tilde{C}$-$\tilde{X}$ 632 nm

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1 3	SrN stretch	458(10)	gas	LF	2

B̃ $^2B_1$ C_{2v}

T_o = 14724(10) gas CL[1]LF[2] B̃-X̃ 670-725 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	SrN stretch	∿450	gas	LF	2

Ã $^2B_2$ C_{2v}

T_o = 14274(10) gas CL[1]LF[2] Ã-X̃ 670-725 nm

X̃ $^2A_1$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	SrN stretch	459(10)	gas	LF	2

References

[1]R. F. Wormsbecher, M. Trkula, C. Martner, R. E. Penn, and D. O. Harris, J. Mol. Spectrosc. 97, 29 (1983).
[2]A. M. R. P. Bopegedera, C. R. Brazier, and P. F. Bernath, J. Phys. Chem. 91, 2779 (1987).

$BaNH_2$

D̃,Ẽ $^2B_1$, $^2B_2$[a]

gas CL[1] D̃,Ẽ-X̃ ∿530 nm

C̃ $^2A_1$[a]

gas CL[1] C̃-X̃ ∿765 nm

Ã,B̃ $^2B_1$, $^2B_2$[a]

gas CL[1] Ã,B̃-X̃ 835-950 nm

X̃ $^2A_1$[a]

[a] *Symmetries proposed by analogy to BaF.*

References

[1]R. F. Wormsbecher, M. Trkula, C. Martner, R. E. Penn, and D. O. Harris, J. Mol. Spectrosc. 97, 29 (1983).

$C_2H_2^+$

B̃ $^2\Sigma_u^+$ $D_{\infty h}$

T_o = 56380(80) gas PE[1,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	CC stretch	2500(20)	gas	PE	1,3
	2	CH stretch	1815(20)	gas	PE	1,3

τ < 14 fs[3]

Ã ^2A_g[a] C_{2h}

T_o = 39486(80) gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	CH stretch	2530(20)	gas	PE	3
	2	CC stretch	1730(20)	gas	PE	3
	3	Bend	492(12)	gas	PE	3
b_u	6	Bend	605(12)	gas	PE	3

Decays in less than one period of bending vibration, possibly into the vinylidene structure.[3]

X̃ $^2\Pi_u$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	2	CC stretch	1829(3)	gas	PE	1,3
Σ_u^+	3	CH a-stretch	3135.98	gas	LD	4
Π_g	4	Deform.	837(12)	gas	PE	3

A = -30.1(1.5) gas LD[4]

B_o = 1.105 LD[4]

$C_2D_2^+$

B̃ $^2\Sigma_u^+$ $D_{\infty h}$

T_o = 56655(80) gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	CC stretch	2275(20)	gas	PE	1,3
	2	CD stretch	1475(20)	gas	PE	1,3

$\tilde{A}\ ^2A_g$ C_{2h}

T_o = 39906(80) gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	CD stretch	2280(20)	gas	PE	3
	2	CC stretch	1450(20)	gas	PE	3
	3	Bend	339(12)	gas	PE	3
b_u	6	Bend	516(12)	gas	PE	3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	CD stretch	2572(16)	gas	PE	3
	2	CC stretch	1651(4)	gas	PE	1,3
Π_g	4	Bend	702(12)	gas	PE	3

[a] Threshold for formation of $HC_2^+ \leq 48000\ cm^{-1}$.[2,3]

References

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[3]J. E. Reutt, L. S. Wang, J. E. Pollard, D. J. Trevor, Y. T. Lee, and D. A. Shirley, J. Chem. Phys. 84, 3022 (1986).
[4]M. W. Crofton, M.-F. Jagod, B. D. Rehfuss, and T. Oka, J. Chem. Phys. 86, 3755 (1987).

HScOH

In an argon matrix,[1] photolyzes with 300-400 nm radiation, producing H_2 + ScO.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ScH stretch	1485.1	Ar	IR	1
		ScO stretch	715.8	Ar	IR	1

DScOD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ScD stretch	1070.0	Ar	IR	1
		ScO stretch	698.2	Ar	IR	1

References

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

HTiOH

In an argon matrix,[1] photolyzes with 400-500 nm radiation, producing H_2 + TiO.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		TiH stretch	1538.9	Ar	IR	1
		TiO stretch	699.7	Ar	IR	1

DTiOD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		TiD stretch	1107.7	Ar	IR	1
		TiO stretch	697.3	Ar	IR	1

References

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

HVOH

In an argon matrix,[1] photolyzes with radiation having a short wavelength cutoff of 400 nm.

$\tilde{X}$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	VH stretch	1583.0	Ar	IR	1
	VO stretch	703.3	Ar	IR	1
	Bend	414.5	Ar	IR	1

DVOD

$\tilde{X}$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	VD stretch	1140.3	Ar	IR	1
	VO stretch	696.6	Ar	IR	1

References

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

$H_2C{=}C$ (Vinylidene)

A transient absorption at 63873 and a structured transient absorption having its strongest member at 72795, formed in the vacuum ultraviolet flash photolysis of C_2H_2,[1], CH_2CO,[1] or C_2H_3Cl,[4] have been assigned[2] to transitions arising from the $\tilde{a}\ ^3B_2$ state of vinylidene.

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

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1 2	C=C stretch	1650(120)	gas	PE	3
3	CH_2 "scissors"	1120(100)	gas	PE	3

$D_2C{=}C$

A transient absorption at 64102 and a structured transient absorption having its strongest member at 72978, formed in the vacuum ultraviolet flash photolysis of C_2D_2,[1], CD_2CO,[1] or C_2D_3Cl,[5] have been assigned[2] to transitions arising from the $\tilde{a}\ ^3B_2$ state of vinylidene.

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

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1 2	C=C stretch	1610(120)	gas	PE	3
3	CD_2 "scissors"	840(100)	gas	PE	3

References

[1]A. H. Laufer, J. Chem. Phys. 73, 49 (1980).
[2]A. H. Laufer, Chem. Phys. Lett. 94, 240 (1983).
[3]S. M. Burnett, A. E. Stevens, C. S. Feigerle, and W. C. Lineberger, Chem. Phys. Lett. 100, 124 (1983).
[4]A. Fahr and A. H. Laufer, J. Phys. Chem. 89, 2906 (1985).
[5]A. Fahr and A. H. Laufer, J. Phys. Chem. 90, 5064 (1986).

H_2CSi

$^1B_2$ C_{2v}

T_o = 29312.883(4) gas AB[1] $^1B_2$-$\tilde{X}$ 310-340 nm

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1 2	CH_2 "scissors"	1101.96	gas	AB	1
3	CSi stretch	702.00	gas	AB	1

A_o = 8.537; B_o = 0.509; C_o = 0.479 AB[1]

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

A_o = 10.193; B_o = 0.553; C_o = 0.521 AB[1]

D_2CSi

$^1B_2$ C_{2v}

T_o = 29272 gas AB[1] $^1B_2$-$\tilde{X}$ 310-340 nm

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1 2	CD_2 "scissors"	829	gas	AB	1
3	CSi stretch	691	gas	AB	1

References

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HAlOH

Photolysis of HAlOH isolated in a Kr matrix with radiation having a 330 nm short wavelength cutoff leads to the formation of AlOH and, in the deuterium-substituted system, of some AlO.[2,3]

In a Kr matrix, very broad absorption between 400 and 630 nm, with maximum near 450 nm.[2,3]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3743	Ar	IR	1
		HAl stretch	1743.3	Ar	IR	1
		AlO stretch	817.9	Ar	IR	1
		HAlO bend	605.4	Ar	IR	1

DAlOD

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		DAl stretch	1280.9	Ar	IR	1
		AlO stretch	797.2	Ar	IR	1
		DAlO bend	473.6	Ar	IR	1

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H_2CN

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

T_o = 35620 gas AB[2,3,5] $\tilde{C}$-$\tilde{X}$ 280-285 nm

35436(25) Ar AB[6] $\tilde{C}$-$\tilde{X}$ 270-285 nm

Gas-phase absorption is diffuse.[5] Photolysis is observed in an argon matrix.[6]

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

T_o = 35075[a] gas AB[2,3,5] $\tilde{B}$-$\tilde{X}$ 280-285 nm

34990(25) Ar AB[6] $\tilde{B}$-$\tilde{X}$ 270-285 nm

All gas-phase bands are diffuse.[5] Photolysis is observed in an argon matrix.[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s-stretch	2774(50)[a]	Ar	AB	6
	2	CN stretch	1883(50)	Ar	AB	6
	3	CH_2 "scissors"	1413(50)	Ar	AB	6

$\tilde{X}\ ^2B_2$ C_{2v} Structure: ESR[1,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CN stretch	1725.4	Ar	IR	6
	3	CH_2 "scissors"	1336.6	Ar	IR	6
b_1	4	OPLA	954.1	Ar	IR	6
b_2	5	CH_2 a-stretch	3103.2	Ar	IR	6
	6	CH_2 rock	912.8	Ar	IR	6

D_2CN

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

T_o = 35481[a] gas AB[2,5] $\tilde{C}$-$\tilde{X}$ 271-285 nm

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

T_o = 35036[a] gas AB[2,5] $\tilde{B}$-$\tilde{X}$ 271-285 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CN stretch	1894[a]	gas	AB	2,5
	3	CD_2 "scissors"	1079[a]	gas	AB	2,5

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CD_2 "scissors"	1073.4	Ar	IR	6
b_1	4	OPLA	776	Ar	IR	6
b_2	5	CD_2 a-stretch	2427.5[a]	Ar	IR	6

[a] Tentative assignment.[6]

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H_2CO^+

C $^2B_2$[a] C_{2v}

T_0 = 43330(50) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1400(50)	gas	PE	1

B $^2A_1$[a] C_{2v}

T_0 = 40100(50) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CO stretch	1270(50)	gas	PE	1

A $^2B_1$ C_{2v}

T_0 = 25910(50) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1400(50)	gas	PE	1
			1210(50)	gas	PE	1

X $^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	2560(50)	gas	PE	1
	2	CO stretch	1590(50)	gas	PE	1
	3	CH_2 "scissors"	1210(50)	gas	PE	1

D_2CO^+

C $^2B_2$[a] C_{2v}

Transition origin not directly measured.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			~990	gas	PE	1

B $^2A_1$[a] C_{2v}

T_0 = 39870(50) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CO stretch	1270(50)	gas	PE	1
	3	CD_2 "scissors"	935(50)	gas	PE	1

A $^2B_1$ C_{2v}

T_0 = 25750(50) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1400(50)	gas	PE	1
			1210(50)	gas	PE	1

τ_0 = 64(22)μs gas PEPICO[3]

X $^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD stretch	1910(50)	gas	PE	1
	2	CO stretch	1560(50)	gas	PE	1
	3	CD_2 "scissors"	870(50)	gas	PE	1

[a] See Ref. 2 for discussion of assignment.

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H_2CS^+

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

$T^a \sim 84900$ gas PE[2]

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

$T^a = 46960(160)$ gas PE[2]

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

$T^a = 36060(160)$ gas PE[2]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		930(100)	gas	PE	2

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

$T^a = 19200(160)$ gas PE[1,2]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		840(100)	gas	PE	1,2

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

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CS stretch	935(100)	gas	PE	1,2

[a] Calculated from vertical ionization potential.

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H_2CSe^+

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

$T^a = 49620(320)$ gas PE[1]

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

$T^a = 34700(320)$ gas PE[1]

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

$T^a = 17350(320)$ gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	CSe stretch	~750	gas	PE	1

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

[a] From vertical ionization potentials.

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$t\text{-}N_2H_2^+$

$\tilde{C}\ ^2A_g$ C_{2h}

$T_o = 53250(160)$ gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g 3	NNH bend	940(30)	gas	PE	1

$\tilde{B}\ ^2B_u$ C_{2h}

$T_o = 41310(160)$ gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g 3	NNH bend	1170(30)	gas	PE	1

$\tilde{A}\ ^2A_u$ C_{2h}

$T_o = 36390(160)$ gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g 2	NN stretch	1110(30)	gas	PE	1

$\tilde{X}\ ^2A_g$ C_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2	NN stretch	∿1850	gas	PE	1
	3	NNH bend	1180(30)	gas	PE	1

t-$N_2D_2^+$

$\tilde{B}\ ^2B_u$ C_{2h}

T_o = 40990(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	3	NND bend	960(30)	gas	PE	1

$\tilde{A}\ ^2A_u$ C_{2h}

T_o = 36310(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2	NN stretch	1110(30)	gas	PE	1

$\tilde{X}\ ^2A_g$ C_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	3	NND bend	1020(30)	gas	PE	1

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H_2CS

$\tilde{E}\ 3p_z\ ^1B_2$ C_{2v}

T_o = 55096 gas AB[8,19] $\tilde{E}$-$\tilde{X}$ 181.5 nm

$\tilde{D}\ 3p_y\ ^1A_1$ C_{2v}

T_o = 53134 gas AB[8,19] $\tilde{D}$-$\tilde{X}$ 188.2 nm

$\tilde{C}\ 3s\ ^1B_2$ C_{2v} Structure: AB[19]

T_o = 47110.821(9) gas AB[1,8,15,19] $\tilde{C}$-$\tilde{X}$ 212.1 nm

A_o = 8.557; B_o = 0.603; C_o = 0.562 AB[19]

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

T_o = 45197 gas AB[8,18] $\tilde{B}$-$\tilde{X}$ 185-215 nm

All but the first absorption band show evidence for predissociation.[18]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CS stretch	476	gas	AB	18
b_1	4	OPLA	363[a]	gas	AB	18

$\tilde{A}\ ^1A_2$ C_{2v} Structure: AB[10,21]

T_o = 16394.475(9) gas AB[7,9,10] $\tilde{A}$-$\tilde{X}$ 440-610 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	3034(2)	gas	AB	9
	2	CH_2 "scissors"	1316(2)	gas	AB	9
	3	CS stretch	820(2)	gas	AB	7,9
b_1	4	OPLA	371.24	gas	AB	9
b_2	5	CH stretch	3081.3(5)	gas	AB	9
	6	CH_2 rock	799(2)	gas	AB	9

A_o = 9.446(2); B_o = 0.539; C_o = 0.509 AB[10]

τ_o = 140(3) μs gas LF[22,24]

$\tilde{a}\ ^3A_2$[c] C_{2v} Structure: AB[11,21]

T_o = 14507.38 gas AB[7,11]LF[20]CL[25] $\tilde{a}$-$\tilde{X}$ 610-800 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_2 "scissors"	1320	gas	AB	11
	3	CS stretch	861.6	gas	AB,LF	11,23
b_1	4	OPLA	312(30)	gas	LF,CL	20,21, 25
b_2	6	CH_2 rock	762.3	gas	LF	23

A_o = 9.383; B_o = 0.552; C_o = 0.521 AB[11]

τ > 1.5 ms gas LF[22,24]

$\tilde{X}\ ^1A_1$ C_{2v} Structure: MW[2,4,5] IR[3,14]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	2971.03	gas	IR	3,14
			2970	Ar	IR	6,17
			2973	N_2	IR	6
	2	CH_2 "scissors"	1457.3	gas	LF	13
			1447.0	gas	IR	14
			1447	Ar	IR	17
	3	CS stretch	1059.20	gas	LS,IR	12,14
			1063	Ar	IR	6,17
			1062	N_2	IR	6
b_1	4	OPLA	990.19	gas	LS,IR	12,14
			993	Ar	IR	6,17
			995	N_2	IR	6
b_2	5	CH stretch	3024.61	gas	IR	3,14
	6	CH_2 rock	991.01	gas	LS,IR	12,14
			988	Ar	IR	6,17

A_o = 9.729; B_o = 0.590; C_o = 0.555 MW[2,4,5] AB[10]

D_2CS

$\tilde{C}$ 3s $^1B_2$ C_{2v}

T_o = 47325.563(4) gas AB[8,19] $\tilde{C}$-$\tilde{X}$ 211.2 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD stretch	1783	gas	AB	8,19
	2	CD_2 "scissors"	746	gas	AB	19

A_o = 4.350; B_o = 0.510; C_o = 0.456 AB[19]

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

$T_o \sim$ 45200 gas AB[18] $\tilde{B}$-$\tilde{X}$ 185-215 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CS stretch	467	gas	AB	18
b_1	4	OPLA	263[a]	gas	AB	18

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

T_o = 16483.502(8) gas AB[7,9,10] $\tilde{A}$-$\tilde{X}$ 440-610 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD stretch	2139(2)	gas	AB	9
	2	CD_2 "scissors"	1013(2)	gas	AB	9
	3	CS stretch	771.3(5)	gas	AB	7,9
b_1	4	OPLA	275.33	gas	AB	9
b_2	5	CD stretch	2324.85	gas	AB	9
	6	CD_2 rock	599(2)	gas	AB	9

A_o = 4.736; B_o = 0.458; C_o = 0.417 AB[10]

τ_o = 182 μs gas LF[24]

$\tilde{a}\ ^3A_2$[c] C_{2v} Structure: AB[21]

T_o = 14613.54 gas AB[7,11] CL[25] $\tilde{a}$-$\tilde{X}$ 610-800 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_2 "scissors"	1012	gas	AB	11
	3	CS stretch	798	gas	AB	7,11
b_1	4	OPLA	223(30)	gas	AB,CL	21,25

A_o = 4.716; B_o = 0.469; C_o = 0.426 AB[11]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD stretch	2158.5	gas	IR	14
			2155	Ar	IR	17
	2	CD_2 "scissors"	1171.8	gas	IR	14
			1167	N_2	IR	17
	3	CS stretch	936.13	gas	IR,LS	14,16
			941	Ar	IR	6,17
			939	N_2	IR	6
b_1	4	OPLA	781.2	gas	IR	14
			783	Ar	IR	6,17
			784	N_2	IR	6
b_2	6	CD_2 rock	757.4	gas	IR	14

A_o = 4.883; B_o = 0.497; C_o = 0.450 MW[2] AB[10] LF[26]

[a] $\frac{1}{2}(2\nu_4)$.
[b] Barrier to inversion ∿ 50.[18]
[c] Barrier to inversion ∿ 7.[21]

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H_2CSe

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

T_o = 13635 gas LF[4] $\tilde{A}$-$\tilde{X}$ 695-735 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	C=Se stretch	700	gas	LF	4
b_1	4	OPLA	∿315	gas	LF	4

$\tilde{a}\ ^3A_2$ C_{2v}

T_o = 12169 gas $AB^1CL^3LF^4$ $\tilde{a}$-$\tilde{X}$ 700-822 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_2 "scissors"	1311	gas	LF	4
	3	C=Se stretch	707	gas	AB,CL LF	1,3,4
b_1	4	OPLA	344[a]	gas	AB,LF	1,4
b_2	6	HCSe bend	812[a]	gas	LF	4

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

A_o = 9.83(6); B_o = 0.414; C_o = 0.396 MW^2

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

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$t\text{-}N_2H_2$

$\tilde{C}\ ^1B_u$[a] C_{2h}

T_o = 67894 gas AB[9] $\tilde{C}$-$\tilde{X}$ 135-147 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2	Bend	1180	gas	AB	9
	3	NN stretch	1849	gas	AB	9

$\tilde{B}\ ^1B_u$ C_{2h} Structure: AB^9

T_o = 57926.5 gas AB[2,9] $\tilde{B}$-$\tilde{X}$ 150-175 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	NH stretch	3092	gas	AB	9
	2	Bend	1180	gas	AB	2,9
	3	NN stretch	1875	gas	AB	2,9

A_o = 15.63; B_o = 1.32; C_o = 1.22 AB[9]

$\tilde{A}\ ^1B_g$ C_{2h}

T_0^c = 23896 gas AB[4,5,8] $\tilde{A}$-$\tilde{X}$ 300-440 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2	Bend	1215(15)	gas	AB	5
	3	NN stretch	1550(20)	gas	AB	5

$\tilde{X}\ ^1A_g$ C_{2h} Structure: IR[2,6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	NH stretch	3128	N_2	Ra	3
	2	NH bend	1583	N_2	Ra	3
	3	N=N stretch	1529	N_2	Ra	3
a_u	4	Torsion	1288.64	gas	IR	10
			1283	Ar	IR	7
			1286	N_2	IR,Ra	1,3,7
b_u	5	NH stretch	3120.28	gas	IR	2,6,10
			3118	Ar	IR	7
			3137	N_2	IR	7
	6	NH bend	1316.41	gas	IR	10
			1313	Ar	IR	7
			1321	N_2	IR	3,7

A_o = 10.000; B_o = 1.304; C_o = 1.150 IR[6,10]

$t\text{-}N_2D_2$

$\tilde{B}\ ^1B_u$ C_{2h}

$T_o \sim 58086^d$ gas AB[2] $\tilde{B}$-$\tilde{X}$ 159-172 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2	Bend	950	gas	AB	2

$\tilde{A}\ ^1B_g$ C_{2h}

gas AB[5] $\tilde{A}$-$\tilde{X}$ 320-430 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2	Bend	910(10)	gas	AB	5
	3	NN stretch	1440(20)	gas	AB	5

$\tilde{X}\ ^1A_g$ C_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2	ND bend	1215	N_2	Ra	3
	3	N=N stretch	1539	N_2	Ra	3
a_u	4	Torsion	946	N_2	IR	1,3,7
b_u	5	ND stretch	2315	gas	IR	6
			2308	N_2	IR	7
	6	ND bend	972	N_2	IR	7

A_o = 6.025; B_o = 1.089; C_o = 0.920 IR[6]

[a] $4p\pi$ Rydberg transition.
[b] $3p\pi$ Rydberg transition.
[c] 5_0^1 vibronic band origin.[8]
[d] 1-0 subband origin.

References

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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]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2865	Ar	IR	1
			2808	Ar	IR	1
			1863[a]	Ar	IR	1
		N=N stretch	1574	Ar	IR	1
			1003	Ar	IR	1

D_2NN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2109	Ar	IR	1
		N=N stretch	1599 1571	Ar	IR	1
			1195	Ar	IR	1
			913	Ar	IR	1
			900	Ar	IR	1
			794	Ar	IR	1

[a] May possibly be contributed by HCO.

References

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H_2CF

5p Rydberg state C_{2v}

T_o = 67265(10) gas MPI[8]

4p Rydberg state C_{2v}

T_o = 63275(10) gas MPI[8] 4p-$\tilde{X}$ 147-158 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF stretch	1580(20)	gas	MPI	8
	3	CH_2 "scissors"	1443(20)	gas	MPI	8
b_1	4	OPLA	1259(20)	gas	MPI	8

3p Rydberg state C_{2v}

T_o = 52863(10) gas MPI[8] 3p-$\tilde{X}$ 167-193 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF stretch	1575(20)	gas	MPI	8
	3	CH_2 "scissors"	1420(20)	gas	MPI	8
b_1	4	OPLA	1223(20)	gas	MPI	8

Threshold for photodecomposition, producing CF, observed[5] near 280 nm in an argon matrix.

$\tilde{X}\ ^2B_1$ C_{2v} Structure: ESR[1]MW[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CF stretch	1170.42	gas	DL	7
			1163	Ar	IR	2,3,5
b_1	4	OPLA	300(30) 260(30)	gas gas	MW MPI	6 8

A_o = 8.846; B_o = 1.032; C_o = 0.925 LMR[4]MW[6]

D_2CF

5p Rydberg state C_{2v}

T_o = 67186(10) gas MPI[8]

4p Rydberg state C_{2v}

T_o = 63195(10) gas MPI[8] 4p-$\tilde{X}$ 154-159 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_2 s-stretch	2190(20)	gas	MPI	8
	2	CF stretch	1513(20)	gas	MPI	8
	3	CD_2 "scissors"	1076(20)	gas	MPI	8
b_1	4	OPLA	1004(20)	gas	MPI	8

3p Rydberg state C_{2v}

T_o = 52786(10) gas MPI[8] 3p-$\tilde{X}$ 167-193 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_2 s-stretch	2176(20)	gas	MPI	8
	2	CF stretch	1504(20)	gas	MPI	8
	3	CD_2 "scissors"	1080(20)	gas	MPI	8
b_1	4	OPLA	976(10)	gas	MPI	8

X $^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF stretch	1191	Ar	IR	2,3,5
	3	CD_2 "scissors"	1013	Ar	IR	5
b_2	4	OPLA	170(30)	gas	MPI	8

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H_2NCl^+

D $^2A''$ C_s

T^a = 61720(560) gas PE[1,2]

C $^2A'$ C_s

T^a = 47360(560) gas PE[1,2]

B $^2A'$ C_s

T_o = 26630(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	4	NCl stretch	450(40)	gas	PE	1,2

A $^2A''$ C_s

T_o = 16700(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH stretch	3040(40)	gas	PE	2
			970(40)	gas	PE	2
			580(40)	gas	PE	1,2

X $^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			760(40)	gas	PE	2

[a] From vertical ionization potential.

References

[1] M. K. Livett, E. Nagy-Felsobuki, J. B. Peel, and G. D. Willett, Inorg. Chem. 17, 1608 (1978).
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H_2NBr^+

C $^2A'$ C_s

T^a = 42600(900) gas PE[1,2]

B $^2A'$ C_s

T^a = 23960(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		NBr stretch	370(60)	gas	PE	1

A $^2A''$ C_s

T^a = 11860(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			840(50)	gas	PE	2

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

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		650(50)	gas	PE	1,2

[a] From vertical ionization potential.

References

[1] E. Nagy-Felsobuki, J. B. Peel, and G. D. Willett, J. Electron Spectrosc. Relat. Phenom. 13, 17 (1978).
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$H_2O_2^+$

$\tilde{C},\tilde{D}\ ^2A,^2B$ C_2

T^a = 55190(320) gas PE[1,2]

$\tilde{B}\ ^2A$ C_2

T^a = 38400(400) gas PE[1,2]

$\tilde{A}\ ^2A$ C_2

T^a = 16800(500) gas PE[1,2]

$\tilde{X}\ ^2B$ C_2

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	Deformation	1080(50)	gas	PE	2

[a] From vertical ionization potential. The first ionization potential of H_2O_2 is taken to equal 10.54 eV, as in Ref. 2.

References

[1] K. Osafune and K. Kimura, Chem. Phys. Lett. 25, 47 (1974).
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$H_2S_2^+$

$\tilde{D}\ ^2A$ C_2

T^a = 46700(1200) gas PE[3]

$\tilde{C}\ ^2B$ C_2

T^a = 37200(400) gas PE[3]

$\tilde{B}\ ^2A$ C_2

T^a = 25900(400) gas PE[3]

$\tilde{A}\ ^2B$ C_2

T^a = 7020(400) gas PE[1-3]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a 3	S-S stretch	500(30)	gas	PE	2

$\tilde{X}\ ^2A$ C_2

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a 3	S-S stretch	480(30)	gas	PE	2

[a] From vertical ionization potential.

References

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6.6. Four-Atomic Monohydrides

CaCCH

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

T_0 = 15521.55 gas LF[1,2] $\tilde{A}$-$\tilde{X}$ 640-665 nm

A = 70.466 gas LF[1,2]

B_0 = 0.118 LF[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	CaC stretch	399(10)	gas	LF	1
Π	5	CaCC bend	91(5)[a]	gas	LF	1

B_0 = 0.116 LF[2]

[a] $\frac{1}{2}(2\nu_5)$.

References

[1]A. M. R. P. Bopegedera, C. R. Brazier, and P. F. Bernath, Chem. Phys. Lett. 136, 97 (1987).
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SrCCH

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

T_0 = 14176(10) gas LF[1] $\tilde{A}$-$\tilde{X}$ 685-725 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	SrC stretch	354(10)	gas	LF	1

A = 275(10) gas LF[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	SrC stretch	343(10)	gas	LF	1
Π	5	SrCC bend	70(5)[a]	gas	LF	1

[a] $\frac{1}{2}(2\nu_5)$.

References

[1]A. M. R. P. Bopegedera, C. R. Brazier, and P. F. Bernath, Chem. Phys. Lett. 136, 97 (1987).

HCCN

$^3\Sigma^-$?

In the gas phase, a prominent absorption band system beginning at 340 nm has been attributed[2,3] to HCCN, but has not been analyzed. An absorption band system assigned to HCCN was observed in an argon matrix between 240 and 340 nm, with band separations of approximately 1050.[4]

$\tilde{X}\ ^3\Sigma^-$ $C_{\infty v}$ Structure: ESR[1]MW[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3229	Ar	IR	4
	2	CCN a-stretch	1735	Ar	IR	4
	3	CCN s-stretch	1178	Ar	IR	4
Π	4	H deform.	458	Ar	IR	4

B_0 = 0.366 MW[5]

DCCN

$\tilde{X}\ ^3\Sigma^-$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2424	Ar	IR	4
	2	CCN a-stretch	1730	Ar	IR	4
	3	CCN s-stretch	1127	Ar	IR	4
Π	4	CCN bend	405	Ar	IR	4
	5	D deform.	318	Ar	IR	4

References

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[2]A. J. Merer and D. N. Travis, Can. J. Phys. 43, 1795 (1965).
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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.

Laser-excited fluorescence studies of the ^{16}O or ^{18}O + C_2H_2 and F + H_2CCO reaction systems[2] and of their fully deuterium-substituted counterparts have demonstrated prominent HCCO emission bands in the 360-500 nm spectral region. Although several of the absorption bands coincide with peaks of the excitation spectrum, the assignment of bands to the two transitions differs. The lifetime for the 353.6 nm band origin was 149(4) ns, with much shorter lifetimes for the higher frequency peaks. The lifetime for the 352.6 nm DCCO band origin was 3.13 μs. Excited-state band separations associated with the 353.6 nm band system of HCCO (DCCO) were 2868, 1183, and 866 (2075, 1167, and 607). The most prominent absorption, at 366.7 nm, appeared only weakly in the excitation spectrum, but the structure of the fluorescence associated with it was similar to that for the 352.6 nm band. Intensity arguments excluded vibrational relaxation in the excited state as an explanation for this phenomenon. The existence of cis and trans rotamers in the lower state, for which band separations of 2373, 1805, and ∿150 (1955, 1751) were observed, was suggested.

Analysis of the submillimeter-wave spectrum[3] 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.

X C_s Structure: MW[3]

A_0 = 41.5(1.5); B_0 = 0.363; C_0 = 0.359 MW[3]

DCCO

X C_s

A_0 = 21.75(12); B_0 = 0.331; C_0 = 0.325 MW[3]

References

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HCCS

Ã $^2\Pi$ $C_{\infty v}$

T_0 = 24299.690(6) gas AB[1,2]EM[3] Ã-X̃ 377-452 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	CC stretch	1843[a]	gas	AB	2
	3	CS stretch	740	gas	AB	1,2
Π	5	CCS bend	328[b]	gas	AB,EM	2,3

B_0 = 0.174 AB^2

X̃ $^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	CC stretch	2189[a]	gas	EM	3
	3	CS stretch	782	gas	EM	3
Π	5	CCS bend	411[b]	gas	EM	3

B_0 = 0.188 AB^2

DCCS

Ã $^2\Pi$ $C_{\infty v}$

T_0 ≈ 24359 gas AB^2 Ã-X̃ 376-420 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	CC stretch	1718[a]	gas	AB	2
	3	CS stretch	725	gas	AB	2

[a] Tentative assignment, suggested by Ref. 3.
[b] $\frac{1}{2}(2\nu_5)$.

References

[1] S. L. N. G. Krishnamachari and T. V. Venkitachalam, Chem. Phys. Lett. 55, 116 (1978).
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HSCC

T_0 = 27475.5 gas AB^1 330-380 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		HSC bend	1062	gas	AB	1
		C-S stretch	746	gas	AB	1
			290	gas	AB	1

X̃ ?

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

DSCC

T_0 = 27501.1 gas AB[1] 330-380 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		DSC bend	854	gas	AB	1
		C-S stretch	650	gas	AB	1

A_0 = 2.258; B_0 = 0.225; C_0 = 0.192 AB[1]

X ?

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

A_0 = 2.936; B_0 = 0.232; C_0 = 0.215 AB[1]

References

[1]S. L. N. G. Krishnamachari and R. Venkatasubramanian, Indian J. Phys. 60B, 37 (1986).

$HCCF^+$

C $^2\Sigma$ $C_{\infty v}$

T^a = 80200(1000) gas PE[2]

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

$T^a \sim$ 54400 gas PE[1,2]

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

T^a = 52800(1000) gas PE[1,2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	C≡C stretch	2180(80)	gas	PE	1
	3	CF stretch	1210(80)	gas	PE	1

[a] From vertical ionization potential.

References

[1]H. J. Haink, E. Heilbronner, V. Hornung, and E. Kloster-Jensen, Helv. Chim. Acta 53, 1073 (1970).
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$HC{\equiv}CCl^+$ [a]

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

T_0 = 27021.3 gas $PE^1EF^{3,4}LF^5$ Ã-X̃ 331-470 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3249.4(2)	gas	LF	5
	2	C≡C stretch	2063.8(2)	gas	LF	5
	3	CCl stretch	595.7(3)	gas	EF,LF	3-5
Π	5	CCCl bend	224	gas	EF	3

τ_1 = 17(3) ns gas EF[1]; ≤25 ns gas PIFCO[2]

τ_2 = 430(90) ns gas EF[1]; 450(45) ns gas PIFCO[2]

A = -400(160) gas PE[1]

B_0 = 0.171 LF[5]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3146[b]	gas	EF	3
	2	C≡C stretch	1984.5(3)	gas	EF	3,4
	3	CCl stretch	836.8(3)	gas	EF	3,4
Π	4	HCC bend	595[b]	gas	EF	3
	5	CCCl bend	235[b]	gas	EF	3

A $\sim$ -150 gas PE[1]

B_0 = 0.195 LF[5]

$DC{\equiv}CCl^+$ [a]

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

T_0 = 26997.5 gas $EF^{3,4}LF^5$ Ã-X̃ 328-488 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2561.5(2)	gas	LF	5
	2	C≡C stretch	1919.7(2)	gas	LF	5
	3	CCl stretch	587.2(3)	gas	EF,LF	3-5
Π	5	CCCl bend	216	gas	EF	3

τ_1 = 17(3) ns gas EF[2]; ≤30 ns gas PIFCO[2]

τ_2 = 430(90) ns gas EF[2]; 500(50) ns gas PIFCO[2]

B_0 = 0.156 LF[5]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2475[b]	gas	EF	3
	2	C≡C stretch	1882.0(3)	gas	EF	3,4
	3	CCl stretch	817.0(3)	gas	EF	3,4
Π	4	DCC bend	476	gas	EF	3

B_0 = 0.177 LF[5]

a ^{35}Cl.
b Tentative assignment.

References

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$HC{\equiv}CBr^+$ a

$\tilde{A}\ ^2\Pi_{3/2}$ $C_{\infty v}$ Structure: LF^3

T_0 = 20550.82(4) gas $PE^1LF^{2,3}EF^4$ $\tilde{A}$-$\tilde{X}$ 416-613 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	C≡C stretch	2051(3)	gas	LF	2
	3	CBr stretch	492(2)	gas	LF,EF	2,4
Π	4	CCH bend	629(3)	gas	LF	2
	5	CCBr bend	207(3)	gas	LF	2

τ_1 = 12(2) ns gas EF^1

τ_2 = 270(54) ns gas EF^1

A = -1610(160) gas PE^1

B_0 = 0.121 LF^3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3280(2)	gas	EF	4
	2	C≡C stretch	1931(2)	gas	EF	4
	3	CBr stretch	673(2)	gas	LF,EF	2,4
Π	4	CCH bend	618(10)	gas	EF	4
	5	CCBr bend	273(10)[b]	gas	EF	4

A = -1000(160) gas PE^1

B_0 = 0.138 LF^3

$DC{\equiv}CBr^+$ a

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

T_0 = 20546.43(4) gas $LF^{2,3}EF^4$ $\tilde{A}$-$\tilde{X}$ 416-604 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2548(3)	gas	LF	2
	2	C≡C stretch	1939(3)	gas	LF	2
	3	CBr stretch	484(2)	gas	LF,EF	2,4
Π	4	CCD bend	488(3)	gas	LF	2
	5	CCBr bend	200(3)	gas	LF	2

B_0 = 0.111 LF^3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2482(2)	gas	EF	4
	2	C≡C stretch	1866(2)	gas	EF	4
	3	CBr stretch	658(2)	gas	EF	4
Π	4	CCD bend	544(10)	gas	EF	4
	5	CCBr bend	258(10)[b]	gas	EF	4

B_0 = 0.126 LF^3

a ^{79}Br.
b $\frac{1}{2}(2\nu_5)$.

References

[1]M. Allan, E. Kloster-Jensen, and J. P. Maier, J. Chem. Soc., Faraday Trans. 2 73, 1406 (1977).
[2]J. P. Maier and L. Misev, J. Chem. Soc., Faraday Trans. 2, 80, 43 (1984).
[3]M. A. King, J. P. Maier, L. Misev, and M. Ochsner, Can. J. Phys. 62, 1437 (1984).
[4]J. Fulara, D. Klapstein, R. Kuhn, and J. P. Maier, J. Phys. Chem. 90, 2061 (1986).

$HC{\equiv}CI^+$

Ã $^2\Pi_{3/2}$ $C_{\infty v}$ Structure: LF^2

T_0 = 17373.94(3) gas $PE^1LF^2EF^3$ Ã-X̃ 521-750 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	C≡C stretch	1822(2)[a]	gas	LF	2
	3	CI stretch	407(2)	gas	LF,EF	2,3
Π	4	HCC bend	612(2)[ab]	gas	LF	2
	5	CCI bend	212	gas	EF	3

τ_1 = 18(4) ns gas EF^1

τ_2 = 500(100) ns gas EF^1

A = -2020(160) gas PE^1

B_0 = 0.097 LF^2

X̃ $^2\Pi_{3/2}$ $C_{\infty v}$ Structure: LF^2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3258(2)	gas	EF	3
	2	C≡C stretch	1805(10)	gas	EF	3
	3	CI stretch	578(2)	gas	EF	3
Π	4	HCC bend	542(10)[b]	gas	EF	3
	5	CCI bend	237(2)	gas	EF	3

A = -3230(160) gas PE^1

B_0 = 0.110 LF^2

$DC{\equiv}CI^+$

Ã $^2\Pi_{3/2}$ $C_{\infty v}$

T_0 = 17388.07(3) gas LF^2 Ã-X̃ 517-575 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	C≡C stretch	1792(2)[a]	gas	LF	2
	3	CI stretch	398(2)	gas	LF,EF	2,3
Π	4	DCC bend	480(2)[b]	gas	LF	2
	5	CCI bend	224(2)[b]	gas	LF,EF	2,3

B_0 = 0.089 LF^2

X̃ $^2\Pi_{3/2}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2618(2)	gas	EF	3
	2	C≡C stretch	1742(10)	gas	EF	3
	3	CI stretch	563(2)	gas	EF	3
Π	5	CCI bend	223(2)	gas	EF	3

B_0 = 0.100 LF^2

[a] Tentative value.
[b] $\frac{1}{2}(2\nu_5)$.

References

[1]M. Allan, E. Kloster-Jensen, and J. P. Maier, J. Chem. Soc., Faraday Trans. 2 73, 1406 (1977).
[2]J. P. Maier and M. Ochsner, J. Chem. Soc., Faraday Trans. 2 81, 1587 (1985).
[3]J. Fulara, D. Klapstein, R. Kuhn, and J. P. Maier, J. Phys. Chem. 90, 2061 (1986).

HNCN

B̃ ?

T_0 = 30500 gas $AB^{2,3}$ B̃-X̃ 289-328 nm

This band system, contributed by a hydrogen-containing species, appears under the same conditions as the Ã-X̃ band of HNCN.[2,3] Its assignment to HNCN is tentative.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1048	gas	AB	3

Ã $^2A'$ C_s Structure: AB^1

T_0 = 28994.1 gas AB^1 Ã-X̃ 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_o = 21.220; B_o = 0.370; C_o = 0.362 AB[1]

References

[1]G. Herzberg and P. A. Warsop, Can. J. Phys. 41, 286 (1963).
[2]N. Basco and K. K. Yee, Chem. Commun. 150 (1968).
[3]H. W. Kroto, T. F. Morgan, and H. H. Sheena, Trans. Faraday Soc. 66, 2237 (1970).

HPCN

By analogy with HNCN, weak, diffuse absorption bands between 314 and 338 nm produced in the flash photolysis of PH_3-C_2N_2-N_2 mixtures have been tentatively assigned to HPCN.[1]

References

[1]N. Basco and K. K. Yee, Chem. Commun. 152 (1968).

$HNCO^+$

$\tilde{D}\ ^2\Sigma$ $C_{\infty v}$?

T^a = 61480(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1000(50)	gas	PE	1

$\tilde{C}\ ^2\Sigma$ $C_{\infty v}$?

T^a = 47440(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			460(50)	gas	PE	1

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

T^a = 33730(1000) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NCO s-stretch	1120(50)	gas	PE	1

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

T^a = 5490(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		NH deform.	610(50)	gas	PE	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	NCO a-stretch	1980(50)	gas	PE	1
	3	NCO s-stretch	1080(50)	gas	PE	1

$DNCO^+$

$\tilde{D}\ ^2\Sigma$ $C_{\infty v}$?

T^a = 61480(320) gas PE[1]

$\tilde{C}\ ^2\Sigma$ $C_{\infty v}$?

T^a = 47440(320) gas PE[1]

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

T^a = 33730(1000) gas PE[1]

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

T^a = 5490(320) gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	NCO a-stretch	2070(50)	gas	PE	1

[a] From vertical ionization potentials.

References

[1]S. Cradock, E. A. V. Ebsworth, and J. D. Murdoch, J. Chem. Soc., Faraday Trans. 2 68, 86 (1972).

$HNCS^+$

$\tilde{C}\ ^2\Sigma$ $C_{\infty v}$?

T^a = 41790(320) gas PE[1]

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

T^a = 27190(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		NCS s-stretch	850(50)	gas	PE	1

A $^2A'$ C_s

T^a = 2900(1000) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		NH deform.	600(50)	gas	PE	1

X $^2A''$ C_s

[a] From vertical ionization potentials.

References

[1]S. Cradock, E. A. V. Ebsworth, and J. D. Murdoch, J. Chem. Soc., Faraday Trans. 2 68, 86 (1972).

$HCNO^+$

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

T_o = 66720(1000) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3000(80)	gas	PE	1

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

T_o = 56160(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	CNO a-stretch	2420(80)	gas	PE	1
	3	CNO s-stretch	1070(80)	gas	PE	1

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

T_o = 36070(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	CNO s-stretch	~1100	gas	PE	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	CNO a-stretch	1700(80)	gas	PE	1
	3	CNO s-stretch	1290(80)	gas	PE	1

References

[1]J. Bastide and J. P. Maier, Chem. Phys. 12, 177 (1976).

HN_3^+

E $^2A'$ C_s

T^a = 87620(1000) gas PE[3]

D $^2A''$ C_s

T^a = 77130(1000) gas PE[2,3]

C $^2A'$ C_s

T^a = 48890(320) gas PE[1-3]

B $^2A'$ C_s

T_o = 38000(320) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	N_3 a-stretch	2380(80)	gas	PE	1-3
	4	N_3 s-stretch	930(80)	gas	PE	1-3
	5	N_3 deform.	570(80)	gas	PE	1-3

Ã $^2A'$ C_s

T_0 = 7750(320) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	5	N_3 deform.	∿480	gas	PE	1-3

X̃ $^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	N_3 a-stretch	1850(80)	gas	PE	1,3
	4	N_3 s-stretch	850(80)	gas	PE	1,3

DN_3

Ẽ $^2A'$ C_s

T^a = 87620(1000) gas PE[3]

D̃ $^2A''$ C_s

T^a = 77130(1000) gas PE[1,3]

C̃ $^2A'$ C_s

T^a = 48890(320) gas PE[1,3]

B̃ $^2A'$ C_s

T_0 = 38000(320) gas PE[1,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	N_3 a-stretch	2300(80)	gas	PE	1,3
	4	N_3 s-stretch	900(80)	gas	PE	1,3
	5	N_3 deform.	490(80)	gas	PE	1,3

Ã $^2A'$ C_s

T_0 = 7750(320) gas PE[1,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	5	N_3 deform.	∿400	gas	PE	3

X̃ $^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	N_3 a-stretch	1850(80)	gas	PE	1,3
	4	N_3 s-stretch	850(80)	gas	PE	1,3

[a] From vertical ionization potential.

References

[1]S. Cradock, E. A. V. Ebsworth, and J. D. Murdoch, J. Chem. Soc., Faraday Trans. 2 68, 86 (1972).
[2]T. H. Lee, R. J. Colton, M. G. White, and J. W. Rabalais, J. Am. Chem. Soc. 97, 4845 (1975).
[3]J. Bastide and J. P. Maier, Chem. Phys. 12, 177 (1976).

HBF_2^+

F̃ $^2A_1$ C_{2v}

T_0 = 57000(500) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	BF stretch	1010(40)	gas	PE	1

Ẽ $^2A_1$ C_{2v}

T^a = 43000(800) gas PE[1]

D̃ $^2B_2$ C_{2v}

T_0 = 36800(560) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	BF stretch	1025(40)	gas	PE	1

C̃ $^2B_1$ C_{2v}

T_0 = 32280(500) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	BF stretch	950(40)	gas	PE	1

Ã,B̃ $^2B_2$,$^2A_2$ C_{2v}

T_o = 16140(1200) gas PE[1]

X̃ $^2A_1$[b] C_{2v}

[a] From vertical ionization potential.
[b] Possibly dissociative.

References

[1]D. P. Chong, C. Kirby, W. M. Lau, T. Minato, and N. P. C. Westwood, Chem. Phys. 59, 75 (1981).

HBCl$_2^+$

F̃ $^2A_1$ C_{2v}

T_o = 46800(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	BH stretch	2510(40)	gas	PE	1
	2	BCl stretch	670(60)	gas	PE	1

Ẽ $^2A_1$ C_{2v}

T_o = 27270(560) gas PE[1]

D̃ $^2B_2$ C_{2v}

T_o = 22110(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	BCl stretch	610(40)	gas	PE	1

C̃ $^2B_1$ C_{2v}

T_o = 13640(320) gas PE[1]

Ã,B̃ $^2A_1$,$^2A_2$ C_{2v}

T_o = 3550(320) gas PE[1]

X̃ $^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	BCl stretch	860(40)	gas	PE	1

References

[1]D. C. Frost, C. Kirby, C. A. McDowell, and N. P. C. Westwood, J. Am. Chem. Soc. 103, 4428 (1981).

HBBr$_2^+$

F̃ $^2A_1$ C_{2v}

T_o ∿ 50700 gas PE[1]

Ẽ $^2A_1$ C_{2v}

T_o = 27760(320) gas PE[1]

D̃ $^2B_2$ C_{2v}

T_o = 23160(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	BBr stretch	500(60)	gas	PE	1

C̃ $^2B_1$ C_{2v}

T_o = 13470(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	BBr stretch	430(60)	gas	PE	1

B̃ $^2A_2$ C_{2v}

T_o = 4030(320) gas PE[1]

Ã $^2A_1$ C_{2v}

T_o = 3230(320) gas PE[1]

X̃ $^2B_2$

References

[1]D. C. Frost, C. Kirby, C. A. McDowell, and N. P. C. Westwood, J. Am. Chem. Soc. 103, 4428 (1981).

HFCO$^+$

D̃ $^2A'$ C_s

T^a = 55100(1000) gas PE[1]

C̃ $^2A''$ C_s

T_o = 42760(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			800(50)	gas	PE	1
			580(50)	gas	PE	1

B $^2A'$ C_s

T^a = 24850(1000) gas PE[1]

A $^2A''$ C_s

T_o = 12830(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1290(50)	gas	PE	1

X $^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1450(50)	gas	PE	1
			1130(50)	gas	PE	1

[a] From vertical ionization potential.

References

[1]K. Wittel, J. Electron Spectrosc. Relat. Phenom. 8, 245 (1976).

$HCOCl^+$

E $^2A'$ C_s

T^a = 45900(1300) gas PE[1]

D $^2A'$ C_s

T_o = 38490(240) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1250(60)	gas	PE	1

C $^2A''$ C_s

T_o = 28720(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CO stretch	1690(30)	gas	PE	1
	4	CCl stretch	770(40)	gas	PE	1
	5	ClCO deform.	340(40)	gas	PE	1

B $^2A'$ C_s

T^a = 7660(320) gas PE[1]

A $^2A''$ C_s

T^a = 7020(320) gas PE[1]

X $^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CH deform.	1390(50)	gas	PE	1
	4	CCl stretch	830(40)	gas	PE	1
	5	ClCO deform.	610(70)	gas	PE	1

[a] From vertical ionization potential.

References

[1]D. C. Frost, C. A. McDowell, and N. P. C. Westwood, Chem. Phys. Lett. 51, 607 (1977).

$HNSO^+$

E $^2A'$ C_s

T^a = 41310(160) gas PE[1]

D $^2A'$ C_s

T^a = 32110(160) gas PE[1]

C $^2A''$ C_s

T^a = 28240(160) gas PE[1]

B $^2A'$ C_s

T^a = 7420(160) gas PE[1]

X,A $^2A'',^2A'$ C_s

[a] From vertical ionization potentials.

References

[1] B. Solouki, P. Rosmus, and H. Bock, Angew. Chem. 88, 381 (1976).

$HCCl_2^{\ddagger}$

A broad, unstructured absorption observed near 250 nm in argon-matrix experiments[2] in which infrared absorptions of $HCCl_2^{\ddagger}$ are prominent has been attributed to an excited state of $HCCl_2^{\ddagger}$ which can undergo proton transfer to the matrix.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	3032.8	Ar	IR	3
	2	CCl stretch	860(30)	gas	PE	4,5
			845	Ar	IR	3
b_2	5	H deformation	1291	Ar	IR	1-3
	6	CCl stretch	1044	Ar	IR	1-3

$DCCl_2^{\ddagger}$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCl stretch	790(30)	gas	PE	4,5
b_2	5	CCl stretch	1122	Ar	IR	1,2
	6	D deformation	864	Ar	IR	1,2

References

[1] M. E. Jacox and D. E. Milligan, J. Chem. Phys. 54, 3935 (1971).
[2] M. E. Jacox, Chem. Phys. 12, 51 (1976).
[3] B. J. Kelsall and L. Andrews, J. Mol. Spectrosc. 97, 362 (1983).
[4] L. Andrews, J. M. Dyke, N. Jonathan, N. Keddar, and A. Morris, J. Chem. Phys. 79, 4650 (1983).
[5] L. Andrews, J. M. Dyke, N. Jonathan, N. Keddar, and A. Morris, J. Am. Chem. Soc. 106, 299 (1984).

t-HONS

Threshold for photoisomerization into t-HSNO < 16400.[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3528.0	Ar	IR	1
	2	HON bend	1363.3	Ar	IR	1
	3	NS stretch	969.5	Ar	IR	1
	4	NO stretch	842.1	Ar	IR	1
	5	ONS bend	476.5	Ar	IR	1
a"	6	Torsion	531.3	Ar	IR	1

t-DONS

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2608.0	Ar	IR	1
	2	DON bend	1103.0	Ar	IR	1
	3	NS stretch	951.8	Ar	IR	1
	4	NO stretch	783.0	Ar	IR	1
	5	ONS bend	465.5	Ar	IR	1

References

[1] M. Nonella, J. R. Huber, and T.-K. Ha, J. Phys. Chem. 91, 5203 (1987).

c-HSNO

In an argon matrix, conversion[2] to t-HSNO and photolysis[1,2] to SNO occur on exposure of the sample to 250 nm radiation.

In an argon matrix, slow conversion to t-HSNO occurs on prolonged exposure of the sample to infrared radiation with $\lambda \geq 2\ \mu$.[2]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SH stretch	2566	Ar	IR	2
	2	NO stretch	1570	Ar	IR	1,2
	3	HSN bend	858.5	Ar	IR	2
	4	SN stretch	503[a]	Ar	IR	1,2
	5	SNO bend	307	Ar	IR	2

X---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a"	6	Torsion	406.5	Ar	IR	2

c-DSNO

X C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	NO stretch	1568	Ar	IR	2
	3	DNS bend	715	Ar	IR	2
	4	SN stretch	435	Ar	IR	2
	5	SNO bend	305.5	Ar	IR	2

[a] Assigned in Ref. 1 to the trans- rotamer.

References

[1] P. O. Tchir and R. D. Spratley, Can. J. Chem. 53, 2318 (1975).
[2] R. P. Müller, M. Nonella, P. Russegger, and J. R. Huber, Chem. Phys. 87, 351 (1984).

t-HSNO

In an argon matrix, converted to c-HSNO by irradiation at 585 nm.[2]

X C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SH stretch	2613 2607	Ar	IR	2
	2	NO stretch	1596	Ar	IR	1,2
	3	HSN bend	877.5	Ar	IR	1,2
	4	SN stretch	543.5	Ar	IR	1,2
	5	SNO bend	297	Ar	IR	1,2
a"	6	Torsion	386.5	Ar	IR	2

t-DSNO

X C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	NO stretch	1595	Ar	IR	1,2
	3	DSN bend	724	Ar	IR	1,2
	4	SN stretch	485.5	Ar	IR	1,2
	5	SNO bend	297	Ar	IR	1,2

References

[1] P. O. Tchir and R. D. Spratley, Can. J. Chem. 53, 2318 (1975).
[2] R. P. Müller, M. Nonella, P. Russegger, and J. R. Huber, Chem. Phys. 87, 351 (1984).

c-HNSO [a]

gas AB[3] 238-269 nm

Diffuse absorption merges into continuum with maximum near 217 nm.[3]

Photolysis in an argon matrix by 254 nm radiation leads to rapid formation of c-HOSN.[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	5	NSO bend	~285	gas	AB	3

ā $^3A'$ [b] C_s

Weak, unstructured absorption 325-350 nm.[3]
In an argon matrix, converted to t-HNSO by irradiation at wavelengths longer than 300 nm.[6]

X $^1A'$ C_s Structure: MW[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH stretch	3345	gas	IR	1
			3308	Ar	IR	3,4
			3303	N_2	IR	4
	2	SO stretch	1261	gas	IR	1
			1249	Ar	IR	3,4
			1252	N_2	IR	4
	3	NS stretch	1090	gas	IR	1
			1083	Ar	IR	3,4
			1094	N_2	IR	4

X $^1A'$---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	4	HNS bend	911	gas	IR	1
			900	Ar	IR	3,4
			923	N_2	IR	4
	5	NSO bend	453	gas	IR	1
			447	Ar	IR	3,4
			455	N_2	IR	4
a"	6	Torsion	759	gas	IR	1
			755	Ar	IR	3,4
			774	N_2	IR	4

c-DNSO

gas AB[3] 242-264 nm

Diffuse, merges into continuum.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	5	NSO bend	~285	gas	AB	3

X C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ND stretch	2480	gas	IR	1
			2453	Ar	IR	3,4
	2	SO stretch	1257	gas	IR	1
			1245	Ar	IR	3,4
	3	NS stretch	1055	gas	IR	1
			1048	Ar	IR	3,4
	4	DNS bend	757	gas	IR	1
			752	Ar	IR	3,4
	5	NSO bend	~410	gas	IR	1
			400	Ar	IR	3,4
a"	6	Torsion	594	gas	IR	1
			594	Ar	IR	3,4

[a] Stable rotamer.
[b] Tentative assignment.

References

[1] H. Richert, Z. Anorg. Allg. Chem. 309, 171 (1961).
[2] W. H. Kirchhoff, J. Am. Chem. Soc. 91, 2437 (1969).
[3] J. M. Allegretti and A. J. Merer, Can. J. Phys. 50, 404 (1972).
[4] P. O. Tchir and R. D. Spratley, Can. J. Chem. 53, 2311 (1975).
[5] P. O. Tchir and R. D. Spratley, Can. J. Chem. 53, 2318 (1975).
[6] P. O. Tchir and R. D. Spratley, Can. J. Chem. 53, 2331 (1975).

t-HNSO

In an argon matrix, prolonged photolysis of c-HNSO samples with 340 nm radiation, the condition under which t-HNSO is formed,[1] leads to the formation of c- and t-HSNO.[2]

X C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	SO stretch	1382	Ar	IR	1
	3	NS stretch	986	Ar	IR	1
	4	HNS bend	881	Ar	IR	1
a"	6	Torsion	651	Ar	IR	1

t-DNSO

X C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	SO stretch	1380	Ar	IR	1
	3	NS stretch	951	Ar	IR	1

References

[1] P. O. Tchir and R. D. Spratley, Can. J. Chem. 53, 2331 (1975).
[2] R. P. Müller, M. Nonella, P. Russegger, and J. R. Huber, Chem. Phys. 87, 351 (1984).

c-HOSN

Photolyzes in an argon matrix on prolonged exposure of the sample to 254-nm radiation, producing c- and t-HSNO.[1,2]

X C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3520	Ar	IR	1
	2	SN stretch	1321	Ar	IR	1
	3	HOS bend	992	Ar	IR	1
	4	SO stretch	674	Ar	IR	1
	5	OSN bend	374	Ar	IR	1
a"	6	Torsion	418	Ar	IR	1

c-DOSN

X C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2597	Ar	IR	1
	2	SN stretch	1319	Ar	IR	1
	4	SO stretch	671	Ar	IR	1
a"	6	Torsion	325	Ar	IR	1

References

[1] P. O. Tchir and R. D. Spratley, Can. J. Chem. 53, 2318 (1975).
[2] R. P. Müller, M. Nonella, P. Russegger, and J. R. Huber, Chem. Phys. 87, 351 (1984).

$HCCl_2$

3d Rydberg state C_{2v}

T_o = 54024(10) gas MPI[3] 3d-X 179-185 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCl_2 s-stretch	845(10)	gas	MPI	3

X C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a"	5	HCCl deform.	1226	Ar	IR	1
	6	CCl_2 a-stretch	902	Ar	IR	1

$DCCl_2$

3d Rydberg state C_{2v}

T_o = 53980(10) gas MPI[3] 3d-X 180-185 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCl_2 s-stretch	814(10)	gas	MPI	3

X C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a"	5	DCCl deform.	974	Ar	IR	1,2
	6	CCl_2 a-stretch	814	Ar	IR	1,2

References

[1] T. G. Carver and L. Andrews, J. Chem. Phys. 50, 4235 (1969).
[2] E. E. Rogers, S. Abramowitz, M. E. Jacox, and D. E. Milligan, J. Chem. Phys. 52, 2198 (1970).
[3] G. R. Long and J. W. Hudgens, J. Phys. Chem. 91, 5870 (1987).

HNF_2^+

F $^2A'$ C_s

T^a = 66480(1100) gas PE[1]

E $^2A''$ C_s

T^a = 60270(1450) gas PE[1]

D $^2A'$ C_s

T^a = 52280(1100) gas PE[1]

C $^2A''$ C_s

T^a = 35900(900) gas PE[1]

B $^2A'$ C_s

T^a = 32350(900) gas PE[1]

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

T^a = 31220(1450) gas PE[1]

X $^2A'$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a' 4	NF_2 "scissors"	580(30)	gas	PE	1

DNF$_2^+$

X $^2A'$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a' 4	NF_2 "scissors"	530(30)	gas	PE	1

[a] From vertical ionization potential.

References

[1] D. Colbourne, D. C. Frost, C. A. McDowell, and N. P. C. Westwood, Chem. Phys. Lett. 72, 247 (1980).

HNCl$_2^+$

F $^2A'$ C_s

T^a = 59800(560) gas PE[1,2]

E $^2A''$ C_s

T^a = 49460(560) gas PE[1,2]

D $^2A'$ C_s

T^a = 37030(560) gas PE[1,2]

C $^2A''$ C_s

T^a = 20330(800) gas PE[1,2]

B $^2A'$ C_s

T^a = 19450(560) gas PE[1,2]

A $^2A''$ C_s

T^a = 15330(560) gas PE[1,2]

X $^2A'$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		560(50)	gas	PE	1

[a] From vertical ionization potential.

References

[1] M. K. Livett, E. Nagy-Felsobuki, J. B. Peel, and G. D. Willett, Inorg. Chem. 17, 1608 (1978).
[2] D. Colbourne, D. C. Frost, C. A. McDowell, and N. P. C. Westwood, J. Chem. Phys. 69, 1078 (1978).

HNBr$_2^+$

F $^2A'$ C_s

T^a = 53250(2000) gas PE[1]

E $^2A''$ C_s

T^a = 41150(2000) gas PE[1]

D $^2A'$ C_s

T^a = 21800(2000) gas PE[1]

C $^2A'$ C_s

T^a = 11860(1000) gas PE[1,2]

B $^2A''$ C_s

T^a = 10730(1000) gas PE[1,2]

A $^2A''$ C_s

T^a = 7260(2000) gas PE[1]

X $^2A'$ C_s

[a] From vertical ionization potentials.

References

[1] E. Nagy-Felsobuki and J. B. Peel, J. Electron Spectrosc. Relat. Phenom. 15, 61 (1979).
[2] D. Colbourne, D. C. Frost, C. A. McDowell, and N. P. C. Westwood, Can. J. Chem. 57, 1279 (1979).

HPF$_2^+$

G $^2A'$ C_s

T^a = 58900(1600) gas PE[1,2]

F $^2A'$ C_s

T^a = 53250(1600) gas PE[1,2]

B,C,D,E $^2A'',^2A'',^2A',^2A''$ C_s

T^a = 38700(1600) gas PE[1,2]

A $^2A'$ C_s

T^a = 33100(1600) gas PE[1,2]

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

[a] From vertical ionization potentials.

References

[1] S. Cradock and D. W. H. Rankin, J. Chem. Soc., Faraday Trans. 2 68, 940 (1972).
[2] A. H. Cowley, R. A. Kemp, M. Lattman, and M. L. McKee, Inorg. Chem. 21, 85 (1982).

6.7. Four-Atomic Nonhydrides

C_4

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

T_o = 19564 Ne AB^2 $\tilde{B}$-$\tilde{X}$ 461-511 nm

19222 Ar AB^2 $\tilde{B}$-$\tilde{X}$ 469-521 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Stretch	2089	Ne	AB	2
			2054	Ar	AB	2

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

T_o < 6000, estimated from ESR data.[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	2164	Ar	IR	1,2

[a] Recent calculations[3] indicate that a rhombic ^1A_g state of C_4 may lie somewhat below this $^3\Sigma_g^-$ state. The barrier to nuclear rearrangement may lead to preferential stabilization of the linear structure in the matrix when C_4 is formed by the photodecomposition of a linear precursor (C_4H_2), as in the experiments of Ref. 2.

References

[1] K. R. Thompson, R. L. DeKock, and W. Weltner, Jr., J. Am. Chem. Soc. 93, 4688 (1971).
[2] W. R. M. Graham, K. I. Dismuke, and W. Weltner, Jr., Astrophys. J. 204, 301 (1976).
[3] D. H. Magers, R. J. Harrison, and R. J. Bartlett, J. Chem. Phys. 84, 3284 (1986).

$B_2O_2^+$

$\tilde{C}\ ^2\Sigma_u$ $D_{\infty h}$

T_o = 18560(320) gas PE[1]

$\tilde{B}\ ^2\Sigma_g$ $D_{\infty h}$

T_o = 13720(320) gas PE[1]

$\tilde{A}\ ^2\Pi_u$ $D_{\infty h}$

T_o = 5080(320) gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	BO stretch	1922[a]	gas	PE	1
	2	BB stretch	499[a]	gas	PE	1

[a] Obtained from Franck-Condon fit to partially resolved structure in the first photoelectron band.

References

[1] B. M. Ruščić, L. A. Curtiss, and J. Berkowitz, J. Chem. Phys. 80, 3962 (1984).

CaNCO [a]

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

T_0 = 17180(30) gas LF[1] $\tilde{B}$-$\tilde{X}$ 582 nm

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

T_0 = 16230(5) gas LF[1] $\tilde{A}$-$\tilde{X}$ 610-635 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	CaN stretch	395(5)	gas	LF	1
Π	4	NCO bend	~650[b]	gas	LF	1

A = 68(7) gas LF[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NCO a-stretch	2200(5)	gas	LF	1
	3	CaN stretch	390(5)	gas	LF	1
Π	4	NCO bend	~640[b]	gas	LF	1
	5	CaNC bend	~50[bc]	gas	LF	1

[a] Originally assigned to CaOCN. For reassignment, see Ref. 2.
[b] Tentative assignment.
[c] This value may correspond to $2\nu_5$.

References

[1] L. C. Ellingboe, A. M. R. P. Bopegedera, C. R. Brazier, and P. F. Bernath, Chem. Phys. Lett. 126, 285 (1986).
[2] L. C. O'Brien and P. F. Bernath, J. Chem. Phys. 88, 2117 (1988).

SrNCO

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

T_0 = 16016(30) gas LF[1] $\tilde{B}$-$\tilde{X}$ 624 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	SrN stretch	314(30)	gas	LF	1

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

T_0 = 15069.62 gas LF[1,2] $\tilde{A}$-$\tilde{X}$ 650-685 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	SrN stretch	320(30)[a]	gas	LF	1

A = 292.57 gas LF[1,2]

B_0 = 0.043 LF[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	SrN stretch	297(30)	gas	LF	1

B_0 = 0.043 LF[2]

[a] For $^2\Pi_{3/2}$ state.

References

[1] L. C. Ellingboe, A. M. R. P. Bopegedera, C. R. Brazier, and P. F. Bernath, Chem. Phys. Lett. 126, 285 (1986).
[2] L. C. O'Brien and P. F. Bernath, J. Chem. Phys. 88, 2117 (1988).

CaN_3

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

T_0 = 17079 gas LF[1] $\tilde{B}$-$\tilde{X}$ 570-590 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	CaN stretch	384	gas	LF	1
Π	5	CaNN bend	42.5[a]	gas	LF	1

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

T_0 = 16255 gas LF[1] $\tilde{A}$-$\tilde{X}$ 600-710 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	CaN stretch	389	gas	LF	1

A = 76 gas LF[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	N_3 a-stretch	2114	gas	LF	1
	2	N_3 s-stretch	1364	gas	LF	1
	3	CaN stretch	396	gas	LF	1
Π	5	CaNN bend	43[a]	gas	LF	1

[a] $\frac{1}{2}(2\nu_5)$.

References

[1]C. R. Brazier and P. F. Bernath, J. Chem. Phys. 88, 2112 (1988).

SrN_3

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

T_0 = 15872 gas LF[1] $\tilde{B}$-$\tilde{X}$ 630 nm

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

T_0 = 15057.69 gas LF[1] $\tilde{A}$-$\tilde{X}$ 640-690 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	SrN stretch	321	gas	LF	1

A = 296.43 gas LF[1]

B_0 = 0.045 LF[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	SrN stretch	316	gas	LF	1
Π	5	SrNN bend	41[a]	gas	LF	1

B_0 = 0.045 LF[1]

[a] $\frac{1}{2}(2\nu_5)$.

References

[1]C. R. Brazier and P. F. Bernath, J. Chem. Phys. 88, 2112 (1988).

$N{\equiv}C{-}C{\equiv}N^+$

$\tilde{C}\ ^2\Pi_u$ $D_{\infty h}$

T_0 = 17020(160) gas PE[1]

17056(6) Ne AB[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡N stretch	2020(10)	Ne	AB	2
	2	C-C stretch	710(40)	gas	PE	1
			740(10)	Ne	AB	2
Π_g	4	Bend	422[a]	Ne	AB	2

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

T_0 = 12100(160) gas PE[1]

12285(40) Ne AB[2]

$\tilde{A}\ ^2\Sigma_g^+$ $D_{\infty h}$

T_0 = 9120(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡N stretch	1860(40)	gas	PE	1

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

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+ 1	C≡N stretch	2120(40)	gas	PE	1

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

References

[1] C. Baker and D. W. Turner, Proc. Roy. Soc. (London) A308, 19 (1968).
[2] J. Fulara, S. Leutwyler, J. P. Maier, and U. Spittel, J. Phys. Chem. 89, 3190 (1985).

$ONCN^+$

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

T_o = 65100(1200) gas PE[1]

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

T_o = 61100(1200) gas PE[1]

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

T_o = 47120(800) gas PE[1]

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

T^a = 28400(560) gas PE[1]

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

T^a = 23080(560) gas PE[1]

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

T^a = 21220(560) gas PE[1]

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

[a] From vertical ionization potential.

References

[1] G. Jonkers, R. Mooyman, and C. A. de Lange, Chem. Phys. 57, 97 (1981).

P_4^+

$\tilde{C}\ ^2T_2$ T_d

$T_o^a \sim 41200$ gas PE[1,2]

Jahn-Teller splitting ∼ 9300 gas PE[1,2]

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

T_o^a = 21860(500) gas PE[1,2]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1 1	Sym. stretch	540(40)	gas	PE	1,2

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

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

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_o values are given with respect to onset of the transition.
[b] Ref. 2 reverses the assignment of these two bands.

References

[1] C. R. Brundle, N. A. Kuebler, M. B. Robin, and H. Basch, Inorg. Chem. 11, 20 (1972).
[2] S. Evans, P. J. Joachim, A. F. Orchard, and D. W. Turner, Int. J. Mass Spectrom. Ion Phys. 9, 41 (1972).

NCNO

An absorption maximum has been reported[3,9] at 216 nm, with absorption extending beyond 200 nm.

A weaker absorption maximum occurs near 270 nm, with a long wavelength threshold near 400 nm.[9]

$\tilde{A}\ ^1A''$ C_s Structure: PF[11]

T_o = 11339 gas AB[1,3,7]PF[11] $\tilde{A}$-$\tilde{X}$ 540-971 nm

Threshold for photodissociation into CN and NO at 17085.[9,10] Extensively perturbed by interaction with high vibrational levels of the ground state.[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	C≡N stretch	1956	gas	PF	11
	2	N=O stretch	1485	gas	PF	11
	3	C-N stretch	918	gas	PF	11
	4	NCN bend	543	gas	AB,PF	7,11
	5	CNO bend	212.5	gas	AB,PF	7,11
a"	6	Torsion	411	gas	PF	11

$\tau_{rad} \sim 14$ μs gas LF[8,12]. $\tau_{fluor} > 40$ μs for all levels below D_0 (17085) LF[12].

A = 4.76(2); B = 0.167(3) PF[11]

X C_s Structure: MW[2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	C≡N stretch	2170.0	gas	IR	6
	2	N=O stretch	1501.0	gas	IR	6
	3	C-N stretch	820.0	gas	IR	3,6
	4	NCN bend	588.5	gas	IR	6
	5	CNO bend	212.0(2)	gas	IR	5
a"	6	Torsion	264.2	gas	IR	5

A_0 = 2.709; B_0 = 0.180; C_0 = 0.168 MW[2,4]IR[5]

References

[1] P. Horsewood and G. W. Kirby, Chem. Commun. 1139 (1971).
[2] R. Dickinson, G. W. Kirby, J. G. Sweeny, and J. K. Tyler, Chem. Commun. 241 (1973).
[3] E. A. Dorko and L. Buelow, J. Chem. Phys. 62, 1869 (1975).
[4] R. Dickinson, G. W. Kirby, J. G. Sweeny, and J. K. Tyler, J. Chem. Soc., Faraday Trans. 2 74, 1393 (1978).
[5] F. M. Nicolaisen and O. J. Nielsen, J. Mol. Struct. 49, 97 (1978).
[6] B. Bak, F. M. Nicolaisen, O. J. Nielsen, and S. Skaarup, J. Mol. Struct. 51, 17 (1979).
[7] J. Pfab, Chem. Phys. Lett. 99, 465 (1983).
[8] I. Nadler, J. Pfab, G. Radhakrishnan, H. Reisler, and C. Wittig, J. Chem. Phys. 79, 2088 (1983).
[9] I. Nadler, J. Pfab, H. Reisler, and C. Wittig, J. Chem. Phys. 81, 653 (1984).
[10] I. Nadler, H. Reisler, M. Noble, and C. Wittig, Chem. Phys. Lett. 108, 115 (1984).
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[12] C. X. W. Qian, H. Reisler, and C. Wittig, Chem. Phys. Lett. 139, 175 (1987).

$C_2F_2^+$

D $^2\Sigma_u$ $D_{\infty h}$

T^a = 84880(1000) gas PE[2]

C $^2\Sigma_g$ $D_{\infty h}$

T^a = 76000(1000) gas PE[1,2]

B $^2\Pi_u$ $D_{\infty h}$

T^a = 59060(1000) gas PE[1,2]

A $^2\Pi_g$ $D_{\infty h}$

T^a = 52600(1000) gas PE[1,2]

X $^2\Pi_u$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2420(80)	gas	PE	2
	2	CF s-stretch	825(80)	gas	PE	2

[a] From vertical ionization potential.

References

[1] G. Bieri, E. Heilbronner, J.-P. Stadelmann, J. Vogt, and W. von Niessen, J. Am. Chem. Soc. 99, 6832 (1977).
[2] G. Bieri, A. Schmelzer, L. Åsbrink, and M. Jonsson, Chem. Phys. 49, 213 (1980).

$C_2Cl_2^+$ [a]

D $^2\Sigma_u^+$ $D_{\infty h}$

T_0 = 62287(160) gas PE[1]

C $^2\Sigma_g^+$ $D_{\infty h}$

T_0 = 53816(160) gas PE[1]

B $^2\Pi_u$ $D_{\infty h}$

T_0 = 35178(160) gas PE[1]

τ = ∿2850 ns gas PEFCO[4]

A $^2\Pi_{g,3/2}$ $D_{\infty h}$

T_0 = 26962.8(3) gas EF[5,8]LF[7] Ã-X̃ 360-496 nm

26637(10) Ne AB[6] Ã-X̃ 341-375 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2223(5)	Ne	AB	6
	2	CCl stretch	484.2(3)[b]	gas	EF,LF	5,7,8
			486(5)	Ne	AB	6
Π_u	5	Bend	205(3)[c]	gas	LF	7
			207(5)[c]	Ne	AB	6

τ = 13(2) ns gas EF[2]PEFCO[4]; ≤30 ns gas PIFCO[3]

A = -565(80) gas EF[5]

$\tilde{X}\ ^2\Pi_{u,3/2}$ $D_{\infty h}$ Structure: UV^2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2107.2(3)[d]	gas	EF,LF	5,7,8
	2	CCl stretch	503.8(3)[e]	gas	EF,LF	5,7,8
Π_g	4	Bend	317.8(3)[c]	gas	EF,LF	5,7,8
Π_u	5	Bend	233[c]	gas	LF	7

A = -240(120) gas EF[5]

a $C_2{}^{35}Cl_2^+$.
b 495 for $\tilde{A}\ ^2\Pi_{g,1/2}$.
c $\frac{1}{2}(2\nu_i)$.
d 2101.0(3) for $\tilde{X}\ ^2\Pi_{u,1/2}$.[8]
e 514.0(3) for $\tilde{X}\ ^2\Pi_{u,1/2}$.[8]

References

[1] E. Heilbronner, V. Hornung, and E. Kloster-Jensen, Helv. Chim. Acta 53, 331 (1970).
[2] M. Allan, E. Kloster-Jensen, and J. P. Maier, J. Chem. Soc., Faraday Trans. 2 73, 1417 (1977).
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[4] J. P. Maier and F. Thommen, Chem. Phys. 70, 325 (1982).
[5] D. Klapstein, J. P. Maier, and W. Zambach, Chem. Phys. 77, 463 (1983).
[6] S. Leutwyler, J. P. Maier, and U. Spittel, Mol. Phys. 51, 437 (1984).
[7] J. P. Maier and L. Misev, Int. J. Mass Spectrom. Ion Proc. 58, 243 (1984).
[8] D. Klapstein, R. Kuhn, and J. P. Maier, J. Electron Spectrosc. Relat. Phenom. 35, 171 (1985).

$ClC{\equiv}CBr^+$

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

T_o = 60432(160) gas PE[1]

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

T_o = 49136(160) gas PE[1]

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

T_o = 33080(160) gas PE[1]

$\tau \geq 1100$ ns gas PEFCO[2]

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

T_o = 21441 gas EF[3] $\tilde{A}$-$\tilde{X}$ 426-550 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡C stretch	2172(2)	gas	EF	3
	2	CCl stretch	878(2)	gas	EF	3
	3	CBr stretch	334(2)	gas	EF	3
Π	4	CCCl bend	304(2)[a]	gas	EF	3
	5	CCBr bend	182(2)[ab]	gas	EF	3

τ = 21(2) ns gas PEFCO[3]

A = ∿-1900 gas EF[3]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡C stretch	2011(2)	gas	EF	3
	2	CCl stretch	1017(2)	gas	EF	3
	3	CBr stretch	405(2)	gas	EF	3
Π	5	CCBr bend	246(2)[a]	gas	LF	3

A = ∿-1000 gas EF[3]

a Tentative assignment.
b $\frac{1}{2}(2\nu_5)$.

References

[1] E. Heilbronner, V. Hornung, and E. Kloster-Jensen, Helv. Chim. Acta 53, 331 (1970).
[2] J. P. Maier and F. Thommen, Chem. Phys. 70, 325 (1982).
[3] D. Klapstein, J. P. Maier, M. Ochsner, and W. Zambach, J. Electron Spectrosc. Relat. Phenom. 34, 161 (1984).

$C_2Br_2^+$ [a]

$\tilde{D}\ ^2\Sigma_u^+$ $D_{\infty h}$

T_o = 58334(160) gas PE[1]

$\tilde{C}\ ^2\Sigma_g^+$ $D_{\infty h}$

T_o = 48168(160) gas PE[1]

$\tilde{B}\ ^2\Pi_u$ $D_{\infty h}$

T_o = 29369(160) gas PE[1]

$\tau \geq 1500$ ns gas PEFCO[3]

A = -323(160) gas PE[1]

$\tilde{A}\ ^2\Pi_{g,1/2}$ $D_{\infty h}$

T_o = 22188(80) gas PE[1]EF[4] $\tilde{A}$-$\tilde{X}$ 467-648 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	2	CBr stretch	278	gas	EF	4
Π_g	4	Bend	257[bc]	gas	EF	4
Π_u	5	Bend	112[b]	gas	EF	4

τ = 27(3) ns gas EF[2]; 25(3) ns gas PEFCO[3]

$\tilde{A}\ ^2\Pi_{g,3/2}$ $D_{\infty h}$

T_o = 19855.9(3) gas EF[4,7],LF[6] $\tilde{A}$-$\tilde{X}$ 438-648 nm

19548(4) Ne AB[5] $\tilde{A}$-$\tilde{X}$ 448-511 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2190	gas	EF,LF	4,6
			2194(5)	Ne	AB	5
	2	CBr stretch	282.7(3)	gas	EF,LF	4,6,7
			293(5)	Ne	AB	5
Π_g	4	Bend	263[b]	gas	EF	4
			259(5)[b] 240(5)[b]	Ne	AB	5
Π_u	5	Bend	119[b]	gas	EF,LF	4,6
			135(5)[b] 126(5)[b]	Ne	AB	5

τ = 29(3) ns gas EF[2]; 31(3) ns gas PEFCO[3]

$\tilde{X}\ ^2\Pi_{u,1/2}$ $D_{\infty h}$

T_o = 1372(80) gas PE[1]EF[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2065.1(3)	gas	EF	4,7
	2	CBr stretch	318.4(3)	gas	EF	4,7
Π_g	4	Bend	294.5(3)[b]	gas	EF	4,7
Π_u	5	Bend	132.6(3)[b]	gas	EF	4,7

$\tilde{X}\ ^2\Pi_{u,3/2}$ $D_{\infty h}$ Structure: UV[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2067.0(3)	gas	EF,LF	4,6,7
	2	CBr stretch	320.7(3)	gas	EF,LF	4,6,7
Π_g	4	Deformation	299.0(3)[b]	gas	EF,LF	4,6,7
Π_u	5	Deformation	134.9(3)[b]	gas	EF,LF	4,6,7

[a] $C_2{}^{79}Br_2^+$.
[b] $\frac{1}{2}(2\nu_i)$.
[c] Tentative value.

References

[1] E. Heilbronner, V. Hornung, and E. Kloster-Jensen, Helv. Chim. Acta 53, 331 (1970).
[2] M. Allan, E. Kloster-Jensen, and J. P. Maier, J. Chem. Soc., Faraday Trans. 2 73, 1417 (1977).
[3] J. P. Maier and F. Thommen, Chem. Phys. 70, 325 (1982).
[4] D. Klapstein, J. P. Maier, and W. Zambach, Chem. Phys. 77, 463 (1983).
[5] S. Leutwyler, J. P. Maier, and U. Spittel, Mol. Phys. 51, 437 (1984).
[6] J. P. Maier and L. Misev, Int. J. Mass Spectrom. Ion Proc. 58, 243 (1984).
[7] D. Klapstein, R. Kuhn, and J. P. Maier, J. Electron Spectrosc. Relat. Phenom. 35, 171 (1985).

$C_2I_2^+$

$\tilde{D}\ ^2\Sigma_u^+$ $D_{\infty h}$

T_o = 52040(160) gas PE[1]

$\tilde{C}\ ^2\Sigma_g^+$ $D_{\infty h}$

T_o = 41874(160) gas PE[1]

$\tilde{B}\ ^2\Pi_u$ $D_{\infty h}$

T_o = 25334(160) gas PE[1]

$\tau \geq$ 3000 ns gas PEFCO[3]

A = -1694(160) gas PE[1]

$\tilde{A}\ ^2\Pi_{g,1/2}$ $D_{\infty h}$

T_o = 17912(80) gas PE[1]EF[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	2	CI stretch	195	gas	EF	4
Π_g	4	Bend	224	gas	EF	4

τ = 52(3) ns gas EF[2]PEFCO[3]

$\tilde{A}\ ^2\Pi_{g,3/2}$ $D_{\infty h}$

T_o = 12971 gas EF[4] $\tilde{A}$-$\tilde{X}$ 670-846 nm

12987(3) Ne AB[5] $\tilde{A}$-$\tilde{X}$ 613-770 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2146(5)	Ne	AB	5
	2	CI stretch	204	gas	EF	4
			195(5)	Ne	AB	5
Π_g	4	Bend	225[ab]	gas	EF	4
			227(5)[a]	Ne	AB	5

τ = 25(3) ns gas PEFCO[3]

$\tilde{X}\ ^2\Pi_{u,1/2}$ $D_{\infty h}$

T_o = 3630(80) gas PE[1]EF[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	1990	gas	EF	4
	2	CI stretch	234	gas	EF	4
Π_g	4	Bend	214[a]	gas	EF	4
Π_u	5	Bend	94[a]	gas	EF	4

$\tilde{X}\ ^2\Pi_{u,3/2}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	2	CI stretch	242	gas	EF	4
Π_g	4	Bend	221[a]	gas	EF	4
Π_u	5	Bend	101[a]	gas	EF	4

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

References

[1] E. Heilbronner, V. Hornung, and E. Kloster-Jensen, Helv. Chim. Acta 53, 331 (1970).
[2] M. Allan, E. Kloster-Jensen, and J. P. Maier, J. Chem. Soc., Faraday Trans. 2 73, 1417 (1977).
[3] J. P. Maier and F. Thommen, Chem. Phys. 70, 325 (1982).
[4] D. Klapstein, J. P. Maier, and W. Zambach, Chem. Phys. 77, 463 (1983).
[5] S. Leutwyler, J. P. Maier, and U. Spittel, Mol. Phys. 51, 437 (1984).

$ClNCO^+$

$F\ ^2A'$ C_s

T^a = 63660(240) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1100(80)	gas	PE	1

$E\ ^2A'$ C_s

T^a = 55430(240) gas PE[1]

Structure with band spacings of either 950 or 1900(50).

$D\ ^2A''$ C_s

T^a = 45180(240) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			910(80)	gas	PE	1

$B,C\ ^2A'',^2A'$ C_s

T^a = 25420(240) gas PE[1]

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

T^a = 7420(240) gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1110(40)	gas	PE	1
			600(40)	gas	PE	1

[a] From vertical ionization potential.

References

[1] D. C. Frost, C. B. MacDonald, C. A. McDowell, and N. P. C. Westwood, Chem. Phys. 47, 111 (1980).

$BrNCO^+$

F $^2A'$ C_s

T^a = 62040(240) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		750(80)	gas	PE[1]	

E $^2A'$ C_s

T^a = 53740(240) gas PE[1]

Structured, with band separations varying from 700 to 850.

D $^2A''$ C_s

T^a = 44540(240) gas PE[1]

C $^2A'$ C_s

T^a = 22190(240) gas PE[1]

B $^2A''$ C_s

T^a = 20820(240) gas PE[1]

A $^2A'$ C_s

T^a = 5970(240) gas PE[1]

X $^2A''$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		1100(40)	gas	PE	1
		520(40)	gas	PE	1

[a] From vertical ionization potential.

References

[1]D. C. Frost, C. B. MacDonald, C. A. McDowell, and N. P. C. Westwood, Chem. Phys. 47, 111 (1980).

$INCO^+$

F $^2A'$ C_s

T^a = 61800(240) gas PE[1]

E $^2A'$ C_s

T^a = 52440(240) gas PE[1]

D $^2A''$ C_s

T^a = 46070(240) gas PE[1]

C $^2A'$ C_s

T^a = 21300(240) gas PE[1]

B $^2A''$ C_s

T^a = 18320(240) gas PE[1]

A $^2A'$ C_s

T^a = 5570(240) gas PE[1]

X $^2A''$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		2070(40)	gas	PE	1
		420(40)	gas	PE	1

[a] From vertical ionization potential.

References

[1]D. C. Frost, C. B. MacDonald, C. A. McDowell, and N. P. C. Westwood, Chem. Phys. 47, 111 (1980).

$FSCN^+$

G $^2A'$ C_s

T^a = 68300(1000) gas PE[1]

F $^2A'$ C_s

T^a = 53800(1000) gas PE[1]

E $^2A''$ C_s

T^a = 52200(1000) gas PE[1]

D $^2A'$ C_s

T^a = 34450(320) gas PE[1]

C $^2A''$ C_s

T^a = 23960(1000) gas PE[1]

B $^2A'$ C_s

T^a = 21460(320) gas PE[1]

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

T^a = 19900(1000) gas PE[1]

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

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	SF stretch	840(50)	gas	PE	1

[a] From vertical ionization potential.

References

[1]G. Jonkers, O. Grabandt, R. Mooyman, and C. A. de Lange, J. Electron Spectrosc. Relat. Phenom. 26, 147 (1982).

ClSCN$^+$

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

T^a = 57280(560) gas PE[1]

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

T^a = 40260(320) gas PE[1]

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

T^a = 32440(320) gas PE[1]

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

T^a = 25900(320) gas PE[1]

$\tilde{C}\ ^2A''$[b] C_s

T^a = 22830(320) gas PE[1]

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

T^a = 20980(320) gas PE[1]

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

T^a = 17910(320) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		680(40)	gas	PE	2

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

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	SCl stretch	570(50)	gas	PE	1

[a] From vertical ionization potential.
[b] May be a vibrational component of the $\tilde{B}$ state.

References

[1]D. C. Frost, C. B. MacDonald, C. A. McDowell, and N. P. C. Westwood, J. Am. Chem. Soc. 103, 4423 (1981).
[2]H. Leung, R. J. Suffolk, and J. D. Watts, Chem. Phys. 109, 289 (1986).

BrSCN$^+$

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

T^a = 55830(560) gas PE[1]

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

T^a = 37680(320) gas PE[1]

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

T^a = 30180(320) gas PE[1]

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

T^a = 25580(320) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		400(60)	gas	PE	1

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

T^a = 19280(320) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a' 1	CN stretch	2050(60)	gas	PE	1

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

T^a = 17180(320) gas PE[1]

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

T^a = 13150(320) gas PE[1]

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

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	SBr stretch	450(50)	gas	PE	1

References

[1] D. C. Frost, C. B. MacDonald, C. A. McDowell, and N. P. C. Westwood, J. Am. Chem. Soc. 103, 4423 (1981).

$ISCN^+$

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

T^a = 24500(800) gas PE[1]

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

T^a = 18000(800) gas PE[1]

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

T^a = 17020(800) gas PE[1]

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

T^a = 13960(800) gas PE[1]

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

[a] From vertical ionization potentials.

References

[1] H. Leung, R. J. Suffolk, and J. D. Watts, Chem. Phys. 109, 289 (1986).

$ClSeCN^+$

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

T^a = 54540(320) gas PE[1]

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

T^a = 38000(320) gas PE[1]

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

T^a = 29530(320) gas PE[1]

$\tilde{D}\ ^2$[illegible] C_s

T^a [illegible]0) gas PE[1]

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

$T^a \sim$ 21800 gas PE[1]

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

T^a = 18070(320) gas PE[1]

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

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	SeCl stretch	440(50)	gas	PE	1

[a] From vertical ionization potentials.

References

[1] G. Jonkers, R. Mooyman, and C. A. de Lange, Mol. Phys. 43, 655 (1981).

$BrSeCN^+$

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

T^a = 54620(320) gas PE[1]

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

T^a = 35660(320) gas PE[1]

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

T^a = 28640(320) gas PE[1]

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

T^a = 26300(320) gas PE[1]

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

T^a = 20740(320) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a' 1	CN stretch	1850(50)	gas	PE	1

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

T^a = 18150(320) gas PE[1]

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

T^a = 13720(320) gas PE[1]

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

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	SeBr stretch	360(50)	gas	PE	1

[a] From vertical ionization potentials.

References

[1]G. Jonkers, R. Mooyman, and C. A. de Lange, Mol. Phys. 43, 655 (1981).

$(NO)_2^+$

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

Dissociative state, with onset at 10700(1000) and maximum at 16400(1000).[1]

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

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1 1	NO stretch	2017(160)	gas	PE	1

References

[1]F. Carnovale, J. B. Peel, and R. G. Rothwell, J. Chem. Phys. 84, 6526 (1986).

$N_2S_2^+$

T^{ab}= 51310(320) gas PE[1,2]

T^{ab} = 32190(320) gas PE[1,2]

$\tilde{C}\ ^2B_{2u}$ D_{2h}

T^a = 15090(320) gas PE[1,2]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		790(80)	gas	PE	1
		450(80)	gas	PE	1

$\tilde{B}\ ^2B_{3u}$ D_{2h}

T^a = 5160(320) gas PE[1,2]

$\tilde{A}\ ^2B_{3g}$ D_{2h}

T^a = 3630(320) gas PE[1,2]

$\tilde{X}\ ^2B_{2g}$ D_{2h}

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		810(80)	gas	PE	1
		470(80)	gas	PE	1

[a] From vertical ionization potential.
[b] A large number of transitions have been calculated[3] to occur in this energy region.

References

[1]D. C. Frost, M. R. LeGeyt, N. L. Paddock, and N. P. C. Westwood, J. Chem. Soc., Chem. Commun. 217 (1977).
[2]R. H. Findlay, M. H. Palmer, A. J. Downs, R. G. Egdell, and R. Evans, Inorg. Chem. 19, 1307 (1980).
[3]W. von Niessen, J. Schirmer, and L. S. Cederbaum, J. Chem. Soc., Faraday Trans. 2 82, 1489 (1986).

ClN_3^+

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

T^a = 67210(500) gas PE[1]

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

T^a = 58010(500) gas PE[1]

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

T^a = 46470(240) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		2100(60)	gas	PE	1
		1280(60)	gas	PE	1

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

T^a = 25740(240) gas PE[1]

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

T^a = 14520(240) gas PE[1]

X $^2A''$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		730(60)	gas	PE	1

[a] From vertical ionization potential. The adiabatic ground-state ionization potential may lie 730(60) lower, increasing each T value by that amount.

References

[1]D. C. Frost, C. B. MacDonald, C. A. McDowell, and N. P. C. Westwood, Chem. Phys. 47, 111 (1980).

BrN_3^+

F $^2A'$ C_s

T^a = 64630(500) gas PE[1]

E $^2A''$ C_s

T^a = 56800(500) gas PE[1]

D $^2A'$ C_s

T^a = 45340(240) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		1940(80)	gas	PE	1

C $^2A'$ C_s

T^a = 22190(240) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		1970(80)	gas	PE	1

B $^2A''$ C_s

T^a = 19690(240) gas PE[1]

A $^2A'$ C_s

T^a = 11130(240) gas PE[1]

X $^2A''$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		710(60)	gas	PE	1

[a] From vertical ionization potential. The adiabatic ground-state ionization potential may lie 710(60) lower, increasing each T value by that amount.

References

[1]D. C. Frost, C. B. MacDonald, C. A. McDowell, and N. P. C. Westwood, Chem. Phys. 47, 111 (1980).

CO_3

A broad, weak absorption with maximum at 406 nm has been assigned[4] to CO_3 trapped in a CO_2 matrix. The threshold for the photodissociation of CO_3 into CO_2 + O in this system lies near 500 nm.

X C_{2v} Structure: IR^3MO^5

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	C=O stretch	2053[a]	Ar	IR	2
			2045	CO_2	IR	1,3
	2	O-O stretch	1070	Ar	IR	2
			1073	CO_2	IR	1,3
	3	C-O stretch	593	CO_2	IR	1,3
b_2	5	C-O stretch	975	Ar	IR	2
			972	CO_2	IR	1,3
	6	O-C=O bend	564	Ar	IR	2
			568	CO_2	IR	1,3

[a] Fermi resonance with overtone of fundamental at 975 leads to appearance of another very prominent absorption at 1894 (1880 in CO_2 matrix experiments).

References

[1]N. G. Moll, D. R. Clutter, and W. E. Thompson, J. Chem. Phys. 45, 4469 (1966).
[2]E. Weissberger, W. H. Breckenridge, and H. Taube, J. Chem. Phys. 47, 1764 (1967).
[3]M. E. Jacox and D. E. Milligan, J. Chem. Phys. 54, 919 (1971).
[4]P. R. Jones and H. Taube, J. Phys. Chem. 75, 2991 (1971).
[5]J. A. Pople, U. Seeger, R. Seeger, and P. von R. Schleyer, J. Comput. Chem. 1, 199 (1980).

F_2BO [a]

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

T_o = 22390.9(4) gas EM[3] $\tilde{C}$-$\tilde{X}$ 446-447 nm

gas EM[1,2] $\tilde{C}$-$\tilde{A}$ 554-633 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	BF stretch	875	gas	EM	1
	3	BF_2 "scissors"	480.6	gas	EM	1,2

C_o = 0.176 EM[3]

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

T_o = 5220[b] gas EM[1,2] $\tilde{C}$-$\tilde{A}$ 554-633 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	BO stretch	1369	gas	EM	1
	2	BF stretch	856.0	gas	EM	1,2
	3	BF_2 "scissors"	491.0	gas	EM	1,2

$\tilde{X}\ ^2B_2$ [b] C_{2v}

C_o = 0.176 EM[3]

a ^{11}B.
b See Ref. 4.

References

1S. L. N. G. Krishnamachari and B. R. Vengsarkar, Proc. C. S. I. R. Sympos. Banaras, 1963, p. 87; Proc. Ind. Acad. Sci. A61, 172 (1965).
2C. W. Mathews and K. K. Innes, J. Mol. Spectrosc. 15, 199 (1965).
3C. W. Mathews, J. Mol. Spectrosc. 19, 203 (1966).
4R. N. Dixon, G. Duxbury, R. C. Mitchell, and J. P. Simons, Proc. Roy. Soc. (London) A300, 405 (1967).

BF_3^+

$\tilde{D}\ ^2E'$ D_{3h}

T_o = 35260(240) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	BF stretch	730(30)	gas	PE	1

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

T_o = 27510(240) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	BF stretch	830(20)	gas	PE	2

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

T_o = 10890(240) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	BF stretch	770(60)	gas	PE	1

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

T_o = 5890(240) gas PE[1]

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

References

1P. J. Bassett and D. R. Lloyd, J. Chem. Soc. A 1551 (1971).
2C. F. Batten, J. A. Taylor, B. P. Tsai, and G. G. Meisels, J. Chem. Phys. 69, 2547 (1978).

BCl_3^+ [a]

$\tilde{E}\ ^2A_1'$ D_{3h}

T_o = 49200(560) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	BCl stretch	440(60)	gas	PE	1

$\tilde{D}\ ^2E'$ D_{3h}

T_o = 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.

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_o = 20800(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	BCl stretch	440(30)	gas	PE	1

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

T^b = 8230(240) gas PE[1]

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

T_o = 4440(480) gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	3	BCl stretch	1090	Ar	IR	2

a 1^1B.
b From vertical ionization potential.

References

1P. J. Bassett and D. R. Lloyd, J. Chem. Soc. A 1551 (1971).
2J. H. Miller and L. Andrews, J. Am. Chem. Soc. 102, 4900 (1980).

BBr_3^+ [a]

$\tilde{F}$

T ~ 53500(480) gas PE[1]

$\tilde{E}\ ^2A_1'$ D_{3h}

T_o = 49380(560) gas PE[1]

$\tilde{D}\ ^2E'$ D_{3h}

T_o^b = 25500(400) gas PE[1]

Spin-orbit splitting = 2180(160)

A broad absorption with maximum at 355 nm (28200) which appears on argon-resonance photolysis of BBr_3 isolated in an argon matrix and which can be destroyed by prolonged exposure of the sample to 340-600 nm radiation has been assigned[2] to the $\tilde{D}$-$\tilde{X}$ transition of BBr_3^+.

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

T_o = 19200(480) gas PE[1]

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

T^c = 9680(480) gas PE[1]

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

T_o^b = 5000(400) gas PE[1]

Spin-orbit splitting ~ 1130.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	3	BBr stretch	930	Ar	IR	2

a 1^1B.
b Onset of transition.
c From vertical ionization potential.

References

1P. J. Bassett and D. R. Lloyd, J. Chem. Soc. A 1551 (1971).
2J. H. Miller and L. Andrews, J. Am. Chem. Soc. 102, 4900 (1980).

BI_3^+

$\tilde{E}\ ^2A_1'$ D_{3h}

T_o = 47200(400) gas PE[1]

$\tilde{D}\ ^2E'$ D_{3h}

T_o^a = 24450(480) gas PE[1]

Spin-orbit splitting = 4030(80).

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

T_o = 18640(400) gas PE[1]

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

T_o^a = 8310(400) gas PE[1]

Spin-orbit splitting = 810(160).

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

T_o^a = 4840(400) gas PE[1]

Spin-orbit splitting = 1450(160).

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

a Onset of transition.

References

[1]P. J. Bassett and D. R. Lloyd, J. Chem. Soc. A 1551 (1971).

AlF_3^+

$\tilde{E}\ ^2A_1'$ D_{3h}

T^a = 37440(320) gas PE[1]

$\tilde{C},\tilde{D}\ ^2A_2'',^2E'$ D_{3h}

T^a = 13070(320) gas PE[1]

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

T^a = 5240(320) gas PE[1]

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

[a] From vertical ionization potentials.

References

[1]J. M. Dyke, C. Kirby, A. Morris, B. W. J. Gravenor, R. Klein, and P. Rosmus, Chem. Phys. 88, 289 (1984).

$AlCl_3^+$

$\tilde{E}\ ^2A_1'$ D_{3h}

T^a = 31950(320) gas PE[1,2]

$\tilde{D}\ ^2E'$ D_{3h}

T^a = 16380(320) gas PE[1,2]

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

T^a = 10650(320) gas PE[1,2]

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

T^a = 5810(320) gas PE[1,2]

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

$T^a \sim 3700$ gas PE[1,2]

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

[a] From vertical ionization potentials.

References

[1]M. F. Lappert, J. B. Pedley, G. J. Sharp, and N. P. C. Westwood, J. Electron Spectrosc. Relat. Phenom. 3, 237 (1974).
[2]G. K. Barker, M. F. Lappert, J. B. Pedley, G. J. Sharp, and N. P. C. Westwood, J. Chem. Soc., Dalton Trans. 1765 (1975).

$AlBr_3^+$

$\tilde{E}\ ^2A_1'$ D_{3h}

T^a = 34860(320) gas PE[1,2]

$\tilde{D}\ ^2E'$ D_{3h}

T^a = 18190(320) gas PE[1,2]

Spin-orbit splitting = 2500(320) gas PE[1,2]

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

T^a = 11780(320) gas PE[1,2]

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

T^a = 6700(320) gas PE[1,2]

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

T^a = 5000(320) gas PE[1,2]

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

[a] From vertical ionization potentials.
[b] $\tilde{A}$ and $\tilde{B}$ levels mixed by spin-orbit interaction.

References

[1]M. F. Lappert, J. B. Pedley, G. J. Sharp, and N. P. C. Westwood, J. Electron Spectrosc. Relat. Phenom. 3, 237 (1974).
[2]G. K. Barker, M. F. Lappert, J. B. Pedley, G. J. Sharp, and N. P. C. Westwood, J. Chem. Soc., Dalton Trans. 1765 (1975).

F_2CN

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

T_o = 27639.8 gas AB[1] $\tilde{C}$-$\tilde{X}$ 338-362 nm

27650(40) Ar AB[2] $\tilde{C}$-$\tilde{X}$ 338-362 nm

27660(40) N_2 AB[2] $\tilde{C}$-$\tilde{X}$ 338-362 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CN stretch	1884	gas	AB	1
			1808(80)	Ar	AB	2
			1879(80)	N_2	AB	2
	2	CF stretch	900	gas	AB	1
	3	CF_2 "scissors"	568	gas	AB	1
			586(80)	Ar	AB	2
			641(80)	N_2	AB	2

C_o = 0.196 AB[1]

X $^2B_2$ C_{2v} Structure: AB[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	C=N stretch	1734[a] 1771	Ar	IR	2
	2	CF stretch	955	Ar	IR	2
b_1	4	OPLA	660	Ar	IR	2
b_2	5	CF stretch	1257	Ar	IR	2
	6	CF_2 rock	497	N_2	IR	2

C_o = 0.195 AB[1]

[a] Strong Fermi resonance interaction with $(\nu_5 + \nu_6)$ (A_1).

References

[1]R. N. Dixon, G. Duxbury, R. C. Mitchell, and J. P. Simons, Proc. Roy. Soc. (London) A300, 405 (1967).
[2]M. E. Jacox and D. E. Milligan, J. Chem. Phys. 48, 4040 (1968).

F_2CO^+

F $^2B_1$ C_{2v}

T^a = 54700(900) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF stretch	760(40)	gas	PE	1,2

E $^2A_1$ C_{2v}

T_o = 49000(500) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			490(40)	gas	PE	2

C,D $^2B_2$,$^2A_2$ C_{2v}

T_o = 31390(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO stretch	1500(40)	gas	PE	2
	3	CF_2 "scissors"	555(40)	gas	PE	2

B $^2A_1$ C_{2v}

T_o = 24850(900) gas PE[1,2]

A $^2B_1$ C_{2v}

T_o = 8630(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO stretch	1430(40)	gas	PE	1,2
	2	CF_2 stretch	920(40)	gas	PE	2
	3	CF_2 "scissors"	505(40)	gas	PE	2

X $^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO stretch	1550(40)	gas	PE	1,2
	3	CF_2 "scissors"	530(40)	gas	PE	1,2

[a] From vertical ionization potential.

References

[1]C. R. Brundle, M. B. Robin, N. A. Kuebler, and H. Basch, J. Am. Chem. Soc. 94, 1451 (1972).
[2]R. K. Thomas and H. Thompson, Proc. Roy. Soc. (London) A327, 13 (1972).

Cl_2CO^+

A $^2A_1$ C_{2v}

$T_o{}^a$ = 62450(320) gas PE[1,2]

G $^2B_2$ C_{2v}

T^{ab} = 44860(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO stretch	~1000	gas	PE	1

F $^2B_1$ C_{2v}

$T_o{}^a$ = 41230(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CCl_2 "scissors"	280(40)	gas	PE	1,2

E $^2A_1$ C_{2v}

T_o[a] = 34290(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO stretch	1460(20)	gas	PE	2
	2	CCl_2 stretch	560(60)	gas	PE	1,2
	3	CCl_2 "scissors"	270(50)	gas	PE	1,2

D $^2A_1$ C_{2v}

T_o[a] = 14850(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CCl_2 "scissors"	290(40)	gas	PE	1,2

C $^2A_2$ C_{2v}

T^{ab} = 12100(560) gas PE[1,2]

Ã,B̃ $^2B_1$,$^2B_2$ C_{2v}

T^{ab} = 8500(1000) gas PE[1,2]

X̃ $^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CCl_2 "scissors"	285(40)	gas	PE	1,2

[a] The first ionization potential is taken as 11.55(2) eV, the value given by Ref. 1. Ref. 2 estimates an adiabatic ionization potential of 11.2 eV.
[b] From vertical ionization potential.

References

[1] D. Chadwick, Can. J. Chem. 50, 737 (1972).
[2] R. K. Thomas and H. Thompson, Proc. Roy. Soc. (London) A327, 13 (1972).

F_2CS^+

D̃ $^2A_2$ C_{2v}

T_o = 57690(320) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF_2 stretch	700(40)	gas	PE	1-3
	3	CF_2 "scissors"	500(40)	gas	PE	1,3

C̃ $^2B_2$ C_{2v}

$T^a \sim$ 48200 gas PE[1,3]

B̃ $^2A_1$ C_{2v}

T_o = 35420(320) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CS stretch	1160(60)	gas	PE	1-3
	2	CF_2 stretch	694(40)	gas	PE	3
	3	CF_2 "scissors"	462(40)	gas	PE	3

Ã $^2B_1$ C_{2v}

T_o = 7020(320) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CS stretch	1360(60)	gas	PE	1-3
	2	CF_2 stretch	730(40)	gas	PE	1-3
	3	CF_2 "scissors"	480(40)	gas	PE	1,3

X̃ $^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CS stretch	1350(40)	gas	PE	1-3
	2	CF_2 stretch	758(40)	gas	PE	3
	3	CF_2 "scissors"	460(40)	gas	PE	1-3

[a] From vertical ionization potential.

References

[1]K. Wittel, A. Haas, and H. Bock, Chem. Ber. 105, 3865 (1972).
[2]H. W. Kroto and R. J. Suffolk, Chem. Phys. Lett. 17, 213 (1972).
[3]G. W. Mines, R. K. Thomas, and H. Thompson, Proc. Roy. Soc. (London) A333, 171 (1973).

$FClCS^+$

F $^2A'$ C_s

T^a = 62930(400) gas PE[1]

E $^2A'$ C_s

T^a = 51640(400) gas PE[1]

D $^2A''$ C_s

T^a = 32110(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CS stretch	1130(40)	gas	PE	1

C $^2A'$ C_s

T^a = 27270(320) gas PE[1]

B $^2A'$ C_s

T^a = 21380(320) gas PE[1]

A $^2A''$ C_s

T^a = 8070(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CS stretch	1080(40)	gas	PE	1

X $^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CS stretch	1130(40)	gas	PE	1

[a] From vertical ionization potentials.

References

[1]K. Wittel, A. Haas, and H. Bock, Chem. Ber. 105, 3865 (1972).

Cl_2CS^+

A $^2A_1$ C_{2v}

T_o = 68420(320) gas PE[1-3]

G $^2B_2$ C_{2v}

T_o = 51480(320) gas PE[1-3]

F $^2B_1$ C_{2v}

T_o = 43410(320) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CCl_2 "scissors"	270(80)	gas	PE	3

E $^2A_1$ C_{2v}

T_o = 37280(320) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCl_2 stretch	380(60)	gas	PE	1,3

D $^2A_2$ C_{2v}

T^a = 24850(320) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CCl_2 "scissors"	260(40)	gas	PE	1,3

C $^2B_2$ C_{2v}

T^a = 22350(320) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CCl_2 "scissors"	255(80)	gas	PE	3

B $^2A_1$ C_{2v}

T_o = 16620(320) gas PE[1-3]

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

T_o = 8390(320) gas PE[1-3]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1 1	CS stretch	900(60)	gas	PE	1-3

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

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1 1	CS stretch	1060(40)[b]	gas	PE	1,3
3	CCl_2 "scissors"	265(40)	gas	PE	1,3

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

References

[1]D. Chadwick, Can. J. Chem. 50, 737 (1972).
[2]K. Wittel, A. Haas, and H. Bock, Chem. Ber. 105, 3865 (1972).
[3]G. W. Mines, R. K. Thomas, and H. Thompson, Proc. Roy. Soc. (London) A333, 171 (1973).

F_2CSe^+

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

T^a = 50800(1600) gas PE[1]

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

T^a = 37900(1600) gas PE[1]

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

T^a = 9700(1600) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		1380(100)	gas	PE	1
		650(100)	gas	PE	1

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

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		1380(50)	gas	PE	1
3	CF_2 "scissors"	400(50)	gas	PE	1

[a] From vertical ionization potentials.

References

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$t\text{-}N_2F_2^+$

T_o = 42000(1600) gas PE[1]

$\tilde{A}\ ^2A_u$ C_{2h}

T_o = 6860(1200) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g		980(80)	gas	PE	1

$\tilde{X}\ ^2A_g$ C_{2h}

References

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NO_3

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

T_o = 15089 gas AB[1,2,4-7]LF[8,9] $\tilde{B}$-$\tilde{X}$ 450-795 nm

All bands are diffuse.[2,7]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1' 1	Sym. stretch	930	gas	AB	2,6
		1450	gas	AB	6
		850	gas	AB	6

τ_o = 340(20) μs gas LF[10]

$\tilde{X}\ ^2A_2'$ D_{3h} Structure: DL[11]

Vib. No. sym.	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_o = 0.457 DL[11]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 proposed the reassignment of the 1492 cm^{-1} absorption to the $\tilde{A}$ state.

References

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FNO_2^+

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

T^a = 52520(160) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		1000(80)	gas	PE	1

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

T^a = 46900(1000) gas PE[1]

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

T_o = 39600(1000) gas PE[1]

$\tilde{C},\tilde{D}\ ^2B_2,^2B_1$ C_{2v}

Transitions between approximately 15400 and 32400.[1]

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

T_o = 8960(1000) gas PE[1]

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

T^a = 6620(160) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		1170(80)	gas	PE	1

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

[a] From vertical ionization potential.

References

[1] D. C. Frost, S. T. Lee, C. A. McDowell, and N. P. C. Westwood, J. Electron Spectrosc. Relat. Phenom. 7, 331 (1975).
[2] M. I. Abbas, J. M. Dyke, and A. Morris, J. Chem. Soc., Faraday Trans. 2 814 (1976).

$ClNO_2^+$

$\tilde{E},\tilde{F},\tilde{G}$ C_{2v}

Transitions between approximately 50500 and 62600.[1]

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

T^a = 14360(160) gas PE[1]

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

T_o = 9440(160) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		850(80)	gas	PE	1

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

T_o = 4520(160) gas PE[1]

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

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3 NO_2 "scissors"	420(80)[b]	gas	PE	1

[a] From vertical ionization potential.
[b] Weak structure in first photoelectron band, possibly contributed by low-lying $\tilde{A}\ ^2B_1$ state.

References

[1]D. C. Frost, S. T. Lee, C. A. McDowell, and N. P. C. Westwood, J. Electron Spectrosc. Relat. Phenom. 7, 331 (1975).

SO_3^+ [a]

E $^2A_1'$ D_{3h}

T^b = 62770(320) gas PE[3]

D $^2E'$ D_{3h}

T_o = 40990(160) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	SO_3 stretch	890(20)	gas	PE	1-4
e'	3	SO_3 stretch	1390	gas	PE	4
	4	Deformation	420(50)	gas	PE	2,4

C $^2A_2''$ D_{3h}

T_o = 16470(120) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	SO_3 stretch	890(50)	gas	PE	1-3

A,B $^2E'$,$^2E''$ D_{3h}

T_o = 7930(120) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	SO_3 stretch	730(50)	gas	PE	1-3
e'	4	Deformation	480(50)	gas	PE	1,3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	SO_3 stretch	920(50)	gas	PE	1,2
e'	4	Deformation	440(50)	gas	PE	1-3

[a] Refs. 1-3 disagree on the assignment of the spectrum. The assignment given here is that of Ref. 2; the calculations of both Ref. 2 and Ref. 3 indicate that the ground state possesses A_2 symmetry, and the detailed analysis of the effect of Jahn-Teller perturbation given by Ref. 4 has provided a good fit to the structure of the 17.86 eV photoelectron band for the D $^2E'$ assignment of Ref. 2.

[b] From vertical ionization potential.

References

[1]G. W. Mines and R. K. Thomas, Proc. Roy. Soc. (London) A336, 355 (1974).
[2]D. S. Alderdice and R. N. Dixon, J. Chem. Soc., Faraday Trans. 2 72, 372 (1976).
[3]D. R. Lloyd, P. J. Roberts, I. H. Hillier, and I. C. Shenton, Mol. Phys. 31, 1549 (1976).
[4]F. T. Chau and L. Karlsson, Phys. Scripta 16, 248 (1977).

S_4

Unstructured absorption maximum at 530 nm in the gas phase and in a Kr matrix.[1,2]

X

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			680	Ar	IR	3
			681	Kr	IR	3
			680	Xe	IR	3
			660	Ar	IR	3
			660	Kr	IR	3
			660	Xe	IR	3
			636	Kr	IR	3
			483	Kr	IR	3
			320	Kr	IR	3
			270	Kr	IR	3

References

[1]B. Meyer, T. V. Oommen, and D. Jensen, J. Phys. Chem. 75, 912 (1971).
[2]B. Meyer, T. Stroyer-Hansen, and T. V. Oommen, J. Mol. Spectrosc. 42, 335 (1972).
[3]B. Meyer and T. Stroyer-Hansen, J. Phys. Chem. 76, 3968 (1972).

CF_3

Rydberg state D_{3h}

gas AB[6]MPI[10] 139-165 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	820	gas	AB,MPI	6,10

4s $^2A_1'$ D_{3h}

$T_o \sim 51665$ gas AB[7]EM[11-14,16,20] $4s^2A_1'$-$\tilde{X}$ 180-300 nm

Calculations[14] suggest that this state is of mixed valence-Rydberg character, with increasing Rydberg contribution at large C-F distances.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	~804	gas	EM	12

τ = 12(3) ns gas EM[17,18]

3p $^2A_2''$, $^2E'$ D_{3h}

$T_o \sim 51600$ gas EM[8,11,13,14] 3p-3s $^2A_1'$ 450-750 nm

The lower state of the visible emission of CF_3, calculated[14] to be the 3s $^2A_1'$ state, which assumes increasing valence character at large C-F distances, is both observed and calculated to be dissociative.

τ = 18(3) ns gas EM[17,18]

$\tilde{X}$ $^2A_1$ C_{3v} Structure: ESR[1]MW[9]DL[15]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF stretch	1089	gas	IR,EM	2,12
					CARS	19
			1083	Ne	IR	5
			1087	Ar	IR	3,4
	2	"Umbrella"	701(3)	gas	IR,EM	2,12
			700	Ne	IR	5
			703	Ar	IR	3,4
e	3	CF stretch	1260.16	gas	IR,DL	2,15
			1252	Ne	IR	5
			1251	Ar	IR	3,4

$\tilde{X}$ $^2A_1$---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	4	Deformation	508	Ne	IR	5
			512	Ar	IR	4

B_o = 0.364 MW[9]; C_o = 0.189 DL[15]

References

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19B. J. Bozlee and J. W. Nibler, J. Chem. Phys. 84, 3798 (1986).
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NF_3^+

E ^2E C_{3v}

T_o^a = 65920(900) gas PE[1]

D $^2A_1$ C_{3v}

T_o = 50600(560) gas PE[1]

C ^2E C_{3v}

T_o = 33800(560) gas PE[1]

B $^2A_2$ C_{3v}

T^a = 28900(720) gas PE[1]

A ^2E C_{3v}

T_o = 20330(650) gas PE[1]

X $^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	"Umbrella"	565(40)	gas	PE	2

Barrier to inversion ~ 6000.[2]

[a] From vertical ionization potential.

References

[1]P. J. Bassett and D. R. Lloyd, J. Chem. Soc., Dalton Trans. 248 (1972).
[2]J. Berkowitz and J. P. Greene, J. Chem. Phys. 81, 3383 (1984).

NCl_3^+

E ^2E C_{3v}

T^a = 53100(1200) gas PE[1]

D $^2A_1$ C_{3v}

T^a = 42700(1200) gas PE[1]

C ^2E C_{3v}

T^a = 23400(1000) gas PE[1]

B ^2E C_{3v}

T^a = 15800(1000) gas PE[1]

A $^2A_2$ C_{3v}

T^a = 12400(1000) gas PE[1]

X $^2A_1$ C_{3v}

[a] From vertical ionization potential.

References

[1]D. Colbourne, D. C. Frost, C. A. McDowell, and N. P. C. Westwood, J. Chem. Phys. 69, 1078 (1978).

PF_3^+

E ^2E C_{3v}

$T_o^a \geq$ 61500(200) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PF stretch	660(30)	gas	PE	2
	2	"Umbrella"	360(30)	gas	PE	2

D $^2A_1$ C_{3v}

$T_o^a \geq$ 55000(200) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PF stretch	690(30)	gas	PE	2
	2	"Umbrella"	395(30)	gas	PE	2

C ^2E C_{3v}

$T_o^a \geq$ 45500(200) gas PE[1,2]

B ^2E C_{3v}

$T^{ab} \geq$ 39300(600) gas PE[1,2]

A $^2A_2$ C_{3v}

$T_o^a \geq$ 31220(500) gas PE[1,2]

X $^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	"Umbrella"	475(30)	gas	PE	1,2

[a] In accord with recent photoionization studies,[3,4] the first ionization potential of PF_3 is taken to be ≤ 11.44 eV.
[b] From vertical ionization potential.

References

[1]P. J. Bassett and D. R. Lloyd, J. Chem. Soc., Dalton Trans. 248 (1972).
[2]J. P. Maier and D. W. Turner, J. Chem. Soc., Faraday Trans. 2 68, 711 (1972).
[3]J. Berkowitz and J. P. Greene, J. Chem. Phys. 81, 4328 (1984).
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PF_2Cl^+

F C_s

T^a = 58900(1600) gas PE[1]

E C_s

T^a = 52400(1600) gas PE[1]

D C_s

T^a = 39500(1600) gas PE[1]

C C_s

T^a = 33900(1600) gas PE[1]

B C_s

T^a = 10500(1600) gas PE[1]

X,A C_s

[a] From vertical ionization potentials.

References

[1]S. Cradock and D. W. H. Rankin, J. Chem. Soc., Faraday Trans. 2 68, 940 (1972).

PF_2Br^+

F C_s

T^a = 59220(1000) gas PE[1]

E C_s

T^a = 54380(1000) gas PE[1]

D C_s

T^a = 40660(1000) gas PE[1]

C $^2A'$ C_s

T^a = 32190(320) gas PE[1]

B $^2A'$ C_s

T^a = 7580(1000) gas PE[1]

A C_s

T^a = 5240(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]S. Cradock and D. W. H. Rankin, J. Chem. Soc., Faraday Trans. 2 68, 940 (1972).

PCl_3^+

F $^2A_1$ C_{3v}

T^a = 67050(320) gas PE[1,3]

E ^2E C_{3v}

T^a = 37840(320) gas PE[1-3]

D $^2A_1$ C_{3v}

T^a = 30010(320) gas PE[1-3]

C ^2E C_{3v}

T^a = 19850(320) gas PE[1-3]

B ^2E C_{3v}

T^a = 12020(320) gas PE[1-3]

A $^2A_2$ C_{3v}

T^a = 9600(320) gas PE[1-3]

X $^2A_1$ C_{3v}

[a] From vertical ionization potentials.

References

[1]P. A. Cox, S. Evans, A. F. Orchard, N. V. Richardson, and P. J. Roberts, Faraday Discuss. Chem. Soc. 54, 26 (1972).
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[3]D. G. Nicholson and P. Rademacher, Acta Chem. Scand. A28, 1136 (1974).

PBr_3^+

E ^2E C_{3v}

T^a = 33560(320) gas PE[1-3]

D $^2A_1$ C_{3v}

T^a = 25580(320) gas PE[1-3]

C ^2E C_{3v}

T^a = 14760(320) gas PE[1-3]

B ^2E C_{3v}

T^a = 8390(320) gas PE[1-3]

Spin-orbit splitting = 2660(320) gas PE[1-3]

$\tilde{A}\ ^2A_2$ C_{3v}

T^a = 5240(320) gas PE[1-3]

$\tilde{X}\ ^2A_1$ C_{3v}

[a] From vertical ionization potentials.

References

[1]P. A. Cox, S. Evans, A. F. Orchard, N. V. Richardson, and P. J. Roberts, Faraday Discuss. Chem. Soc. 54, 26 (1972).
[2]J. L. Berkosky, F. O. Ellison, T. H. Lee, and J. W. Rabalais, J. Chem. Phys. 59, 5342 (1973).
[3]D. G. Nicholson and P. Rademacher, Acta Chem. Scand. A28, 1136 (1974).

AsF_3^+

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

T^a = 38890(320) gas PE[1]

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

T^a = 34050(320) gas PE[1]

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

T^a = 25900(320) gas PE[1]

$\tilde{A},\tilde{B}\ ^2E,^2A_2$ C_{3v}

T^a = 18070(320) gas PE[1]

$\tilde{X}\ ^2A_1$ C_{3v}

[a] From vertical ionization potentials.

References

[1]A. W. Potts, H. J. Lempka, D. G. Streets, and W. C. Price, Phil. Trans. Roy. Soc. (London) A268, 59 (1970).

$AsCl_3^+$

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

T^a = 32760(320) gas PE[1,3]

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

T^a = 25820(320) gas PE[1,3]

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

T^a = 16460(320) gas PE[1,3]

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

T^a = 10000(320) gas PE[1,3]

$\tilde{A}\ ^2A_2$ C_{3v}

T^a = 8470(320) gas PE[3]

$\tilde{X}\ ^2A_1$ C_{3v}

[a] From vertical ionization potential. The first ionization potential of $AsCl_3$ is taken as 10.55(2) eV, as in the photoionization and photoelectron spectroscopic studies of Ref. 2.

References

[1]A. W. Potts, H. J. Lempka, D. G. Streets, and W. C. Price, Phil. Trans. Roy. Soc. (London) A268, 59 (1970).
[2]R. A. W. Johnstone and F. A. Mellon, J. Chem. Soc., Faraday Trans. 2 68, 1209 (1972).
[3]T. H. Lee and J. W. Rabalais, J. Chem. Phys. 60, 1172 (1974).

$AsBr_3^+$

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

T^a = 27510(400) gas PE[1,2]

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

T^a = 20650(400) gas PE[1,2]

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

T^a = 10650(400) gas PE[1,2]

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

T^a = 5360(320) gas PE[1,2]

Spin-orbit splitting = 2500(320) gas PE[1]

$\tilde{A}\ ^2A_2$ C_{3v}

T^a = 2500(320) gas PE[1]

$\tilde{X}\ ^2A_1$ C_{3v}

[a] From vertical ionization potentials.

References

[1]T. H. Lee and J. W. Rabalais, J. Chem. Phys. 60, 1172 (1974).
[2]J. B. Peel and G. D. Willett, J. Electron Spectrosc. Relat. Phenom. 9, 175 (1976).

SbF_3^+

$\tilde{F}\ ^2A_1$ C_{3v}

T^a = 50350(320) gas PE[1]

E ^2E C_{3v}

T^a = 32110(320) gas PE[1]

D $^2A_1$ C_{3v}

T^a = 27750(320) gas PE[1]

C ^2E C_{3v}

T^a = 22030(320) gas PE[1]

A,B $^2A_2$,^2E C_{3v}

T^a = 16460(320) gas PE[1]

X $^2A_1$ C_{3v}

[a] From vertical ionization potentials.

References

[1] I. Novak and A. W. Potts, J. Chem. Soc., Dalton Trans. 635 (1983).

$SbCl_3^+$

E ^2E C_{3v}

T^a = 25660(320) gas PE[1,2]

D $^2A_1$ C_{3v}

T^a = 19610(320) gas PE[1,2]

C ^2E C_{3v}

T^a = 12590(320) gas PE[1,2]

A,B $^2A_2$,^2E C_{3v}

T^a = 7020(320) gas PE[1,2]

X $^2A_1$ C_{3v}

[a] From vertical ionization potentials.

References

[1] T. H. Lee and J. W. Rabalais, J. Chem. Phys. 60, 1172 (1974).
[2] D. G. Nicholson and P. Rademacher, Acta Chem. Scand. A28, 1136 (1974).

$SbBr_3^+$

E ^2E C_{3v}

T^a = 24120(320) gas PE[1,2]

D $^2A_1$ C_{3v}

T^a = 17670(320) gas PE[1,2]

C ^2E C_{3v}

T^a = 10090(320) gas PE[1,2]

B ^2E C_{3v}

T^a = 5890(320) gas PE[1,2]

Spin-orbit splitting = 2340(320) gas PE[1]

A $^2A_2$ C_{3v}

T^a = 2740(320) gas PE[1,2]

X $^2A_1$ C_{3v}

[a] From vertical ionization potential. The first ionization potential of $SbBr_3$ is taken as 10.07 eV, as in Ref. 1, and values from the photoelectron spectrum of that study, run at a somewhat lower temperature than that of Ref. 2, were used for the table.

References

[1] T. H. Lee and J. W. Rabalais, J. Chem. Phys. 60, 1172 (1974).
[2] D. G. Nicholson and P. Rademacher, Acta Chem. Scand. A28, 1136 (1974).

F_2SO^+

E C_s

T_o = 47120(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	SF_2 stretch	705(40)	gas	PE	1
	4	SF_2 "scissors"	390(40)	gas	PE	1

D $^2A'$ C_s

T^a = 38570(320) gas PE[1,2]

C $^2A''$ C_s

T^a = 34800(1000) gas PE[1,2]

B $^2A''$ C_s

T_o = 18960(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SO stretch	1180(40)	gas	PE	1,2
	2	SF_2 s-stretch	790(40)	gas	PE	1,2
	4	SF_2 "scissors"	350(40)	gas	PE	1,2

Ã $^2A''$ C_s

T^a = 15330(500) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SO stretch	∿1000	gas	PE	2

X̃ $^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			420(40)	gas	PE	1,2

[a] From vertical ionization potential.

References

[1]G. W. Mines, R. K. Thomas, and H. Thompson, Proc. Roy. Soc. (London) A329, 275 (1972).
[2]D. Chadwick, D. C. Frost, F. G. Herring, A. Katrib, C. A. McDowell, and R. A. N. McLean, Can. J. Chem. 51, 1893 (1973).

Cl_2SO^+

H̃ $^2A''$ C_s

T^a = 44600(1000) gas PE[4]

G̃ $^2A'$ C_s

T^a = 41790(320) gas PE[1,3,4]

F̃ $^2A'$ C_s

T^a = 37360(320) gas PE[1,3,4]

D̃,Ẽ $^2A'$,$^2A''$ C_s

T^a = 16400(1000) gas PE[1,3,4]

C̃ $^2A'$ C_s

T^a = 11780(320) gas PE[1-4]

B̃ $^2A''$ C_s

T^a = 8710(320) gas PE[1-4]

Ã $^2A''$ C_s

T^a = 6620(320) gas PE[1-4]

X̃ $^2A'$ C_s

References

[1]G. W. Mines, R. K. Thomas, and H. Thompson, Proc. Roy. Soc. (London) A329, 275 (1972).
[2]H. Bock and B. Solouki, Angew. Chem. Intern. Ed. 11, 436 (1972).
[3]D. Chadwick, D. C. Frost, F. G. Herring, A. Katrib, C. A. McDowell, and R. A. N. McLean, Can. J. Chem. 51, 1893 (1973).
[4]H. Bock and B. Solouki, Chem. Ber. 107, 2299 (1974).

F_2SS^+

D̃ C_s

T^a = 38900(1000) gas PE[1]

C̃ C_s

T^a ∿ 35700 gas PE[1]

B̃ C_s

T^a = 17180(320) gas PE[1]

Ã C_s

T^a = 5240(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]G. Wagner, H. Bock, R. Budenz, and F. Seel, Chem. Ber. 106, 1285 (1973).

$FSSF^+$

D̃ C_2

T^a = 38400(1000) gas PE[1]

C̃ C_2

T^a = 34400(1000) gas PE[1]

B̃ C_2

T^a = 16940(320) gas PE[1]

Ã C_2

T^a = 3310(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]G. Wagner, H. Bock, R. Budenz, and F. Seel, Chem. Ber. 106, 1285 (1973).

$S_2Cl_2^+$

$\tilde{G}\ ^2B$ C_2

T^a = 48330(400) gas PE[1,2]

$F\ ^2A$ C_2

T^a = 35580(400) gas PE[1,2]

$E\ ^2B$ C_2

$T^a \sim$ 23700 gas PE[1,2]

$D\ ^2A$ C_2

T^a = 23080(400) gas PE[1,2]

$\tilde{C}\ ^2B$ C_2

T^a = 20500(400) gas PE[1,2]

$B\ ^2A$ C_2

T^a = 14280(400) gas PE[1,2]

$\tilde{A}\ ^2B$ C_2

$T^a \sim$ 5160 gas PE[1,2]

$X\ ^2A$ C_2

[a] From vertical ionization potential. The first ionization potential of S_2Cl_2 is taken to equal 9.66(3) eV, from the photoionization study of Ref. 3.

References

[1]R. J. Colton and J. W. Rabalais, J. Electron Spectrosc. Relat. Phenom. 3, 345 (1974).
[2]B. Solouki and H. Bock, Inorg. Chem. 16, 665 (1977).
[3]R. Kaufel, G. Vahl, R. Minkwitz, and H. Baumgärtel, Z. Anorg. Allg. Chem. 481, 207 (1981).

$S_2Br_2^+$

$\tilde{H}$ C_2

T^a = 43300(1000) gas PE[1,2]

$\tilde{G}$ C_2

T^a = 34370(400) gas PE[1,2]

F C_2

$T^a \sim$ 31200 gas PE[1,2]

E C_2

T^a = 20700(1000) gas PE[1,2]

D C_2

T^a = 19100(1000) gas PE[1,2]

$\tilde{C}$ C_2

T^a = 15980(400) gas PE[1,2]

B C_2

T^a = 12590(400) gas PE[1,2]

$\tilde{A}$ C_2

T^a = 5000(400) gas PE[1,2]

[a] From vertical ionization potential. The first ionization potential of S_2Br_2 is taken to equal 9.23(3) eV, from the photoionization study of Ref. 3.

References

[1]R. J. Colton and J. W. Rabalais, J. Electron Spectrosc. Relat. Phenom. 3, 345 (1974).
[2]B. Solouki and H. Bock, Inorg. Chem. 16, 665 (1977).
[3]R. Kaufel, G. Vahl, R. Minkwitz, and H. Baumgärtel, Z. Anorg. Allg. Chem. 481, 207 (1981).

$Se_2Cl_2^+$

$\tilde{H}\ ^2A$ C_2

$T^a \sim$ 39100 gas PE[1]

$\tilde{G}\ ^2B$ C_2

$T^a \sim$ 31000 gas PE[1]

$F\ ^2A$ C_2

$T^a \sim$ 29000 gas PE[1]

$E\ ^2A$ C_2

$T^a \sim$ 21700 gas PE[1]

$D\ ^2B$ C_2

$T^a \sim$ 19900 gas PE[1]

$\tilde{C}\ ^2B$ C_2

$T^a \sim$ 17900 gas PE[1]

B ^2A C_2

$T^a \sim 10000$ gas PE[1]

X,Ã $^2A,^2B$ C_2

[a] From vertical ionization potentials.

References

[1]E. Nagy-Felsobuki and J. B. Peel, J. Chem. Soc., Faraday Trans. 2 76, 148 (1980).

ClF_3^+

F $^2B_2$ C_{2v}

T_o = 33640(900) gas PE[1]

E $^2B_1$ C_{2v}

T^a = 27590(480) gas PE[1]

D $^2A_2$ C_{2v}

T^a = 21860(720) gas PE[1]

C̃ $^2B_2$ C_{2v}

T^a = 17590(720) gas PE[1]

B̃ $^2A_1$ C_{2v}

T_o = 8960(900) gas PE[1]

X̃,Ã $^2B_1,^2A_1$ C_{2v}

[a] From vertical ionization potential.

References

[1]R. L. DeKock, B. R. Higginson, D. R. Lloyd, A. Breeze, D. W. J. Cruickshank, and D. R. Armstrong, Mol. Phys. 24, 1059 (1972).

BrF_3^+

I $^2B_2$ C_{2v}

T^a = 53330(640) gas PE[1]

G̃,H̃ $^2A_1,^2B_1$ C_{2v}

T^a = 43890(480) gas PE[1]

F $^2B_2$ C_{2v}

T_o = 33160(560) gas PE[1]

E $^2B_1$ C_{2v}

T^a = 27920(560) gas PE[1]

D $^2A_2$ C_{2v}

T^a = 23400(560) gas PE[1]

C̃ $^2B_2$ C_{2v}

T^a = 19770(640) gas PE[1]

B̃ $^2A_1$ C_{2v}

T_o = 14440(400) gas PE[1]

X̃,Ã $^2B_1,^2A_1$ C_{2v}

[a] From vertical ionization potential.

References

[1]R. L. DeKock, B. R. Higginson, D. R. Lloyd, A. Breeze, D. W. J. Cruickshank, and D. R. Armstrong, Mol. Phys. 24, 1059 (1972).

6.8. CH_4^+, SiH_4^+, GeH_4^+, NH_4, and Five-Atomic Trihydrides

CH_4^+

$\tilde{C}\ ^2A_1$ T_d

T_o = 78870(160)[a] gas PE[3,6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	2190(80)	gas	PE	6

$\tilde{B}$ [b] C_s ?

T[c] ~ 19240 gas PE[1-3,5,6]

$\tilde{A}$ [b] C_s ?

$T_o \leq$ 13350[a] gas PE[1-3,5,6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1300(100)	gas	PE	5

$\tilde{X}$ [b] C_{2v} Structure: ESR[7] MO[8,10]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1700(100)[d]	gas	PE	5
			1200(100)	gas	PE	3,5

CD_4^+

$\tilde{C}\ ^2A_1$ T_d

T_o = 79400(200) gas PE[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD stretch	1460(80)	gas	PE	3,6

[a] Based on adiabatic ionization potential of 12.615(10) eV for CH_4[4,5] and of 12.658(15) eV for CD_4.[9]
[b] Resulting from Jahn-Teller distortion of the ground $^2T_2$ state of CH_4^+.
[c] From vertical ionization potential.
[d] Two progressions, with onset near 3670.

References

[1] A. D. Baker, C. Baker, C. R. Brundle, and D. W. Turner, Int. J. Mass Spectrom. Ion Phys. 1, 285 (1968).
[2] B. P. Pullen, T. A. Carlson, W. E. Moddeman, G. K. Schweitzer, W. E. Bull, and F. Grimm, J. Chem. Phys. 53, 768 (1970).
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[10] R. F. Frey and E. R. Davidson, J. Chem. Phys. 88, 1775 (1988).

SiH_4^+

$\tilde{C}\ ^2A_1$ T_d

T_o = 56070(240)[a] gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiH stretch	1690(30)	gas	PE	2

$\tilde{A},\tilde{B}$ [b]

$T_o \leq$ 14930(240)[a] gas PE[1,2]

$\tilde{X}$ [bc] C_s Structure: MO[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			760(10)	gas	PE,PI	1,2,4

[a] Based on adiabatic ionization potential of 11.00(2) eV for SiH_4.[4]
[b] Resulting from Jahn-Teller distortion of the ground $^2T_2$ state of SiH_4^+.
[c] Threshold for formation of $SiH_2^+ + H_2$ = 4360(240) and for formation of $SiH_3^+ + H \leq$ 8760.[4]

References

[1] B. P. Pullen, T. A. Carlson, W. E. Moddeman, G. K. Schweitzer, W. E. Bull, and F. A. Grimm, J. Chem. Phys. 53, 768 (1970).
[2] A. W. Potts and W. C. Price, Proc. Roy. Soc. (London) A326, 165 (1972).
[3] J. A. Pople and L. A. Curtiss, J. Phys. Chem. 91, 155 (1987).
[4] J. Berkowitz, J. P. Greene, H. Cho, and B. Ruščić, J. Chem. Phys. 86, 1235 (1987).

GeH_4^+

$\tilde{C}\ ^2A_1$ T_d

$T_o \geq 55430(160)$[a] gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	GeH stretch	1534(30)	gas	PE	2

$\tilde{A},\tilde{B}$ [b]

$T_o \geq 9040(160)$[a] gas PE[1,2]

$\tilde{X}$ [b]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			670(20)	gas	PE	1,2

[a] Based on an adiabatic ionization potential of 11.34 eV.[2] As for CH_4 and SiH_4, the true adiabatic ionization potential is likely to be substantially lower than the value obtained by photoelectron spectroscopy.
[b] Resulting from Jahn-Teller distortion of the ground $^2T_2$ state of GeH_4^+.

References

[1]B. P. Pullen, T. A. Carlson, W. E. Moddeman, G. K. Schweitzer, W. E. Bull, and F. A. Grimm, J. Chem. Phys. 53, 768 (1970).
[2]A. W. Potts and W. C. Price, Proc. Roy. Soc. (London) A326, 165 (1972).

NH_4

3p $^2F_2$ T_d

$T_o \sim 15078$[ab] gas EM[1,2,4] $3p^2F_2$-$3s^2A_1$ 663.5 nm

Diffuse.

3s $^2A_1$ T_d

gas $3p^2F_2$-$3s^2A_1$ 663.5 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NH stretch[c]	2552	gas	EM	1,4
e	2	Deformation[c]	1581	gas	EM	1,4

ND_4

3p $^2F_2$ T_d

T_o[a] = 14828.285(4) gas EM[1,2,4] AB[3,5]

$3p^2F_2$-$3s^2A_1$ 675 nm

Three weak bands have been observed[4] 775, 1138, and 1722 cm^{-1} above the band origin. However, the assignment of these bands has not yet been established.

B_o = 3.122 gas AB[5]

3s $^2A_1$ T_d

gas $3p^2F_2$-$3s^2A_1$ 675 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ND stretch[c]	1960	gas	EM	1,4
e	2	Deformation	1080.25(7)	gas	EM	7

$\tau \sim 30$ μs gas AB[5]

B_o = 3.041 gas AB[5]

[a] Measured with respect to the lowest Rydberg state, 3s $^2A_1$. The ground state is dissociative.
[b] Estimated[5] by scaling of data for ND_4.
[c] Tentative assignment.

References

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[7]J. K. G. Watson, Proc. 17th International Symposium on Free Radicals, Nat. Bur. Stand. (U. S.) Spec. Publ. 716, K. M. Evenson, Ed., pp. 650-670 (1986).

$CaCH_3$

$\tilde{B}\ ^2A_1$ C_{3v}

T_o = 16003(10) gas LF[1] $\tilde{B}$-$\tilde{X}$ 620-630 nm

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

T_o = 14700(10)[a] gas LF[1] $\tilde{A}$-$\tilde{X}$ 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 = 79(20) gas LF[1]

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 "umbrella"	1085(10)	gas	LF	1
	3	CaC stretch	419(10)	gas	LF	1
e	6	CaCH deform.	319(5)[b]	gas	LF	1

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

References

[1]C. R. Brazier and P. F. Bernath, J. Chem. Phys. 86, 5918 (1987).

$SrCH_3$

$\tilde{B}\ ^2A_1$ C_{3v}

T_o = 14777(10) gas LF[1] $\tilde{B}$-$\tilde{X}$ 670-680 nm

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

T_o = 13653(10)[a] gas LF[1] $\tilde{A}$-$\tilde{X}$ 670-740 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 "umbrella"	1054(10)	gas	LF	1
	3	SrC stretch	373(10)	gas	LF	1
e	6	SrCH deform.	342(5)[b]	gas	LF	1

A = 273(20) gas LF[1]

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 "umbrella"	1072(10)	gas	LF	1
	3	SrC stretch	362(10)	gas	LF	1
e	6	SrCH deform.	279(5)[b]	gas	LF	1

[a] Predissociated above ∿ 15000.[1]
[b] $\frac{1}{2}(2\nu_6)$.

References

[1]C. R. Brazier and P. F. Bernath, J. Chem. Phys. 86, 5918 (1987).

C_2H_3

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

$T_o \leq 20020$ gas AB[1] 500-400 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CC stretch	1200	gas	AB	2
		CCH bend	920	gas	AB	2

References

[1]H. E. Hunziker, H. Kneppe, A. D. McLean, P. Siegbahn, and H. R. Wendt, Can. J. Chem. 61, 993 (1983).

CH_2NH^+

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

T ∿ 52400 gas PE[1]

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

T ∿ 34600 gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2530(160)	gas	PE	1
			1660(160)	gas	PE	1

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

T ∿ 18300 gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CN stretch	1370(160)	gas	PE	1

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

References

[1]J. B. Peel and G. D. Willett, J. Chem. Soc., Faraday Trans. 2 71, 1799 (1975).

CH_2NH

Photodissociates, producing HNC, on irradiation at 254 nm.[2]

$\tilde{X}\ ^1A'$ C_s Structure: MW[3,4,6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH stretch	3262.62	gas	IR	10,12
	2	CH stretch	3024.45	gas	IR	14
			3036	Ar	IR	1,5
	3	CH stretch	2914.18	gas	IR	10,14
			2926	Ar	IR	1,5
	4	C=N stretch	1638.30	gas	LS,IR	7,8,10
			1641	Ar	IR	1,5
	5	CH_2 "scissors"	1452.04	gas	IR	8-10
			1453	Ar	IR	1,5
	6	HCNH deform.	1344.27	gas	IR	8-10
			1348	Ar	IR	1,5
	7	HCNH deform.	1058.18	gas	IR	10,13, 15
			1059	Ar	IR	1,5
a"	8	Torsion	1126.99	gas	IR	10,11, 13,15
			1123	Ar	IR	1,5
	9	H_2CN OPLA	1060.76	gas	IR	10,13, 15
			1063	Ar	IR	1,5

A_o = 6.545; B_o = 1.156; C_o = 0.979 MW[3]

CD_2ND

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CD stretch	2269	Ar	IR	1,5
	3	CD stretch	2184	Ar	IR	1,5
	4	C=N stretch	1577	Ar	IR	1,5
	5	DCND deform.	1089	Ar	IR	1,5
a'	6	CD_2 "scissors"	1067	Ar	IR	1,5
	7	DCND deform.	770	Ar	IR	1,5
a"	9	Torsion	821	Ar	IR	1,5

A_o = 3.406; B_o = 0.904; C_o = 0.712 MW[6]

References

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CH_3N

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

T_o = 31823.915(7)	gas	AB[1],EM[1,2,4]	$\tilde{A}$-$\tilde{X}$ 300-348 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		CH_3 rock	748(4)[a]	gas	EM	2

A = -22.872(7) gas EM^4

B_o = 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 s-stretch	2938(4)	gas	EM	2
	2	CH_3 deform.	1350(4)	gas	EM	2
	3	CN stretch	1039(4)	gas	EM	2
			1029	N_2	AB	3
e	4	CH_3 a-stretch	3065(4)	gas	EM	2
	6	CH_3 rock	902(4)	gas	EM	2

B_o = 0.931 EM^4

CD_3N

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

T_o = 31774.158(2)[b] gas AB^1,$EM^{2,4}$ $\tilde{A}$-$\tilde{X}$ 308-340 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
e		CD_3 rock	579(4)[a]	gas	EM	2

B_o = 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	1	CD_3 s-stretch	2108(4)	gas	EM	2
	2	CD_3 deform.	932(4)	gas	EM	2
	3	CN stretch	1108(4)	gas	EM	2

$\tilde{X}\ ^3A_2$---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	6	CD_3 rock	745(4)	gas	EM	2

B_o = 0.744 EM^4

[a] Observed as sequence band.
[b] Calculated assuming $A(CD_3N) = A(CH_3N)$.

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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.[14]

$\tilde{A}\ ^2A_1$ C_{3v}

T_o = 31614.5 gas $EM^{1,2,11,12}$ AB^5 $LF^{6,8,16}$

$\tilde{A}$-$\tilde{X}$ 271-421 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	16
	2	"Umbrella"	1315	gas	LF	16
	3	CO stretch	660	gas	AB,EM LF	5,12,16
e	4	CH_3 stretch	2962	gas	LF	16
	5	CH_2 "scissors"	1407	gas	LF	16
	6	HCO deform.	595	gas	LF	16

τ = 2.2(2)μs gas $EM^{2,9}$ $LF^{4,15}$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 stretch	2840	gas	LF	16
	2	CH_3 "umbrella"	1362	gas	LF	16
	3	CO stretch	1047	gas	LF,EM	6,9,12 16
e	4	CH_3 stretch	2774[b]	gas	LF	16
	5	CH_2 "scissors"	1487	gas	LF	16
	6	HCO deform.	653	gas	LF	16

A = -62.24(17) gas LMR[7]MW[10]EM[11,12]LF[16]

A_o = 5.21; B_o = 0.932 LMR[7]MW[10]

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.[14]

$\tilde{A}\ ^2A_1$

T_o = 31554 gas LF[6,16]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	16
	2	CD_3 "umbrella"	971	gas	LF	16
	3	CO stretch	663	gas	EM,LF	12,16
e	5	CD_2 "scissors"	1047	gas	LF	16

$\tilde{X}\ ^2E$ 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	16
	3	CD_3 "umbrella"	893[b]	gas	LF	16
e	5	CD_2 "scissors"	1174	gas	LF,EM	6,12,16
	6	DCO deform.	496	gas	LF	16

A = -56(2) gas EM[12]

[a] Somewhat distorted by Jahn-Teller coupling.
[b] Tentative assignment.

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CH_2OH

3p Rydberg state C_s

T_o = 41064 gas MPI[3,4] 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
a'	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

$\tilde{A}$

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

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OH stretch	3650	Ar	IR	1,2
			3637	N_2	IR	1
	4	CH_2 "scissors"	1459	Ar	IR	2
	5	OH deform.	1334	Ar	IR	1,2
	6	CO stretch	1183	Ar	IR	1,2
			1183	N_2	IR	1
	7	HCOH deform.	1048	Ar	IR	1,2
			1056	N_2	IR	1
	8	CH_2 rock	607(15)	gas	MPI	4
	9	Torsion	420	Ar	IR	1,2
			482	N_2	IR	1

CD_2OD

3p Rydberg state C_s

T_o = 40913 gas MPI[3,4] 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	3
	5	COD bend + CD_2 rock	803	gas	MPI	3
	6	CO stretch	1565	gas	MPI	3,4
a"	9	Torsion	440	gas	MPI	3

$\tilde{A}$

Threshold for photodecomposition into D_2CO + D near 280 nm.[1,2]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OD stretch	2694	Ar	IR	2
			2682	N_2	IR	1
	4	CO stretch	1223	Ar	IR	2
			1222	N_2	IR	1
	5		1041	Ar	IR	2

$\tilde{X}$---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	7		765	Ar	IR	2
	8	CD_2 rock	498(15)	gas	MPI	4

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CH_3S

A diffuse, unstructured band at 218.5 nm, observed on flash photolysis of a number of sulfur-containing compounds, has been attributed[1] to CH_3S.

$\tilde{A}\ ^2A_1$ C_{3v}

T_o = 26531 gas EM^{2}LF[6] $\tilde{A}$-$\tilde{X}$ 365-520 nm

Predissociation threshold ≦ 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	403(1)	gas	EM,LF	2,6

τ_o = 310(20) ns gas LF[6]; 760(60) ns gas LF[8]

$\tilde{X}\ ^2E$ C_{3v} Structure: MW[7]

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 = -220.3 gas MW[7]

B_o = 0.45 MW[7]

CD_3S

$\tilde{A}\ ^2A_1$ C_{3v}

T_o = 26574 gas LF[6] $\tilde{A}$-$\tilde{X}$ 352-378 nm

Predissociation threshold ≦ 27728.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_3 "umbrella"	837(1)	gas	LF	6
	3	CS stretch	395(1)	gas	LF	6

τ_o = 0.45(11) μs gas LF[6]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_3 "umbrella"	1100(50)	gas	PD	4
	3	CS stretch	667(1)	gas	PD,LF	4,6
e	5	DCS deform.	780[a]	gas	PD	4

[a] $\frac{1}{2}(2\nu_5)$; $2\nu_5$ = 1560(50).

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CH_3F^+

$\tilde{C}\ ^2A_1$ C_{3v}

$T_o \sim 87700$ gas PE[2,4]

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

$T_o \sim 30400$ gas PE[1-5]

A weak, broad absorption maximum at 255 nm (39200) which appears on argon-resonance photolysis of CH_3F isolated in solid argon and which can be destroyed by mercury-arc photolysis has been attributed[6] to the $\tilde{A},\tilde{B}$-$\tilde{X}$ transition of CH_3F^+.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CF stretch	695(80)	gas	PE	5
e	5	CH_3 deform.	1315(80)	gas	PE	5
	6	HCF deform.	880(80)	gas	PE	5

[a] The high resolution PE spectrum[5] suggests a Jahn-Teller splitting of ∿ 4800, with excitation of a progression in ν_5 (∿1050) in the higher energy component.

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CH_3Cl^+

$\tilde{C}\ ^2A_1$ C_{3v}

T^a = 82400(900) gas PE[2]

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

T^a = 33170(900) gas PE[1-4,7]

Position of first maximum is given. A Jahn-Teller splitting of ∿ 5000 is observed.[4,7]

A weak, broad absorption with onset near 400 nm (25000) and maximum at 335 nm (29800) which appears on argon-resonance photolysis of CH_3Cl isolated in an argon matrix and which is destroyed by exposure of the sample to 290-1000 nm radiation has been attributed[6] to the $\tilde{B}$-$\tilde{X}$ and $\tilde{A}$-$\tilde{X}$ transitions of CH_3Cl^+.

$\tilde{A}\ ^2A_1$ C_{3v}

T_o = 20260(900) gas PE[1-4,7]

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

Analysis of Ref. 5 suggests that the observed splitting of 218(50) is predominantly due to the Jahn-Teller effect and that the structure is distorted to C_s or C_1 symmetry. Small differences between the vibrational spacings observed for the two components of the overall transition are within the experimental error.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 "umbrella"	1073(50)	gas	PE	2,4
	3	CCl stretch	654(50)	gas	PE	3,4
e	5	CH_3 deform.	1550(50)	gas	PE	3,4
	6	CH_3 rock	870(50)	gas	PE	3,4

[a] From vertical ionization potential.

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CH_3Br^+

$\tilde{C}\ ^2A_1$ C_{3v}

T^a = 75500(900) gas PE[1]

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

T_o = 31930(900) gas PE[1,3]

A Jahn-Teller splitting of ~ 5600 is observed.[1-3] (Onset of the transition is given.)

A broad absorption with maximum at 267 nm (37400) which appears on argon-resonance photolysis of CH_3Br isolated in an argon matrix and which has a photodecomposition threshold at a wavelength longer than 500 nm has been assigned[5] to the $\tilde{B}$-$\tilde{X}$ transition of CH_3Br^+.

$\tilde{A}\ ^2A_1$ C_{3v}

T_o = 19820(900) gas PE[1-3]

A broad absorption with maximum at 348 nm (28700) which appears on argon-resonance photolysis of CH_3Br isolated in an argon matrix and which has a photodecomposition threshold at a wavelength longer than 500 nm has been assigned[5] to the $\tilde{A}$-$\tilde{X}$ transition of CH_3Br^+.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 stretch[b]	2930(120)	gas	PE	3
	2	CH_3 "umbrella"	1290(80)	gas	PE	1-3
	3	CBr stretch	468(80)	gas	PE	3
e	4	CH_3 stretch	3130(100)	gas	PE	2,3
	6	CH_3 rock	850(80)	gas	PE	1-3

Spin-orbit splitting = 2570(100) gas PE[2-4]

CD_3Br^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_3 "umbrella"	947(80)	gas	PE	2
e	4	CD_3 stretch	2165(80)	gas	PE	2

Spin-orbit splitting = 2730(100) gas PE[2]

[a] From vertical ionization potential.
[b] Identified for $^2E_{1/2}$, but not for $^2E_{3/2}$.

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CH_3I^+

$\tilde{C}\ ^2A_2$ C_{3v}

T^a = 81200(900) gas PE[1]

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

T_o = 35180(900) gas PE[1-3]
A Jahn-Teller splitting of ~ 5600 is observed.[1-3] (Onset of the transition is given.)

$\tilde{A}\ ^2A_1$ C_{3v}

T_o = 18816 gas PE[1-3]PF[6-10]

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"	1185	gas	PF	9,10
	3	CI stretch	303	gas	PE,PF	3,9,10

A^b = 5.07(5); B^b = 0.185 PF[6,8]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 stretch[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 = 5045 gas PE[1-4]PF[9]

CD_3I^+

$\tilde{A}\ ^2A_1$ C_{3v}

T_o = 18946 gas PE,PF[7,9,10]

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"	916	gas	PF	10
	3	CI stretch	282	gas	PF	10

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_3 "umbrella"	952	gas	PF	7

[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 $^2E_{3/2}$.

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SiH_3F^+

$\tilde{C}\ ^2A_1$ C_{3v}

T^a = 52400(400) gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			~800	gas	PE	2

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

$T^a \sim$ 28900 gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiH_3 stretch	1470(80)	gas	PE	2

$\tilde{A}\ ^2A_1$ C_{3v}

$T^a \sim$ 26900 gas PE[1,2]

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

Jahn-Teller splitting = 3550(160).[2]

[a] From vertical ionization potentials. Transitions are measured from first maximum in the photoelectron spectrum.

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. 67, 3425 (1971).
[2]D. C. Frost, F. G. Herring, A. Katrib, R. A. N. McLean, J. E. Drake, and N. P. C. Westwood, Can. J. Chem. 49, 4033 (1971).

SiH_3Cl^+

C $^2A_1$ C_{3v}

T^a = 51900(500) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiH_3 stretch	1760(80)[b]	gas	PE	1,2

B ^2E C_{3v}

T^a ∿ 18000 gas PE[1,2]

A $^2A_1$ C_{3v}

T^a = 14400(1000) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	SiCl stretch	480(40)	gas	PE	1

X ^2E C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	SiCl stretch	520(40)	gas	PE	1,2

[a] From vertical ionization potentials.
[b] ∿1320 for SiD_3Cl^+.[2]

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. 67, 3425 (1971).
[2]D. C. Frost, F. G. Herring, A. Katrib, R. A. N. McLean, J. E. Drake, and N. P. C. Westwood, Can. J. Chem. 49, 4033 (1971).

SiH_3Br^+

D $^2A_1$ C_{3v}

T^a = 68900(1000) gas PE[1]

C $^2A_1$ C_{3v}

T^a = 57120(320) gas PE[1,2]

B ^2E C_{3v}

T^a = 20500(1000) gas PE[1,2]

Jahn-Teller splitting = 3200(320) gas PE[2]

A $^2A_1$ C_{3v}

T^a = 15250(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	SiBr stretch	400(80)	gas	PE	2

X $^2E_{3/2}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			∿320	gas	PE	2

Spin-orbit splitting = 1600(320) gas PE[2]

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. 67, 3425 (1971).
[2]D. C. Frost, F. G. Herring, A. Katrib, R. A. N. McLean, J. E. Drake, and N. P. C. Westwood, Can. J. Chem. 49, 4033 (1971).

SiH_3I^+

B ^2E C_{3v}

T^a = 24400(1000) gas PE[1]

A $^2A_1$ C_{3v}

T^a = 18230(320) gas PE[1]

X $^2E_{3/2}$ C_{3v}

Spin-orbit splitting = 4440(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. 67, 3425 (1971).

GeH_3F^+

Ã,B̃ $^2A_1$,^2E C_{3v}

$T^a \sim 22000$ gas PE[1]

X̃ ^2E C_{3v}

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. 67, 3425 (1971).

GeH_3Cl^+

B̃ ^2E C_{3v}

T^a = 16100(1000) gas PE[1]

Ã $^2A_1$ C_{3v}

T^a = 14120(320) gas PE[1]

X̃ ^2E C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	GeCl stretch	∿400	gas	PE	1

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. 67, 3425 (1971).

GeH_3Br^+

B̃ ^2E C_{3v}

T^a = 18500(1000) gas PE[1]

Ã $^2A_1$ C_{3v}

T^a = 15330(320) gas PE[1]

X̃ $^2E_{3/2}$ C_{3v}

Spin-orbit splitting = 1775(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. 67, 3425 (1971).

GeH_3I^+

B̃ ^2E C_{3v}

T^a = 24300(1000) gas PE[1]

Ã $^2A_1$ C_{3v}

T^a = 17100(320) gas PE[1]

X̃ $^2E_{3/2}$ C_{3v}

Spin-orbit splitting = 4440(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. 67, 3425 (1971).

NH_2OH^+

D̃ $^2A''$ C_s

T^a = 54500(1000) gas PE[2]

C̃ $^2A'$ C_s

T^a = 50100(1000) gas PE[1,2]

B̃ $^2A'$ C_s

T^a = 39620(320) gas PE[1,2]

Ã $^2A''$ C_s

T^a = 8960(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3100(160)	gas	PE	1,2

X̃ $^2A'$ C_s

[a] From vertical ionization potentials.

References

[1]K. Kimura and S. Katsumata, J. Chem. Phys. 67, 1225 (1977).
[2]P. Rademacher and B. Freckmann, J. Electron Spectrosc. Relat. Phenom. 19, 251 (1980).

6.9. Five-Atomic Dihydrides

$(C_2H_2)Ni$

Exposure of the sample isolated in solid argon to radiation of wavelength longer than 400 nm results in isomerization to $NiC{=}CH_2$.[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		C=C stretch	1647.4	Ar	IR	1
		CH bend	847.3	Ar	IR	1
b_1		CH bend	730.9	Ar	IR	1
b_2		CH bend	658.1	Ar	IR	1
?		CNi stretch	548.6	Ar	IR	1

$(C_2D_2)Ni$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		C=C stretch	1540.6	Ar	IR	1
		CD bend	718.6	Ar	IR	1
b_1		CD bend	548.4	Ar	IR	1
b_2		CD bend	506.2	Ar	IR	1
?		CNi stretch	507.4	Ar	IR	1

References

[1]E. S. Kline, Z. H. Kafafi, R. H. Hauge, and J. L. Margrave, J. Am. Chem. Soc. 109, 2402 (1987).

$NiC{=}CH_2$

In an argon matrix, isomerizes to $(C_2H_2)Ni$ on exposure to radiation of wavelength between 280 and 360 nm.[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s-stretch	2889.1	Ar	IR	1
	2	C=C stretch	1635.0	Ar	IR	1
b_1	6	H_2CC OPLA	758.6	Ar	IR	1

$\tilde{X}$---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	8	CH_2 a-stretch	2983.5	Ar	IR	1
	9	CH_2 rock	833.6	Ar	IR	1

$NiC{=}CD_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C=C stretch	1626.2	Ar	IR	1
b_1	6	H_2CC OPLA	606.3	Ar	IR	1

References

[1]E. S. Kline, Z. H. Kafafi, R. H. Hauge, and J. L. Margrave, J. Am. Chem. Soc. 109, 2402 (1987).

cyclo-C_3H_2

Photodecomposition threshold in an argon matrix near 360 nm; linear C_3H_2 formed.[1,6]

$\tilde{X}$ C_{2v} Structure: MW[4,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1278.6 1277.7	Ar	IR	1,6
			1063.6	Ar	IR	1,6
			887.1	Ar	IR	1,6
			787.8	Ar	IR	1,6

$A_o = 1.171$; $B_o = 1.075$; $C_o = 0.559$ MW[2-5]

References

[1]H. P. Reisenauer, G. Maier, A. Riemann, and R. W. Hoffmann, Angew. Chem. 96, 596 (1984); Angew. Chem. Int. Ed. Engl. 23, 641 (1984).
[2]P. Thaddeus, J. M. Vrtilek, and C. A. Gottlieb, Astrophys. J. 299, L63 (1985).
[3]M. Bogey, C. Demuynck, and J. L. Destombes, Chem. Phys. Lett. 125, 383 (1986).
[4]M. Bogey, C. Demuynck, J. L. Destombes, and H. Dubus, J. Mol. Spectrosc. 122, 313 (1987).
[5]J. M. Vrtilek, C. A. Gottlieb, and P. Thaddeus, Astrophys. J. 314, 716 (1987).

[6]G. Maier, H. P. Reisenauer, W. Schwab, P. Čársky, B. A. Hess, Jr., and L. J. Schaad, J. Am. Chem. Soc. 109, 5183 (1987).

$H_2C=C=C:$

Photoisomerization to HCCCH occurs at 254 nm.[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s-stretch	3059.6 3049.5	Ar	IR	1
	2	C_3 a-stretch	1963.2 1952.2	Ar	IR	1
	3	CH_2 "scissors"	1449.3 1446.9	Ar	IR	1
b_1	5	H_2CC OPLA	1004.8 999.5	Ar	IR	1
b_2	8	CH_2 rock	1025.0	Ar	IR	1

$D_2C=C=C:$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_2 s-stretch	2212.5 2200.5	Ar	IR	1
	2	C_3 a-stretch	1944.4 1933.4	Ar	IR	1
	3	CD_2 "scissors" + C_3 s-stretch	1208.7	Ar	IR	1
	4	C_3 s-stretch + CD_2 "scissors"	950.8	Ar	IR	1
b_1	5	D_2CC OPLA	803.2 800.3	Ar	IR	1
b_2	8	CD_2 rock	832.6 829.2	Ar	IR	1

[a] Singlet state.

References

[1]G. Maier, H. P. Reisenauer, W. Schwab, P. Čársky, B. A. Hess, Jr., and L. J. Schaad, J. Am. Chem. Soc. 109, 5183 (1987).

HCCCH

Prolonged 313-nm irradiation of HCCCH isolated in solid argon leads to its isomerization to $H_2C=C=C:$, which has a singlet ground state.[5]

An absorption band system of singlet HCCCH has been identified[2] in the 310-370-nm spectral region, but a detailed analysis has not been reported. Beyond 28900 the bands are diffuse, and a continuous absorption is superposed on the short wavelength end of the band system. The molecule is linear in at least one of the states of the transition. A progression involving an upper-state vibrational frequency of 1094 has been tentatively identified. The preliminary analysis found B' = 0.310 and B" = 0.324.

$\tilde{X}\ ^3\Sigma$ $D_{\infty h}$ Structure: ESR[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	CH stretch	3293.0 3266.0	Ar	IR	5
			3285	Kr	IR	3
	4	C_3 a-stretch	2140	Kr	IR	3
Π_u	6	C_3 deform.	408.8 402.6	Ar	IR	4,5
			408	Kr	IR	3
	7	HCC deform.	259.9 245.9	Ar	IR	4,5
			258	Kr	IR	3

DCCCD

$\tilde{X}\ ^3\Sigma$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	CD stretch	2472	Ar	IR	4
			2482	Kr	IR	3
	4	C_3 a-stretch	2065?	Kr	IR	3
Π_u	6	C_3 deform.	392	Kr	IR	3
	7	DCC deform.	171	Ar	IR	4

References

[1]R. A. Bernheim, R. J. Kempf, J. V. Gramas, and P. S. Skell, J. Chem. Phys. 43, 196 (1965).
[2]A. J. Merer, Can. J. Phys. 45, 4103 (1967).
[3]F. K. Chi, Ph.D. thesis, Michigan State University (1972).
[4]M. E. Jacox and D. E. Milligan, Chem. Phys. 4, 45 (1974).
[5]G. Maier, H. P. Reisenauer, W. Schwab, P. Čársky, B. A. Hess, Jr., and L. J. Schaad, J. Am. Chem. Soc. 109, 5183 (1987).

H_2CCO^+

E $^2A_1$ C_{2v}

T^b = 69270(900)[a] gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CH_2 "scissors"	~1210	gas	PE	2

D $^2A_1$ C_{2v}

T^b = 57170(900)[a] gas PE[2]

C $^2B_2$ C_{2v}

T_o = 52170(230)[a] gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CH_2 "scissors"	1020(80)	gas	PE	1,2

B $^2B_1$ C_{2v}

T_o = 40230(230)[a] gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4	CCO s-stretch	950(80)	gas	PE	1,2

A $^2B_2$ C_{2v}

T_o = 34100(230)[a] gas PE[1-3]

X $^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCO a-stretch	2220(80)	gas	PE	2,3
	4	CCO s-stretch	1080(80)	gas	PE	2,3

D_2CCO^+

E $^2A_1$ C_{2v}

T^b = 69270(900)[a] gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CD_2 "scissors"	~810	gas	PE	2

D $^2A_1$ C_{2v}

T^b = 57170(900)[a] gas PE[2]

C $^2B_2$ C_{2v}

T_o = 52170(230)[a] gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CD_2 "scissors"	860(80)	gas	PE	2

B $^2B_1$ C_{2v}

T_o = 40230(230)[a] gas PE[2,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4	CCO s-stretch	950(80)	gas	PE	2

A $^2B_2$ C_{2v}

T_o = 34100(230)[a] gas PE[2,3]

X $^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCO a-stretch	2220(80)	gas	PE	2,3
	4	CCO s-stretch	1080(80)	gas	PE	2,3

[a] Calculated using first ionization potential of 9.614(8) eV, from photoionization measurements of Ref. 3.
[b] From vertical ionization potential.

References

[1] D. Baker and D. W. Turner, J. Chem. Soc. D 480 (1969).
[2] D. Hall, J. P. Maier, and P. Rosmus, Chem. Phys. 24, 373 (1977).
[3] J. Vogt, A. D. Williamson, and J. L. Beauchamp, J. Am. Chem. Soc. 100, 3478 (1978).

H_2CCN^-

Threshold for electron detachment from ground-state H_2CCN^- ∿ 12500 gas PD[1,3] PE[2]

Dipole-Bound State C_{2v}

T_o = 12428.665(2) gas PD[3]

A_o = 9.510; B_o = 0.341; C_o = 0.329 PD[3]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	5	H_2CC deform.	424.77[a]	gas	PD,PE	1-3

Barrier to inversion = 100(50) gas PE[2]

A_o = 9.294; B_o = 0.338; C_o = 0.327 PD[1,3] PE[2]

D_2CCN^-

Threshold for electron detachment from ground-state D_2CCN^- ∿ 12430 gas PD[1,3] PE[2]

Dipole-Bound State C_{2v}

T_o = 12360.434 gas PD[3]

A_o = 4.771; B_o = 0.302; C_o = 0.284 PD[3]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	5	D_2CC deform.	289.13[b]	gas	PD,PE	1-3

A_o = 4.695; B_o = 0.300; C_o = 0.283 PD[1,3] PE[2]

[a] $1^+ - 0^+$ band separation.[3] $0^\pm$ inversion splitting = 152.[2]
[b] $1^+ - 0^+$ band separation.[3] $0^\pm$ inversion splitting = 101.[2]

References

[1] J. Marks, D. M. Wetzel, P. B. Comita, and J. I. Brauman, J. Chem. Phys. 84, 5284 (1986).
[2] S. Moran, H. B. Ellis, Jr., D. J. DeFrees, A. D. McLean, and G. B. Ellison, J. Am. Chem. Soc. 109, 5996 (1987).
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H_2CNC^-

Threshold for electron detachment from ground-state H_2CNC^- = 8540(190) gas PE[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	5	H_2CN deform.	374[a]	gas	PE	1

Barrier to inversion = 650(50) gas PE[1]

A = 8.07(28); B = 0.366(10); C = 0.357 PE[1]

D_2CNC^-

Threshold for electron detachment from ground-state D_2CNC^- = 8630(190) gas PE[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	5	D_2CN deform.	335[b]	gas	PE	1

A = 4.18(17); B = 0.327; C = 0.312 PE[1]

[a] From computer fit. $0^\pm$ inversion splitting = 5 PE[1]
[b] From computer fit. $0^\pm$ inversion splitting = 1 PE[1]

References

[1] S. Moran, H. B. Ellis, Jr., D. J. DeFrees, A. D. McLean, S. E. Paulson, and G. B. Ellison, J. Am. Chem. Soc. 109, 6004 (1987).

H_2CCS^+

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

T_e ∿ 67000 gas PE[1,2]

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

T_e ∿ 53300 gas PE[1,2]

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

T_e = 45670(160) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			950(80)	gas	PE	1,2

B $^2B_1$ C_{2v}

T^a = 26220(160) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			710(80)	gas	PE	1,2

Ã $^2B_2$ C_{2v}

T^a = 19610(160) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCS a-stretch	1660(80)	gas	PE	1,2
			680(80)	gas	PE	1,2

X̃ $^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCS a-stretch	1450(80)	gas	PE	1,2
			700(80)	gas	PE	1,2

[a] From vertical ionization potentials.

References

[1]H. Bock, B. Solouki, G. Bert, and P. Rosmus, J. Am. Chem. Soc. 99, 1663 (1977).
[2]P. Rosmus, B. Solouki, and H. Bock, Chem. Phys. 22, 453 (1977).

NH_2CN^+

D̃ $^2A''$ C_s

T^a = 65760(900) gas PE[1]

C̃ $^2A'$ C_s

T^a = 28880(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		C-N stretch	1040(80)	gas	PE	1
		NCN deform.	480(80)	gas	PE	1

B̃ $^2A'$ C_s

T^a = 18800(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		C-N stretch	800(80)	gas	PE	1
		NCN deform.	400(80)	gas	PE	1

Ã $^2A''$ C_s

T^a = 14930(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	C≡N stretch	2080(80)	gas	PE	1

X̃ $^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	C≡N stretch	2000(80)	gas	PE	1
	3	C-N stretch	1600(80)	gas	PE	1
	4	Inversion	720(80)	gas	PE	1

[a] From vertical ionization potentials.

References

[1]H. Stafast and H. Bock, Chem. Ber. 107, 1882 (1974).

$CH_2N_2^+$

Ẽ $^2A_1$ C_{2v}

T^a = 85520(1000) gas PE[1]

D̃ $^2B_2$ C_{2v}

T^a = 76650(1000) gas PE[1]

C̃ $^2B_1$ C_{2v}

T^a = 63980(320) gas PE[1]

B̃ $^2A_1$ C_{2v}

T_o = 49460(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	NN stretch	2180(80)	gas	PE	1
	3	CH_2 "scissors"	1360(80)	gas	PE	1

Ã $^2B_2$ C_{2v}

T_o = 38490(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s-stretch	2780(80)	gas	PE	1
	2	NN stretch	2040(80)	gas	PE	1
	3	CH_2 "scissors"	1200(80)	gas	PE	1

X̃ $^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	NN stretch	2180(80)	gas	PE	1
	4	CN stretch	970(80)	gas	PE	1

$CD_2N_2^+$

Ẽ $^2A_1$ C_{2v}

T^a = 85520(1000) gas PE[1]

D̃ $^2B_2$ C_{2v}

T^a = 76650(1000) gas PE[1]

C̃ $^2B_1$ C_{2v}

T^a = 63980(320) gas PE[1]

B̃ $^2A_1$ C_{2v}

T_o = 49460(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	NN stretch	2250(80)	gas	PE	1
	3	CD_2 "scissors"	1020(80)	gas	PE	1

Ã $^2B_2$ C_{2v}

T_o = 38490(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_2 s-stretch	2170(80)	gas	PE	1
	2	NN stretch	1930(80)	gas	PE	1
	4	CD_2 "scissors"	800(80)	gas	PE	1

X̃ $^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	NN stretch	2180(80)	gas	PE	1
	4	CN stretch	970(80)	gas	PE	1

[a] From vertical ionization potential.

References

[1] J. Bastide and J. P. Maier, Chem. Phys. 12, 177 (1976).

$CH_2N_2^+$

(Diazirine Cation)

D̃ $^2B_1$ C_{2v}

T^a = 58090(1600) gas PE[1]

C̃ $^2A_1$ C_{2v}

$T_o \sim$ 46000 gas PE[1]

B̃ $^2A_1$ C_{2v}

T_o = 31060(1000) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1330(80)	gas	PE	1

Ã $^2B_1$ C_{2v}

T_o = 20170(1600) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			2200(80)[b]	gas	PE	1
			890(80)	gas	PE	1

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

[a] From vertical ionization potential.
[b] Comparison with the spectrum of the neutral molecule suggests that this relatively prominent progression may be contributed by (890 + 1300) combinations.

References

[1] M. B. Robin, C. R. Brundle, N. A. Kuebler, G. B. Ellison, and K. B. Wiberg, J. Chem. Phys. 57, 1758 (1972).

H_2CCS

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

$T_o \sim 17995$ gas AB[10] $\tilde{A}$-$\tilde{X}$ 450-550 nm

Diffuse bands.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	C=C stretch	1402	gas	AB	10
	8	CCS bend	∿284	gas	AB	10

$\tilde{X}\ ^1A_1$ C_{2v} Structure: $MW^{2-5}IR^9$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s-stretch	3020	gas	IR	9
			3012	Ar	IR	1,6,7
	2	C=C stretch	1757	gas	IR	9
			1755	Ar	IR	1,6-8
	3	CH_2 "scissors"	1331	gas	IR	9
			1323	Ar	IR	1,6,7
	4	C=S stretch	850	gas	IR	9
			858	Ar	IR	7
b_1	5	H_2C=C OPLA	692	Ar	IR	1,6-8
	6	CCS bend	404	Ar	IR	1,7

$\tilde{X}\ ^1A_1$---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	7	CH_2 a-stretch	3107	gas	IR	9
			3097 3068	Ar	IR	7
	8	CH_2 rock	922	gas	IR	9
			918	Ar	IR	7
	9	CCS bend	356	Ar	IR	7

$A_o = 9.555$; $B_o = 0.189$; $C_o = 0.185$ $MW^{2-5}IR^9$

D_2CCS

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

$T_o \sim 18002$ gas AB[10] $\tilde{A}$-$\tilde{X}$ 450-550 nm

Diffuse bands.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	C=C stretch	1400	gas	AB	10
	8	CCS bend	∿256	gas	AB	10

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_2 s-stretch	2229	Ar	IR	1,7
	2	C=C stretch	1738	Ar	IR	1,7
	3	CD_2 "scissors"	1030	Ar	IR	7
	4	C=S stretch	775	Ar	IR	7
b_1	5	D_2C=C OPLA	555	Ar	IR	1,7
	6	CCS bend	375	Ar	IR	7
b_2	7	CD_2 a-stretch	2330[a]	Ar	IR	7
	8	CD_2 rock	755	Ar	IR	7
	9	CCS bend	308	Ar	IR	7

[a] Tentative.

References

[1]A. Krantz and J. Laureni, J. Am. Chem. Soc. 96, 6768 (1974).
[2]K. Georgiou, H. W. Kroto, and B. M. Landsberg, J. Chem. Soc., Chem. Commun., 739 (1974).
[3]B. Bak, O. J. Nielsen, H. Svanholt, A. Holm, N. H. Toubro, A. Krantz, and J. Laureni, Acta Chem. Scand. A33, 161 (1979).
[4]K. Georgiou, H. W. Kroto, and B. M. Landsberg, J. Mol. Spectrosc. 77, 365 (1979).
[5]M. Winnewisser and E. Schäfer, Z. Naturforsch. 35a, 483 (1980).
[6]A. Krantz and J. Laureni, J. Am. Chem. Soc. 103, 486 (1981).
[7]M. Torres, I. Safarik, A. Clement, R. K. Gosavi, and O. P. Strausz, Can. J. Chem. 62, 2777 (1984).
[8]M. Hawkins, M. J. Almond, and A. J. Downs, J. Phys. Chem. 89, 3326 (1985).
[9]H. W. Kroto and D. McNaughton, J. Mol. Spectrosc. 114, 473 (1985).
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$HCOOH^+$

E $^2A'$ C_s

T^a = 49700(320) gas PE[1,3]

D $^2A'$ C_s

T_o = 45500(320) gas PE[1,3]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	CO stretch	1300(40)	gas	PE	1,2

C $^2A''$ C_s

$T_o \sim$ 32800 gas PE[1,3]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		940	gas	PE	1

B $^2A'$ C_s

$T_o \sim$ 23200 gas PE[1,3]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		940	gas	PE	1

A $^2A''$ C_s

T_o = 8390(320) gas PE[1,3]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	C=O stretch	2340(40)	gas	PE	2
	C-O stretch	1080(60)	gas	PE	1,2

X $^2A'$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	CO stretch	1460(30)	gas	PE	1,2

$DCOOD^+$

D $^2A'$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	CO stretch	1210(40)	gas	PE	2
	COD bend ?	880(40)	gas	PE	2

A $^2A''$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	C=O stretch	2280(40)	gas	PE	2
	C-O stretch	1090(40)	gas	PE	2

X $^2A'$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	CO stretch	1494(40)	gas	PE	2
	COD bend	970(40)	gas	PE	2

[a] From vertical ionization potential.

References

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[2]I. Watanabe, Y. Yokoyama, and S. Ikeda, Chem. Phys. Lett. 19, 406 (1973).
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H_2CSO^+

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

T^a = 64550(320) gas PE[1]

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

T^a = 55910(320) gas PE[1]

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

T^a = 43650(320) gas PE[1]

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

T^a = 36230(320) gas PE[1]

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

T^a = 11620(320) gas PE[1]

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

[a] From vertical ionization potentials.

References

[1]E. Block, H. Bock, S. Mohmand, P. Rosmus, and B. Solouki, Angew. Chem. 88, 380 (1976); Angew. Chem. Int. Ed. Engl. 15, 383 (1976).

$CH_2F_2^+$

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

T_o = 83900(1000) gas PE[1,3]

$\tilde{D},\tilde{E},\tilde{F}\ ^2B_1,^2A_1,^2B_2$ C_{2v}

T_o = 44380(400) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CF_2 stretch	700(100)	gas	PE	1-3

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

T^a = 24300(400) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CF_2 stretch	970(80)	gas	PE	1-3
	4	CF_2 "scissors"	500(80)	gas	PE	1,3

$\tilde{A},\tilde{B}\ ^2A_1,^2B_1$ C_{2v}

T_o = 14760(400) gas PE[1-3]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	2744	Ar	IR	4
	2	CH_2 "scissors"	1120(80)	gas	PE	1-3
b_1	6	CH stretch	2854	Ar	IR	4
b_2	8	CH_2 wag	1408	Ar	IR	4
	9	CF stretch	1255	Ar	IR	4

$CD_2F_2^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CF_2 stretch	970(80)	gas	PE	3
	4	CF_2 "scissors"	500(80)	gas	PE	3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD stretch	2062	Ar	IR	4
b_1	7		980	Ar	IR	4
b_2	8	CD_2 wag	1063	Ar	IR	4
	9	CF stretch	1262	Ar	IR	4

[a] From vertical ionization potential.

References

[1]A. W. Potts, H. J. Lempka, D. G. Streets, and W. C. Price, Phil. Trans. Roy. Soc. (London) A268, 59 (1970).
[2]B. P. Pullen, T. A. Carlson, W. E. Moddeman, G. K. Schweitzer, W. E. Bull, and F. A. Grimm, J. Chem. Phys. 53, 768 (1970).
[3]C. R. Brundle, M. B. Robin, and H. Basch, J. Chem. Phys. 53, 2196 (1970).
[4]L. Andrews and F. T. Prochaska, J. Chem. Phys. 70, 4714 (1979).

CH_2FCl^+

T^a = 62610(1000) gas PE[1]

T^a = 50510(1000) gas PE[1]

T^a = 41230(400) gas PE[1]

T^a = 23080(1000) gas PE[1]

T^a = 21060(400) gas PE[1]

T^a = 19040(1000) gas PE[1]

T^a = 17020(1000) gas PE[1]

T^a = 4520(1000) gas PE[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_2 stretch	2902	Ar	IR	2
		CH_2 "scissors"	1200(80)	gas	PE	1
		CCl stretch	874	Ar	IR	2

CD_2FCl^+

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD_2 stretch	2162[b]	Ar	IR	2
		CCl stretch	843	Ar	IR	2

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

References

[1] J. Doucet, P. Sauvageau, and C. Sandorfy, J. Chem. Phys. 58, 3708 (1973).
[2] F. T. Prochaska and L. Andrews, J. Chem. Phys. 73, 2651 (1980).

$CH_2Cl_2^+$

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

T^a = 72500(1000) gas PE[1]

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

T^a = 43970(240) gas PE[1]

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

T^a = 37280(240) gas PE[1]

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

T^a = 32110(240) gas PE[1]

A broad absorption with maximum at 342 nm (29200) which appears on argon-resonance photolysis of CH_2Cl_2 isolated in solid argon and which has a photodecomposition threshold at a wavelength longer than 650 nm has been assigned[5] to the $\tilde{D}$-$\tilde{X}$ transition of $CH_2Cl_2^+$.

$\tilde{B}$,$\tilde{C}$ $^2A_2$,$^2A_1$[b] C_{2v}

T^a = 7260(240) gas PE[1]

$\tilde{X}$,$\tilde{A}$ $^2B_2$,$^2B_1$[b] C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CCl_2 stretch	640(80)	gas	PE	1
b_2	8	CH_2 wag	1193	Ar	IR	5,6
	9	CCl_2 stretch	764	Ar	IR	5,6

$CD_2Cl_2^+$

$\tilde{X}$,$\tilde{A}$ $^2B_2$,$^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	8	CD_2 wag	1083	Ar	IR	6
	9	CCl_2 stretch	603	Ar	IR	5,6

[a] From vertical ionization potential. The first ionization potential of CH_2Cl_2 is taken as 11.32(1) eV, as in the photoionization study of Ref. 3.
[b] The order of these states is uncertain.[2,4]

References

[1] A. W. Potts, H. J. Lempka, D. G. Streets, and W. C. Price, Phil. Trans. Roy Soc. (London) A268, 59 (1970).
[2] R. N. Dixon, J. N. Murrell, and B. Narayan, Mol. Phys. 20, 611 (1971).
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[5]L. Andrews, F. T. Prochaska, and B. S. Ault, J. Am. Chem. Soc. 101, 9 (1979).
[6]B. J. Kelsall and L. Andrews, J. Mol. Spectrosc. 97, 362 (1983).

$CH_2Br_2^+$

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

T^a = 74070(800) gas PE[1]

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

T^a = 46230(560) gas PE[1]

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

T^a = 34130(560) gas PE[1]

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

T^a = 29040(560) gas PE[1]

A prominent absorption at 362 nm (27600) which appears on argon-resonance photolysis of CH_2Br_2 isolated in solid argon and which has a photodecomposition threshold at a wavelength longer than 650 nm has been assigned[4] to the $\tilde{D}$-$\tilde{X}$ transition of $CH_2Br_2^+$.

$\tilde{B},\tilde{C}\ ^2A_2,^2A_1$[b] C_{2v}

T^a = 6130(560) gas PE[1]

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

T^a = 2420(560) gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	8	CH_2 wag	1129	Ar	IR	4
	9		695	Ar	IR	4
			684	Ar	IR	4,5

$CD_2Br_2^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	9		546	Ar	IR	4,5

[a] From vertical ionization potential. The first ionization potential of CH_2Br_2 has been taken as 10.52(5) eV, as determined in the photoelectron-photoion coincidence study of Ref. 3.
[b] For assignment, see Ref. 2.

References

[1]A. W. Potts, H. J. Lempka, D. G. Streets, and W. C. Price, Phil. Trans. Roy. Soc. (London) A268, 59 (1970).
[2]R. N. Dixon, J. N. Murrell, and B. Narayan, Mol. Phys. 20, 611 (1971).
[3]B. P. Tsai, T. Baer, A. S. Werner, and S. F. Lin, J. Phys. Chem. 79, 570 (1975).
[4]L. Andrews, F. T. Prochaska, and B. S. Ault, J. Am. Chem. Soc. 101, 9 (1979).
[5]B. J. Kelsall and L. Andrews, J. Mol. Spectrosc. 97, 362 (1983).

$CH_2I_2^+$

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

T^a = 81000(1000) gas PE[1]

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

T^a = 48410(320) gas PE[1]

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

T^a = 33970(320) gas PE[1]

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

T^a = 26540(320) gas PE[1]

A prominent absorption at 379 nm (26400) which appears on argon-resonance photolysis of CH_2I_2 isolated in solid argon and which has a photodecomposition threshold at a wavelength longer than 650 nm has been assigned[3] to the $\tilde{D}$-$\tilde{X}$ transition of $CH_2I_2^+$.

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

T^a = 8880(320) gas PE[1]

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

T^a = 6050(320) gas PE[1]

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

T^a = 2420(320) gas PE[1]

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

[a] From vertical ionization potential. The first ionization potential of CH_2I_2 has been taken as 9.46(2) eV, as determined in the photoelectron-photoion coincidence study of Ref. 2.

References

[1]A. W. Potts, H. J. Lempka, D. G. Streets, and W. C. Price, Phil. Trans. Roy. Soc. (London) A268, 59 (1970).
[2]B. P. Tsai, T. Baer, A. S. Werner, and S. F. Lin, J. Phys. Chem. 79, 570 (1975).
[3]L. Andrews, F. T. Prochaska, and B. S. Ault, J. Am. Chem. Soc. 101, 9 (1979).

$SiH_2F_2^+$

G $^2A_1$ C_{2v}

T^a = 59220(480) gas PE[2]

F $^2A_1$ C_{2v}

T^a = 44000(1200) gas PE[2]

E $^2B_2$ C_{2v}

T^a = 41000(1200) gas PE[2]

D $^2B_1$ C_{2v}

T^a = 38300(1200) gas PE[1,2]

C $^2A_2$ C_{2v}

T^a = 28400(900) gas PE[2]

B $^2B_2$ C_{2v}

T^a = 26000(900) gas PE[1,2]

A $^2A_1$ C_{2v}

T^a = 18960(560) gas PE[1,2]

X $^2B_1$ C_{2v}

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. 67, 3425 (1971).
[2]D. C. Frost, F. G. Herring, A. Katrib, R. A. N. McLean, J. E. Drake, and N. P. C. Westwood, Can. J. Chem. 49, 4033 (1971).

$SiH_2Cl_2^+$

G $^2A_1$ C_{2v}

$T^a \sim$ 53400 gas PE[1,2]

F $^2B_1$ C_{2v}

T^a = 23400(720) gas PE[2]

E $^2A_1$ C_{2v}

T^a = 22180(720) gas PE[2]

D $^2B_2$ C_{2v}

T^a = 20170(720) gas PE[1,2]

C $^2A_1$ C_{2v}

T^a = 8550(480) gas PE[2]

B $^2A_2$ C_{2v}

T^a = 6700(480) gas PE[1,2]

A $^2B_1$ C_{2v}

T^a = 3150(320) gas PE[1,2]

X $^2B_2$ C_{2v}

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. 67, 3425 (1971).
[2]D. C. Frost, F. G. Herring, A. Katrib, R. A. N. McLean, J. E. Drake, and N. P. C. Westwood, Can. J. Chem. 49, 4033 (1971).

$SiH_2Br_2^+$

D C_{2v}

T^a = 22400(1000) gas PE[1]

C C_{2v}

T^a = 19600(320) gas PE[1]

B C_{2v}

T^a = 5570(320) gas PE[1]

A C_{2v}

T^a = 1610(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. 67, 3425 (1971).

$SiH_2I_2^+$

F C_{2v}

T^a = 28640(320) gas PE[1]

E C_{2v}

T^a = 23720(320) gas PE[1]

D C_{2v}

T^a = 19690(320) gas PE[1]

C C_{2v}

T^a = 8390(320) gas PE[1]

B C_{2v}

T^a = 5320(320) gas PE[1]

A C_{2v}

T^a = 2420(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. 67, 3425 (1971).

$GeH_2F_2^+$

B C_{2v}

T^a = 26600(1600) gas PE[1]

A C_{2v}

T^a = 12900(1600) gas PE[1]

X $^2B_1$ C_{2v}

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. 67, 3425 (1971).

$GeH_2Cl_2^+$

C C_{2v}

T^a = 18880(320) gas PE[1]

B C_{2v}

T^a = 5320(320) gas PE[1]

A C_{2v}

T^a = 2420(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. 67, 3425 (1971).

$GeH_2Br_2^+$

E C_{2v}

T^a = 24370(320) gas PE[1]

D C_{2v}

T^a = 20010(320) gas PE[1]

C C_{2v}

T^a = 18070(320) gas PE[1]

B C_{2v}

T^a = 4760(320) gas PE[1]

A C_{2v}

T^a = 1290(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. 67, 3425 (1971).

$GeH_2I_2^+$

F C_{2v}

T^a = 27920(320) gas PE[1]

E C_{2v}

T^a = 22270(320) gas PE[1]

D C_{2v}

T^a = 18800(320) gas PE[1]

C C_{2v}

T^a = 7830(320) gas PE[1]

B C_{2v}

T^a = 5000(320) gas PE[1]

A C_{2v}

T^a = 2100(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, Trans. Faraday Soc. 67, 3425 (1971).

H_2CCl-I

In a nitrogen matrix, very strong absorption maximum at 370 nm and much weaker absorption maximum at 545 nm. Irradiation in either of these absorption regions results in re-formation of the more stable

CH_2ClI structure in which both halogen atoms are bonded to the carbon atom.

X

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CH_2 a-stretch	3168.8	Ar	IR	1
	CH_2 s-stretch	3042.3 3039.4	Ar	IR	1
	CCl stretch	886.2	Ar	IR	1
	H_2CCl OPLA	639.0 633.5	Ar	IR	1

D_2CCl-I

X

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CD_2 a-stretch	2395.2	Ar	IR	1
	CD_2 s-stretch	2228.2 2226.6	Ar	IR	1
	CD_2 "scissors"	1072.5	Ar	IR	1
	CCl stretch	836.5	Ar	IR	1
	D_2CCl OPLA	502.9 498.8	Ar	IR	1

References

[1]G. Maier and H. P. Reisenauer, Angew. Chem. 98, 829 (1986); Angew. Chem. Int. Ed. Engl. 25, 819 (1986).

H_2CBr-I

In a nitrogen matrix, very strong absorption maximum at 403 nm and much weaker absorption maximum at 660 nm. Irradiation in either of these absorption regions results in re-formation of the more stable CH_2BrI structure in which both halogen atoms are bonded to the carbon atom.

X

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CH_2 a-stretch	3165.2	Ar	IR	1
	CH_2 s-stretch	3035.7	Ar	IR	1
	H_2CBr OPLA	638.1 630.6	Ar	IR	1

References

[1]G. Maier and H. P. Reisenauer, Angew. Chem. 98, 829 (1986); Angew. Chem. Int. Ed. Engl. 25, 819 (1986).

H_2CI-I

In a nitrogen matrix, very strong absorption maximum at 438 nm and much weaker absorption maximum at 745 nm. Irradiation in either of these absorption regions results in re-formation of the more stable CH_2I_2 structure in which both iodine atoms are bonded to the carbon atom.

X

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CH_2 a-stretch	3151.2	Ar	IR	1
	CH_2 s-stretch	3028.0	Ar	IR	1
	CH_2 "scissors"	1372.8	Ar	IR	1
	CI stretch	713.6 704.6	Ar	IR	1
	H_2CI OPLA	622.7 618.3 611.1	Ar	IR	1

D_2CI-I

X

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CD_2 a-stretch	2377.6	Ar	IR	1
	CD_2 s-stretch	2213.0	Ar	IR	1
	CD_2 "scissors"	1032.7	Ar	IR	1
	CI stretch	645.3	Ar	IR	1
	D_2CI OPLA	498.0 488.6	Ar	IR	1

References

[1]G. Maier and H. P. Reisenauer, Angew. Chem. 98, 829 (1986); Angew. Chem. Int. Ed. Engl. 25, 819 (1986).

6.10. Five-Atomic Monohydrides

C_4H

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

T_0 = 33740 Ne AB[1] 259-296 nm

33797 Ar AB[1] 248-295 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3100(10)	Ar	AB	1
	2	C≡C stretch	2130(10)	Ar	AB	1
	3	C≡C stretch	2028(10)	Ne	AB	1
			2060(10)	Ar	AB	1
	4	C-C stretch	800(10)	Ne	AB	1
			760(10)	Ar	AB	1
Π	5	HCC bend	570[a]	Ar	AB	1

Groups of absorptions observed in an argon matrix[1] between 13408 and 13906, 17629 and 17939, 21972 and 25667, and 26867 and 32104 have also tentatively been attributed to C_4H.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	3	C≡C a-stretch	2060	Ar	IR	1

B_0 = 0.165 MW[2-5]

C_4D

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

T_0 = 33900 Ar AB[1] 258-294 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2640(10)	Ar	AB	1
	2	C≡C s-stretch	2140(10)	Ar	AB	1
	4	C-C stretch	760(10)	Ar	AB	1
Π	5	DCC bend	485[a]	Ar	AB	1

An absorption at 17685 and a group of bands between 26925 and 30883 in the argon-matrix observations[1] have also tentatively been assigned to C_4D.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	3	C≡C a-stretch	2050	Ar	IR	1

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

References

[1] K. I. Dismuke, W. R. M. Graham, and W. Weltner, Jr., J. Mol. Spectrosc. 57, 127 (1975).
[2] M. Guélin, S. Green, and P. Thaddeus, Astrophys. J. 224, L27 (1978).
[3] M. B. Bell, P. A. Feldman, and H. E. Matthews, Astrophys. J. 273, L35 (1983).
[4] M. B. Bell, H. E. Matthews, and T. J. Sears, Astron. Astrophys. 127, 241 (1983).
[5] C. A. Gottlieb, E. W. Gottlieb, P. Thaddeus, and H. Kawamura, Astrophys. J. 275, 916 (1983).

$HC{\equiv}C{-}C{\equiv}N^+$

$\tilde{C}$

T_0 = 48570(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1320(40)	gas	PE	1

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

T_0 = 19600(160) gas PE[1]

19374(43) Ne AB[2] $\tilde{B}$-$\tilde{X}$ 474-516 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+			1940(40)	gas	PE	1
	4	C-C stretch	810(40)	gas	PE	1
			820(60)	Ne	AB	2

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

T_0 = 15650(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	4	C-C stretch	860(40)	gas	PE	1

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

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		2180(40)	gas	PE	1

References

[1]C. Baker and D. W. Turner, Proc. Roy. Soc. (London) A308, 19 (1968).
[2]J. Fulara, S. Leutwyler, J. P. Maier, and U. Spittel, J. Phys. Chem. 89, 3190 (1985).

HCOCN

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

T_o = 26276(2) gas LF[1] $\tilde{A}$-$\tilde{X}$ 358-385 nm

Vib. No. sym.		Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CO stretch	1310.6	gas	LF	1
	4	HCO bend	1124.3	gas	LF	1
	5	CC stretch	940.0	gas	LF	1
	6	CCO bend	517.0	gas	LF	1
	7	CCN bend	216.9	gas	LF	1
a"	8	CH wag	408.2	gas	LF	1
	9	CCN bend	365.9	gas	LF	1

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

Vib. No. sym.		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

References

[1]R. H. Judge, D. C. Moule, A. Biernacki, M. Benkel, J. M. Ross, and J. Rustenburg, J. Mol. Spectrosc. 116, 364 (1986).
[2]D. J. Clouthier and D. C. Moule, J. Am. Chem. Soc. 109, 6259 (1987).

HNO_3^+

$\tilde{F}$ C_s

T_o = 56800(900) gas PE[1,2]

$\tilde{E}$ C_s

T_o = 51640(160) gas PE[1,2]

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

T_o = 33400(160) gas PE[1,2]

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

T_o = 11620(900) gas PE[1,2]

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

T_o = 9760(160) gas PE[1,2]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		1210(30)	gas	PE	1

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

T^a = 3950(240) gas PE[1,2]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		1490(30)	gas	PE	1,2
		1070(30)	gas	PE	1,2

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

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		1370(80)	gas	PE	2
		650(30)	gas	PE	1

[a] First detectable component.

References

[1]D. R. Lloyd, P. J. Roberts, and I. H. Hillier, J. Chem. Soc., Faraday Trans. 2 71, 496 (1975).
[2]D. C. Frost, S. T. Lee, C. A. McDowell, and N. P. C. Westwood, J. Electron Spectrosc. Relat. Phenom. 7, 331 (1975).

HCF_3^+

F $^2A_1$ C_{3v}

T^a = 85360(400) gas PE[1,3,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	2660(80)	gas	PE	4
	3	CF_3 stretch	1050(80)	gas	PE	4

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

T^a ~ 54400 gas PE[1-4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			480(80)	gas	PE	1

C ^2E C_{3v}

T_o = 26220(400) gas PE[1-4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF_3 stretch	1050(80)	gas	PE	1-4
	3	CF_3 "umbrella"	550(80)	gas	PE	1,3,4

B ^2E C_{3v}

T^a = 18800(1000) gas PE[1-4]

A $^2A_2$ C_{3v}

T^a = 13200(1000) gas PE[1-4]

X $^2A_1$ C_{3v}

DCF_3^+

C ^2E C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF_3 stretch	1050(80)	gas	PE	3
	3	CF_3 "umbrella"	500(80)	gas	PE	3

[a] From vertical ionization potential.

References

[1] A. W. Potts, H. J. Lempka, D. G. Streets, and W. C. Price, Phil. Trans. Roy. Soc. (London) A268, 59 (1970).
[2] B. P. Pullen, T. A. Carlson, W. E. Moddeman, G. K. Schweitzer, W. E. Bull, and F. A. Grimm, J. Chem. Phys. 53, 768 (1970).
[3] C. R. Brundle, M. B. Robin, and H. Basch, J. Chem. Phys. 53, 2196 (1970).
[4] G. Bieri, L. Åsbrink, and W. von Niessen, J. Electron Spectrosc. Relat. Phenom. 23, 281 (1981).

HCF_2Cl^+

G,H $^2A'$,$^2A''$ C_s

T^a = 59870(800) gas PE[1,2]

F $^2A'$ C_s

T^a = 50910(800) gas PE[1,2]

C,D,E $^2A''$,$^2A''$,$^2A'$ C_s

T^a = 27270(800) gas PE[1,2]

B $^2A'$ C_s

T^a = 10890(800) gas PE[1,2]

X,A $^2A''$,$^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		FCCl deform.	410(80)	gas	PE	2

[a] From vertical ionization potentials.

References

[1] J. Doucet, P. Sauvageau, and C. Sandorfy, J. Chem. Phys. 58, 3708 (1973).
[2] I. Novak, T. Cvitaš, L. Klasinc, and H. Güsten, J. Chem. Soc., Faraday Trans. 2 77, 2049 (1981).

$HCFCl_2^+$

F,G $^2A'$,$^2A''$ C_s

T^a = 47360(800) gas PE[1,2]

E $^2A'$ C_s

T^a = 22830(800) gas PE[1,2]

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

T^a = 20570(800) gas PE[1,2]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	CCl_2 stretch	610(80)	gas	PE	2
	FCCl deform.	400(80)	gas	PE	2

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

T^a = 8470(800) gas PE[1,2]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	CCl_2 "scissors"	280(80)	gas	PE	2

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

T^a = 3630(800) gas PE[1,2]

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

T^a = 1600(800) gas PE[1,2]

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

[a] From vertical ionization potentials.

References

[1] J. Doucet, P. Sauvageau, and C. Sandorfy, J. Chem. Phys. 58, 3708 (1973).
[2] I. Novak, T. Cvitaš, L. Klasinc, and H. Güsten, J. Chem. Soc., Faraday Trans. 2 77, 2049 (1981).

$HCCl_3^+$

$\tilde{F}\ ^2A_1$ C_{3v}

T^a = 68000(1000) gas PE[1]

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

T^a = 45100(320) gas PE[1]

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

T^a = 37280(320) gas PE[1]

A strong, broad absorption with maximum at 388 nm (25800) which appears on argon-resonance photolysis of $HCCl_3$ isolated in solid argon and which has a photodecomposition threshold at a wavelength longer than 470 nm has been assigned[5] to the $\tilde{D}$-$\tilde{X}$ transition of $HCCl_3^+$. The energy difference is attributed to structural relaxation in the condensed phase.

$\tilde{C}\ ^2E^b$ C_{3v}

T^a = 11940(320) gas PE[1]

$\tilde{B}\ ^2A_1{}^b$ C_{3v}

T^a = 5160(320) gas PE[1]

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

T^a = 4360(320) gas PE[1]

$\tilde{X}\ ^2A_2{}^b$ C_{3v}

[a] From vertical ionization potential. The first ionization potential of $HCCl_3$ is taken as 11.37(2) eV, as in the photoelectron-photoion coincidence study of Ref. 4.
[b] The assignment of Ref. 2 has been used. An alternate assignment has been proposed by Ref. 3.

References

[1] A. W. Potts, H. J. Lempka, D. G. Streets, and W. C. Price, Phil. Trans. Roy Soc. (London) A268, 59 (1970).
[2] R. N. Dixon, J. N. Murrell, and B. Narayan, Mol. Phys. 20, 611 (1971).
[3] S. Katsumata and K. Kimura, Bull. Chem. Soc. Japan 46, 1342 (1973).
[4] A. S. Werner, B. P. Tsai, and T. Baer, J. Chem. Phys. 60, 3650 (1974).
[5] L. Andrews, B. J. Kelsall, J. H. Miller, and B. W. Keelan, J. Chem. Soc., Faraday Trans. 2 79, 1417 (1983).

$HCBr_3^+$

$\tilde{F}\ ^2A_1$ C_{3v}

T^a = 75200(1000) gas PE[1]

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

T^a = 43000(320) gas PE[1]

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

T^a = 34130(320) gas PE[1]

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

T^a = 10000(320) gas PE[1]

Spin-orbit splitting = 1290(320) gas PE[1]

$\tilde{B}\ ^2A_1$ C_{3v}

T^a = 6450(320) gas PE[1]

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

T^a = 2660(320) gas PE[1]

Spin-orbit splitting = 1130(320) gas PE[1]

X $^2A_2$ C_{3v}

[a] From vertical ionization potential. The first ionization potential of $HCBr_3$ is taken as 10.48(2) eV, as in the photoelectron-photoion coincidence study of Ref. 2.

References

[1]A. W. Potts, H. J. Lempka, D. G. Streets, and W. C. Price, Phil. Trans. Roy. Soc. (London) A268, 59 (1970).
[2]B. P. Tsai, T. Baer, A. S. Werner, and S. F. Lin, J. Phys. Chem. 79, 570 (1975).

$HSiF_3$

F $^2A_1$ C_{3v}

T^a = 52120(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	SiF_3 stretch	725(40)	gas	PE	1
	3	Deformation	330(40)	gas	PE	1

E ^2E C_{3v}

T^a = 33320(320) gas PE[1]

D $^2A_1$ C_{3v}

T^a = 30010(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	SiF_3 stretch	790(40)	gas	PE	1

C ^2E C_{3v}

T^a = 22270(320) gas PE[1]

B ^2E C_{3v}

T^a = 15330(320) gas PE[1]

A $^2A_2$ C_{3v}

T^a = 11780(320) gas PE[1]

X $^2A_1$ C_{3v}

[a] From vertical ionization potentials.

References

[1]S. Cradock, E. A. V. Ebsworth, and R. A. Whiteford, J. Chem. Soc., Dalton Trans. 22, 2401 (1973).

$HSiCl_3$

F $^2A_1$ C_{3v}

T^a = 50020(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiH stretch	∿2000	gas	PE	1

E $^2A_1$ C_{3v}

T^a = 24530(320) gas PE[1]

D ^2E C_{3v}

T^a = 22670(320) gas PE[1]

C ^2E C_{3v}

T^a = 9120(320) gas PE[1]

A,B $^2A_1$,^2E C_{3v}

T^a = 3790(320) gas PE[1]

X $^2A_2$ C_{3v}

[a] From vertical ionization potentials.

References

[1]D. C. Frost, F. G. Herring, A. Katrib, R. A. N. McLean, J. E. Drake, and N. P. C. Westwood, Can. J. Chem. 49, 4033 (1971).

6.11. Five-Atomic Nonhydrides

N_3CN^+

F $^2A''$ C_s

T^a = 57280(900) gas PE[1]

E $^2A'$ C_s

T^a = 45500(240) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	NN stretch	1520(40)	gas	PE	1

D $^2A''$ C_s

T^a = 28720(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	C≡N stretch	1960(40)	gas	PE	1
	5	NNN bend	620(40)	gas	PE	1
	6	CNN bend	430(40)	gas	PE	1

C $^2A'$ C_s

T_o = 24930(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	NN stretch	1380(40)	gas	PE	1
	4	NC stretch	1090(40)	gas	PE	1
	5	NNN bend	620(40)	gas	PE	1

B $^2A'$ C_s

T^a = 19120(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	C≡N stretch	2190(40)	gas	PE	1
	3	NN stretch	1130(40)	gas	PE	1
	5	NNN bend	810(40)	gas	PE	1

A $^2A'$ C_s

T_o = 8550(240) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	6	CNN bend	640(40)	gas	PE	1

X $^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	NN stretch	1900(40)	gas	PE	1
			1120(40)	gas	PE	1
			800(40)	gas	PE	1

[a] From vertical ionization potential.

References

[1] D. C. Frost, H. W. Kroto, C. A. McDowell, and N. P. C. Westwood, J. Electron Spectrosc. Relat. Phenom. 11, 147 (1977).

$C_3O_2^+$

D $^2\Pi_u$ $D_{\infty h}$

T_o = 53680(50) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	CO stretch	2195(40)	gas	PE	1
	2	C_3 s-stretch	629(40)	gas	PE	1

C $^2\Sigma_g$[a]

T_o = 51420(50) gas PE[1]

B $^2\Pi_u$[a]

T_o = 41520(50) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Bend	662(40)	gas	PE	1

Ã $^2\Pi_g$[a]

T_o = 31440(50) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CO a-stretch	2364(40)	gas	PE	1
	Bend	718(30)	gas	PE	1

X̃ $^2\Pi_u$ $D_{\infty h}$

Vib. No. sym.		Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	CO stretch	2105(40)	gas	PE	1
Π_u	7	Bend	435(40)[b]	gas	PE	1

[a] Symmetry of the orbital which is depopulated on ionization is given. Photoelectron spectrum indicates that the product ion is bent.
[b] Observed as sequence bands. This vibration is highly anharmonic.

References

[1] J. W. Rabalais, L. O. Werme, T. Bergmark, L. Karlsson, M. Hussain, and K. Siegbahn, "Electron Spectroscopy," D. A. Shirley, Ed., (North-Holland Publishing Co., Amsterdam, 1972), p. 425.

$NCNCO^+$

Ẽ $^2A'$ C_s

T^a = 45990(320) gas PE[1]

D̃ $^2A''$ C_s

$T^a \sim$ 26220 gas PE[1]

C̃ $^2A'$ C_s

T_o = 24450(320) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		730(60)	gas	PE	1

B̃ $^2A'$ C_s

T^a = 15900(320) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		2340(60)	gas	PE	1
		1410(60)	gas	PE	1
		600(60)	gas	PE	1

Ã $^2A'$ C_s

T^a = 4120(320) gas PE[1]

X̃ $^2A''$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		2130(60)	gas	PE	1
		540(60)	gas	PE	1

[a] From vertical ionization potential.

References

[1] D. C. Frost, H. W. Kroto, C. A. McDowell, and N. P. C. Westwood, J. Electron Spectrosc. Relat. Phenom. 11, 147 (1977).

$S(CN)_2^+$

H̃ $^2B_2$ C_{2v}

T^a = 67600(1000) gas PE[1]

G̃ $^2A_1$ C_{2v}

T^a = 41800(1000) gas PE[1]

F̃ $^2B_1$ C_{2v}

T^a = 29850(320) gas PE[1]

Vib. No. sym.		Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CS stretch	560(40)	gas	PE	1

Ẽ $^2A_1$ C_{2v}

T^a = 23400(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CS stretch	840(40)	gas	PE	1

D $^2B_2$ C_{2v}

T^a = 21780(320) gas PE[1]

C $^2A_2$ C_{2v}

T^a = 18320(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CN stretch	1980(40)	gas	PE	1

B $^2B_2$ C_{2v}

T^a = 15730(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CN stretch	1840(40)	gas	PE	1

A $^2A_1$ C_{2v}

T^a = 15200(1000) gas PE[1]

X $^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CN stretch	2040(40)	gas	PE	1
	2	SC_2 stretch	640(40)	gas	PE	1

[a] From vertical ionization potentials.

References

[1] P. Rosmus, H. Stafast, and H. Bock, Chem. Phys. Lett. 34, 275 (1975).

$NCNCS^+$

G $^2A'$ C_s

T^a = 43730(560) gas PE[1]

E,F $^2A''$,$^2A'$ C_s

T^a = 39450(560) gas PE[1]

D $^2A'$ C_s

T^a = 21540(560) gas PE[1]

C $^2A''$ C_s

T^a = 18800(320) gas PE[1]

B $^2A'$ C_s

T^a = 16860(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		NCS a-stretch	1940(60)	gas	PE	1
		NCS bend	645(60)	gas	PE	1

A $^2A'$ C_s

T^a = 2180(560) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			400(60)	gas	PE	1

X $^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		NCS a-stretch	1690(60)	gas	PE	1

[a] From vertical ionization potentials.

References

[1] M. A. King and H. W. Kroto, J. Am. Chem. Soc. 106, 7347 (1984).

$FC{\equiv}CCN^+$

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

T_0 = 79100(500) gas PE[1]

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

T_0 = 58900(500) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		1300(80)	gas	PE	1
		730(80)	gas	PE	1

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

T_0 = 20170(160) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		1300(80)	gas	PE	1
		730(80)	gas	PE	1

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

T_0 = 16060(160) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		2200(80)	gas	PE	1
		680(80)	gas	PE	1

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

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		2360(80)	gas	PE	1
		600(80)	gas	PE	1

References

[1]G. Bieri, E. Heilbronner, V. Hornung, E. Kloster-Jensen, J. P. Maier, F. Thommen, and W. Von Niessen, Chem. Phys. 36, 1 (1979).

$ClC{\equiv}CCN^+$

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

T_0 = 56500(500) gas PE[1]

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

T_0 = 31900(500) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		480(80)	gas	PE	1

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

T_0 = 20352(3) gas LF[3]

20392(16) Ne AB[3] $\tilde{B}$-$\tilde{X}$ 446-490 nm

Vib. No. sym.		Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	C≡C stretch	1990(20)	Ne	AB	3
	3	C-C stretch	970(80)	gas	PE	1
	4	CCl stretch	538(20)	Ne	AB	3

τ = 190(10) ns gas PEFCO[2]

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

T_0 = 18870(160) gas PE[1]

19662(16) Ne AB[3] $\tilde{A}$-$\tilde{X}$ 461-509 nm

Vib. No. sym.		Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	C≡C stretch	2007(20)[a]	Ne	AB	3
	4	CCl stretch	471(20)	Ne	AB	3

τ = 394(20) ns gas PEFCO[2]

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

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		2140(80)	gas	PE	1
	CCl stretch	500(80)	gas	PE	1

[a] Tentative value.

References

[1]G. Bieri, E. Heilbronner, V. Hornung, E. Kloster-Jensen, J. P. Maier, F. Thommen, and W. Von Niessen, Chem. Phys. 36, 1 (1979).
[2]R. Kuhn, J. P. Maier, and F. Thommen, J. Electron Spectrosc. Relat. Phenom. 34, 253 (1984).
[3]S. Leutwyler, J. P. Maier, and U. Spittel, J. Chem. Soc., Faraday Trans. 2 81, 1565 (1985).

$BrC{\equiv}CCN^+$

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

T_0 = 50750(500) gas PE[1]

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

T_0 = 27400(500) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CBr stretch	400(80)	gas	PE	1

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

T_0 = 20570(160) gas PE[1]

PEFCO[2] and neon-matrix [3] observations suggest that the $\tilde{A}$ and $\tilde{B}$ states are strongly mixed.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C-C stretch	1020(80)	gas	PE	1

τ = 11(2) ns gas PEFCO[2]

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

T_0 = 18621(1) gas EF[3,4]LF[3,4] $\tilde{A}$-$\tilde{X}$ 460-540 nm

18347(3) Ne AB[3] $\tilde{A}$-$\tilde{X}$ 427-545 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡N stretch	2219(4)	Ne	AB	3
	2	C≡C stretch	2020(2)	gas	LF	4
			1976(4)	Ne	AB	3
	3	C-C stretch	1140(2)	gas	LF	4
			1149(4)	Ne	AB	3
	4	CBr stretch	359(2)	gas	LF	4
			354(4)	Ne	AB	3
Π	6	CCC deform.	259(2)[a]	gas	LF	4
	7	CCBr deform.	108(2)[a]	gas	LF	4

τ = 17(2) ns gas PEFCO[2]

A = -1130(160) gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡N stretch	2120(2)	gas	EF	4
	2	C≡C stretch	1983(2)	gas	EF	4
	3	C-C stretch	1095(2)	gas	EF	4
	4	CBr stretch	438(2)	gas	EF	4
Π	6	CCC deform.	302(2)[a]	gas	EF	4
	7	CCBr deform.	111(2)[a]	gas	EF	4

A = -890(160) gas PE[1]

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

References

[1] G. Bieri, E. Heilbronner, V. Hornung, E. Kloster-Jensen, J. P. Maier, F. Thommen, and W. Von Niessen, Chem. Phys. 36, 1 (1979).
[2] R. Kuhn, J. P. Maier, and F. Thommen, J. Electron Spectrosc. Relat. Phenom. 34, 253 (1984).
[3] S. Leutwyler, J. P. Maier, and U. Spittel, J. Chem. Soc., Faraday Trans. 2 81, 1565 (1985).
[4] R. Kuhn, J. P. Maier, L. Misev, and T. Wyttenbach, J. Electron Spectrosc. Relat. Phenom. 41, 265 (1986).

$IC{\equiv}CCN^+$

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

T_0 = 43700(500) gas PE[1]

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

T_0 = 28400(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C-C stretch	1050(80)	gas	PE	1

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

T_0 = 23870(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2100(80)	gas	PE	1
		CI stretch	400(80)	gas	PR	1

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

T_o = 15560(160) gas PE[1]

15371(2) Ne AB[3] $\tilde{A}$-$\tilde{X}$ 530-650 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡N stretch	2214(4)	Ne	AB	3
	2	C≡C stretch	2060(80)	gas	PE	1
	3	C-C stretch	1007(4)	Ne	AB	3
	4	CI stretch	308(4)	Ne	AB	3

τ < 6 ns gas PEFCO[2]

A = -2340(160) gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2060(80)	gas	PE	1
		CI stretch	400(80)	gas	PE	1

A = -2820(160) gas PE[1]

References

[1]G. Bieri, E. Heilbronner, V. Hornung, E. Kloster-Jensen, J. P. Maier, F. Thommen, and W. Von Niessen, Chem. Phys. 36, 1 (1979).
[2]R. Kuhn, J. P. Maier, and F. Thommen, J. Electron Spectrosc. Relat. Phenom. 34, 253 (1984).
[3]S. Leutwyler, J. P. Maier, and U. Spittel, J. Chem. Soc., Faraday Trans. 2 81, 1565 (1985).

$Se(CN)_2^+$

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

T^a = 62450(320) gas PE[1]

$\tilde{G}\ ^2S_1$ C_{2v}

T^a = 42360(320) gas PE[1]

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

T^a = 27670(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	SeC stretch	460(50)	gas	PE	1

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

T^a = 24120(560) gas PE[1]

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

T^a = 23080(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CN stretch	2150(50)	gas	PE	1

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

T^a = 19360(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CN stretch	1900(50)	gas	PE	1

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

$T^a \sim$ 18480 gas PE[1]

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

T^a = 17510(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CN stretch	1900(50)	gas	PE	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CN stretch	1900(50)	gas	PE	1
	2	SeC stretch	530(50)	gas	PE	1

[a] From vertical ionization potentials.

References

[1]G. Jonkers, R. Mooyman, and C. A. de Lange, Mol. Phys. 43, 655 (1981).

Cl_2CCO^+

I $^2A_1$ C_{2v}

T^a = 73100(560) gas PE[1]

H $^2B_2$ C_{2v}

T^a = 65430(560) gas PE[1]

G $^2A_1$ C_{2v}

T^a = 61960(560) gas PE[1]

F $^2B_1$ C_{2v}

T^a = 52850(560) gas PE[1]

E $^2B_2$ C_{2v}

T^a = 47040(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			930(60)	gas	PE	1

D $^2B_1$ C_{2v}

T^a = 38970(320) gas PE[1]

C $^2A_1$ C_{2v}

T^a = 30420(320) gas PE[1]

B $^2A_2$ C_{2v}

T^a = 27840(320) gas PE[1]

A $^2B_2$ C_{2v}

T^a = 25090(320) gas PE[1]

X $^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CCO a-stretch	2200(40)	gas	PE	1
	2	CCO s-stretch	1100(40)	gas	PE	1
	4	CCl_2 "scissors"	330(40)	gas	PE	1

[a] From vertical ionization potentials.

References

[1] D. Colbourne, D. C. Frost, C. A. McDowell, and N. P. C. Westwood, J. Chem. Soc., Chem. Commun. 250 (1980).

$CF_2N_2^+$

F $^2B_2$ C_{2v}

T_o = 62930(1600) gas PE[1]

E $^2A_2$ C_{2v}

T^a = 53250(1600) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			600(80)	gas	PE	1

C,D $^2B_1$,$^2A_1$ C_{2v}

T^a = 44780(1000) gas PE[1]

A,B $^2B_1$,$^2A_1$ C_{2v}

T_o = 30660(1000) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1330(80)	gas	PE	1

X $^2B_2$ C_{2v}

[a] From vertical ionization potential.

References

[1] M. B. Robin, C. R. Brundle, N. A. Kuebler, G. B. Ellison, and K. B. Wiberg, J. Chem. Phys. 57, 1758 (1972).

PF_2CN^+

E C_s

T^a = 58900(1600) gas PE[1]

D C_s

T^a = 50800(1600) gas PE[1]

C C_s

T^a = 37900(1600) gas PE[1]

$\tilde{B}$ C_s

T^a = 16900(1600) gas PE[1]

$\tilde{A}$ C_s

T^a = 12900(1600) gas PE[1]

[a] From vertical ionization potentials.

References

[1]S. Cradock and D. W. H. Rankin, J. Chem. Soc., Faraday Trans. 2 68, 940 (1972).

FSO_3^+

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

T^b = 53700(1200) gas PE[1]

$\tilde{C}$ $^3A_2$[a] C_{3v}

T^b = 40700(1200) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SO_3 s-stretch	920(40)	gas	PE	1
	3	SO_3 "umbrella"	550(40)	gas	PE	1

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

T^b = 17300(1200) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			850(40)	gas	PE	1

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

T^b = 10100(1200) gas PE[1]

$\tilde{X}$ $^1A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SO_3 s-stretch	1220(40)	gas	PE	1

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

References

[1]A. B. Cornford, D. C. Frost, F. G. Herring, and C. A. McDowell, Faraday Discuss. Chem. Soc. 54, 56 (1972).

CF_4^+

$\tilde{D}$ $^2A_1$ T_d Structure: PE,EF[6]

T_o^a = 78830(160) gas PE[1,2,4]

gas EF[5] $\tilde{D}$-$\tilde{C}$ 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.[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF stretch	800(1)	gas	PE,EF	2,4,5

B_o = 0.180(3)[b] EF[6]

$\tilde{C}$ $^2T_2$ T_d Structure: PE,EF[6]

T_o^a = 51230(160) gas PE[1,2,4]

gas EF[5] $\tilde{D}$-$\tilde{C}$ 350-420 nm

Broad, unstructured emission maxima at 290 and 230 nm (34500 and 43500) which appear on He^+ or electron impact on CF_4 have been interpreted as arising from the $\tilde{C}$-$\tilde{A}$ and $\tilde{C}$-$\tilde{X}$ transitions of CF_4^+, respectively.[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF stretch	729	gas	PE,EF	1,2,4,5

Spin-orbit splitting = +16(1) EF[5-7]

$B_o \sim 0.168$[c] PE,EF[6]

$\tilde{B}$ ^2E

T_o^a = 23800(1000) gas PE[1-4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF stretch	810(80)	gas	PE	2-4
e		Deformation	500(100)	gas	PE	2-4

$\tilde{A}$ $^2T_2$

T_o^a = 14100(1000) gas PE[1-4]

$\tilde{X}\ ^2T_1$

[a] Measured with respect to onset of first photoelectron band, estimated by Ref. 2 at 15.35 eV.
[b] From computer simulation of emission bands.
[c] From Franck-Condon analysis of photoelectron spectrum.

References

[1] A. W. Potts, H. J. Lempka, D. G. Streets, and W. C. Price, Phil. Trans. Roy. Soc. (London) A268, 59 (1970).
[2] C. R. Brundle, M. B. Robin, and H. Basch, J. Chem. Phys. 53, 2196 (1970).
[3] A. E. Jonas, G. K. Schweitzer, F. A. Grimm, and T. A. Carlson, J. Electron Spectrosc. Relat. Phenom. 1, 29 (1972/73).
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[5] J. F. M. Aarts, S. M. Mason, and R. P. Tuckett, Mol. Phys. 60, 761 (1987).
[6] S. M. Mason and R. P. Tuckett, Mol. Phys. 62, 175 (1987).
[7] R. N. Dixon and R. P. Tuckett, Chem. Phys. Lett. 140, 553 (1987).

CF_3Cl^+

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

T_o[a] ≤ 66130(400) gas PE[2,4]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_o 2	CF_3 "umbrella"	589(80)	gas	PE	4
3	CCl stretch	420(80)	gas	PE	4

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

T_o[a] = 60420(400) gas PE[2,4]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1 2	CF_3 "umbrella"	637(80)	gas	PE	4

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

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

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1 2	CF_3 "umbrella"	726(80)	gas	PE	4
3	CCl stretch	387(80)	gas	PE	4
e 4	CF_3 stretch	1130(80)	gas	PE	4

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

T^{ab} = 34610(400) gas PE[1,2,4]

A broad, unstructured absorption with onset near 400 nm (25000) and maximum at 295 nm (33900) which appears on argon-resonance photolysis of CF_3Cl isolated in solid argon and which has a photodecomposition threshold at a wavelength longer than 340 nm has been assigned[7] to the $\tilde{C}$-$\tilde{X}$ transition of CF_3Cl^+.

$\tilde{B}\ ^2A_2$ C_{3v}

T^{ab} = 26950(400) gas PE[1,2,4]

$\tilde{A}\ ^2A_1$ C_{3v}

T^{ab} = 22110(400) gas PE[1,2,4]

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

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CF stretch	1299	Ar	IR	5,6
	CCl stretch	734	Ar	IR	5,6
	Deformation	460 451	Ar	IR	5,6
	Deformation	416	Ar	IR	5,6

[a] The first ionization potential of CF_3Cl is taken as 12.42(4) eV, the mean of the values reported in the photoionization studies of Refs. 2 and 3.
[b] From vertical ionization potential.

References

[1] J. Doucet, P. Sauvageau, and C. Sandorfy, J. Chem. Phys. 58, 3708 (1973).
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[7] L. Andrews and F. T. Prochaska, J. Phys. Chem. 83, 368 (1979).

CF_3Br^+

$\tilde{G}\ ^2A_1$ C_{3v}

T^a = 93800(1200) gas PE[2]

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

T^a = 71200(1200) gas PE[2]

E $^2A_1$ C_{3v}

T^a = 62300(1200) gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF_3 "umbrella"	620(80)	gas	PE	2
	3	CBr stretch	360(80)	gas	PE	2

D ^2E C_{3v}

T^a = 44300(800) gas PE[1,2]

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

C ^2E C_{3v}

T^a = 36100(800) gas PE[1,2]

A broad, unstructured absorption with maximum near 295 nm (33600) which appears on argon-resonance photolysis of CF_3Br isolated in solid argon and which has a photodecomposition threshold near 340 nm[5] may be contributed by the $\tilde{C}$-$\tilde{X}$ transition of CF_3Br^+.

B $^2A_2$ C_{3v}

T^a = 30500(800) gas PE[1,2]

A $^2A_1$ C_{3v}

T^a = 17750(800) gas PE[1,2]

X ^2E C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1293	Ar	IR	3,4
		CF stretch	1255	Ar	IR	3,4
			469	Ar	IR	3,4

[a] From vertical ionization potentials.

References

[1] J. Doucet, P. Sauvageau, and C. Sandorfy, J. Chem. Phys. 58, 3708 (1973).
[2] T. Cvitaš, H. Güsten, L. Klasinc, I. Novadj, and H. Vančik, Z. Naturforsch. 32a, 1528 (1977).
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CF_3I^+

G $^2A_1$ C_{3v}

T^a = 107700(1200) gas PE[1]

F ^2E C_{3v}

T^a = 81900(1200) gas PE[1]

E $^2A_1$ C_{3v}

T^a = 70200(800) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF_3 stretch	1090(80)	gas	PE	1
	2	CF_3 "umbrella"	600(80)	gas	PE	1
	3	CI stretch	190(80)	gas	PE	1

D ^2E C_{3v}

T^a = 55100(800) gas PE[1]

C ^2E C_{3v}

T^a = 47360(800) gas PE[1]

B $^2A_2$ C_{3v}

T^a = 41230(800) gas PE[1]

A $^2A_1$ C_{3v}

T^a = 22600(800) gas PE[1]

X $^2E_{3/2}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1229	Ar	IR	2
		CF_3 s-stretch	1090(80)	gas	PE	1
			677	Ar	IR	2

$\tilde{X}\ ^2E_{3/2}$---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			497	Ar	IR	2
		CI stretch	240(80)	gas	PE	1

Spin-orbit splitting = 5890(80).[1]

[a] From vertical ionization potentials.

References

[1] T. Cvitaš, H. Güsten, L. Klasinc, I. Novadj, and H. Vančik, Z. Naturforsch. 32a, 1528 (1977).
[2] F. T. Prochaska and L. Andrews, J. Am. Chem. Soc. 100, 2102 (1978).

$CF_2Cl_2^+$

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

T^{ab} = 68200(1000) gas PE[2,4,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCl_2 stretch	~565	gas	PE	5

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

T_o^a = 56160(160) gas PE[1,2,4,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCl_2 stretch	550(80)	gas	PE	5

$\tilde{E},\tilde{F}\ ^2A_2,^2A_1$ C_{2v}

T^{ab} = 36500(160) gas PE[1,2,4,5]

A broad absorption with maximum near 310 nm (32300) which appears on argon-resonance photolysis of CF_2Cl_2 isolated in solid argon and which has a photodecomposition threshold between 420 and 340 nm has been assigned[7] to the $\tilde{E},\tilde{F}$-$\tilde{X}$ transitions of $CF_2Cl_2^+$.

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

T_o^a = 19150(110) gas PE[1,2,4,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CF_2 "scissors"	370(40)	gas	PE	1,4,5

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

T^{ab} = 13880(160) gas PE[1,2,4,5]

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

T_o^a = 11050(120) gas PE[1,2,4,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF_2 stretch	1097(80)	gas	PE	4,5
	2	CCl_2 stretch	565(80)	gas	PE	5
	4	CCl_2 "scissors"	210(80)	gas	PE	5

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

T^{ab} = 6370(160) gas PE[1,2,4,5]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF_2 a-stretch	1234	Ar	IR	6
		CCl_2 a-stretch	1067	Ar	IR	6
		CF_2 bend	609	Ar	IR	6
		FCCl deform.	424	Ar	IR	6
		FCCl deform.	406	Ar	IR	6

[a] The first ionization potential of CF_2Cl_2 is taken as 11.75 eV, as determined in the photoionization studies of Refs. 2 and 3.
[b] From vertical ionization potential.

References

[1] J. Doucet, P. Sauvageau, and C. Sandorfy, J. Chem. Phys. 58, 3708 (1973).
[2] H. W. Jochims, W. Lohr, and H. Baumgärtel, Ber. Bunsenges. Phys. Chem. 80, 130 (1976).
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$CF_2Br_2^+$

G C_{2v}

T^a = 60700(1000) gas PE[1]

F C_{2v}

T^a = 42900(1000) gas PE[1]

E C_{2v}

T^a = 34530(400) gas PE[1]

A very strong, broad absorption with maximum at 357 nm (28000) which appears on argon-resonance photolysis of CF_2Br_2 isolated in solid argon and which has a photodecomposition threshold at a wavelength longer than 420 nm has been assigned[3] to the $\tilde{E}$-$\tilde{X}$ transition of $CF_2Br_2^+$.

D C_{2v}

T^a = 16700(400) gas PE[1]

C C_{2v}

T^a = 9760(400) gas PE[1]

B C_{2v}

T^a = 6780(400) gas PE[1]

A C_{2v}

T^a = 3310(400) gas PE[1]

X C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF_2 stretch	1244	Ar	IR	2
			873	Ar	IR	2
			868	Ar	IR	2
			428	Ar	IR	2
			406	Ar	IR	2

[a] From vertical ionization potentials.

References

[1]J. Doucet, R. Gilbert, P. Sauvageau, and C. Sandorfy, J. Chem. Phys. 62, 366 (1975).
[2]F. T. Prochaska and L. Andrews, J. Phys. Chem. 82, 1731 (1978).
[3]L. Andrews and F. T. Prochaska, J. Phys. Chem. 83, 368 (1979).

$CFCl_3^+$

E,F $^2A_1$,^2E C_{3v}

T^a = 53650(160) gas PE[1-4]

D ^2E C_{3v}

T_o = 25390(120) gas PE[1-4]

A prominent, broad absorption with maximum near 405 nm (24700) which appears on argon-resonance photolysis of $CFCl_3$ isolated in solid argon and which has a photodecomposition threshold at a wavelength longer than 500 nm has been assigned[6] to the $\tilde{D}$-$\tilde{X}$ transition of $CFCl_3^+$.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCl_3 stretch	~460	gas	PE	4
	3	CCl_3 "umbrella"	275(40)	gas	PE	1,4

C $^2A_1$ C_{3v}

T_o = 13430(100) gas PE[1-4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF stretch	1010(80)	gas	PE	2
	2	CCl_3 stretch	640(80)	gas	PE	2
	3	CCl_3 "umbrella"	340(40)	gas	PE	4

B ^2E C_{3v}

T^a = 9680(160) gas PE[1-4]

Band shows a splitting of 1130(240).[4]

A ^2E C_{3v}

T^a = 2980(160) gas PE[1-4]

Band shows a splitting of 1530(160).[4]

$\tilde{X}\ ^2A_2$ C_{3v}

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CF stretch	1214	Ar	IR	5
	CCl a-stretch	1041	Ar	IR	5
	CCl s-stretch	585	Ar	IR	5
	Deformation	432	Ar	IR	5
	Deformation	324[b]	Ar	IR	5

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

References

[1]J. Doucet, P. Sauvageau, and C. Sandorfy, J. Chem. Phys. 58, 3708 (1973).
[2]F. T. Chau and C. A. McDowell, J. Electron Spectrosc. Relat. Phenom. 6, 357 (1975).
[3]H. W. Jochims, W. Lohr, and H. Baumgärtel, Ber. Bunsenges. Phys. Chem. 80, 130 (1976).
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$CFBr_3^+$

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

T^a = 55830(160) gas PE[1]

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

T^a = 26540(160) gas PE[1]

A prominent, broad absorption with maximum near 435 nm (23000) which appears on argon-resonance photolysis of $CFBr_3$ isolated in solid argon and which has a photodecomposition threshold at a wavelength longer than 500 nm has been assigned[3] to the $\tilde{D}$-$\tilde{X}$ transition of $CFBr_3^+$.

$\tilde{C}\ ^2A_1$ C_{3v}

T_0 = 12750(320) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1 3	CBr_3 "umbrella"	210(80)	gas	PE	1

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

T^a = 9200(160) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1 1	CF stretch	874(80)	gas	PE	1

Splitting of 1690(160) observed.[1]

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

T^a = 3790(160) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1 3	CBr_3 "umbrella"	213(80)	gas	PE	1

Splitting of 4030(160) observed.[1]

$\tilde{X}\ ^2A_2$ C_{3v}

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CF stretch	1167 1160	Ar	IR	2
		853	Ar	IR	2
		423	Ar	IR	2
		399	Ar	IR	2
		316	Ar	IR	2

[a] From vertical ionization potential.

References

[1]F. T. Chau and C. A. McDowell, J. Electron Spectrosc. Relat. Phenom. 6, 357 (1975).
[2]F. T. Prochaska and L. Andrews, J. Phys. Chem. 82, 1731 (1978).
[3]L. Andrews and F. T. Prochaska, J. Phys. Chem. 83, 368 (1979).

CCl_4^+

$\tilde{D}\ ^2A_1$ T_d

T^{ab} = 68800(900) gas PE[2]

$\tilde{C}\ ^2T_2$

T_0^a = 39290(900) gas PE[2-4]

A strong, broad (FWHM ~ 5200) absorption with maximum at 425 nm (23500) which appears on argon-resonance photolysis of CCl_4 isolated in an argon matrix, with counterparts in krypton and xenon matrices and in various condensed-phase radiolysis systems, has been assigned[6,7] to the $\tilde{C}$-$\tilde{X}$ transition of CCl_4^+. The energy difference is attributed to structural

relaxation in the condensed phase. The absorption can be destroyed by exposure of the sample to 500-1000 nm radiation.

B ^2E

T^{ab} = 15330(240) gas PE[2-4]

A $^2T_2$

T_o[a] = 6450(320) gas PE[2-4]

X $^2T_1$ [c] C_{2v} ?

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CCl_2 a-stretch	927	Ar	IR	5
	C··Cl_2 stretch	374	Ar	IR	5

[a] The first ionization potential is taken as 11.47(1) eV, as in the photoionization study of Ref. 1.
[b] From vertical ionization potential.
[c] Distorted by Jahn-Teller interaction.

References

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[3]J. C. Green, M. L. Green, P. J. Joachim, A. F. Orchard, and D. W. Turner, Phil. Trans. Roy. Soc. (London) A268, 111 (1970).
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CBr_4^+

D $^2A_1$ T_d

T^{ab} = 75000(1000) gas PE[1,2]

C $^2T_2$

T^{ab} = 38600(600) gas PE[1,2]

A strong, broad absorption with maximum at 475 nm (21000) which appears on argon-resonance photolysis of CBr_4 isolated in an argon matrix and which has a photodecomposition threshold at a wavelength longer than 650 nm has been assigned[5] to the C̃-X̃ transition of CBr_4^+. The energy difference is attributed to structural relaxation in the condensed phase.

B ^2E

T^{ab} = 14320(400) gas PE[1,2]

A $^2T_2$

T^{ab} = 6050(320) gas PE[1,2]

X $^2T_1$ [c]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CBr stretch	778	Ar	IR	4
	C··Br_2 stretch	326	Ar	IR	4

[a] The first ionization potential of CBr_4 is taken as 10.31(2) eV, as in the photoionization study of Ref. 3.
[b] From vertical ionization potential.
[c] Distorted by Jahn-Teller interaction.

References

[1]A. W. Potts, H. J. Lempka, D. G. Streets, and W. C. Price, Phil. Trans. Roy. Soc. (London) A268, 59 (1970).
[2]J. C. Green, M. L. Green, P. J. Joachim, A. F. Orchard, and D. W. Turner, Phil. Trans. Roy. Soc. (London) A268, 111 (1970).
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SiF_4^+

D̃ $^2A_1$ T_d Structure: PE,EF[8]

T^{ab} = 50800(200) gas PE[1]

EF[6]EM[7,9] D̃-C̃ 530-590 nm

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 D̃-B̃ and D̃-Ã transitions of SiF_4^+, respectively.[5,7]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1 1	SiF stretch	743.4(5)	gas	EF	6

B_o = 0.136(1)[c] EF[8]

C̃ $^2T_2$ T_d[d] Structure: PE,EF[8]

T_o[a] = 33130(100) gas PE[1,2,4]

EF[6]EM[7,9] D̃-C̃ 530-590 nm

D̃-C̃ band origin measured at 18146.8 in emission studies on a cooled beam.[6]

Continuous emission between 570 and 730 nm (13700 and 17550) may arise either from the C̃-Ã transition[6] or from an extension of the D̃-C̃ transition.[7,9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiF stretch	706.6(5)	gas	PE,EF	2,4,6
e	2	Deformation	159.0(5)	gas	EF	6
t_2	4	Deformation	431.0(5)	gas	PE,EF	2,4,6

Spin-orbit splitting = +6.9(2) EF[6,8,10]

B_o = 0.132[c] PE,EF[8]

B̃ ^2E

T_o[a] = 22580(100) gas PE[1,2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiF stretch	685(50)	gas	PE	4

Ã $^2T_2$

T_o[a] = 17000(1000) gas PE[1,2,4]

X̃ $^2T_1$

[a] Measured with respect to a first ionization potential of 15.19 eV, estimated[3] 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 D̃ - C̃ emission.
[d] Dynamic Jahn-Teller distortion, probably to C_{3v}.[6,8]

References

[1] T. P. Fehlner and D. W. Turner, Inorg. Chem. 13, 754 (1974).
[2] D. R. Lloyd and P. J. Roberts, J. Electron Spectrosc. Relat. Phenom. 7, 325 (1975).
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SiF_3Cl^+

G̃ $^2A_1$ C_{3v}

T[a] = 59870(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiF_3 stretch	890(40)	gas	PE	1
	3	Deformation	200(40)	gas	PE	1

F̃ ^2E C_{3v}

T[a] = 44210(320) gas PE[1]

Ẽ $^2A_1$ C_{3v}

T[a] = 38890(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiF_3 stretch	965(40)	gas	PE	1
	2	SiCl stretch	605(40)	gas	PE	1

D̃ ^2E C_{3v}

T[a] = 32680(320) gas PE[1]

C̃ ^2E C_{3v}

T[a] = 26300(320) gas PE[1]

B̃ $^2A_2$ C_{3v}

T[a] = 23480(320) gas PE[1]

Ã $^2A_1$ C_{3v}

T[a] = 15250(320) gas PE[1]

X̃ ^2E C_{3v}

[a] From vertical ionization potentials.

References

[1] S. Cradock, E. A. V. Ebsworth, and R. A. Whiteford, J. Chem. Soc., Dalton Trans. 2401 (1973).

SiF_3Br^+

G̃ $^2A_1$ C_{3v}

T[a] = 67290(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiF_3 stretch	755(40)	gas	PE	1
	3	Deformation	240(40)	gas	PE	1

F ^2E C_{3v}

T^a = 51150(320) gas PE[1]

E $^2A_1$ C_{3v}

T^a = 45500(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiF_3 stretch	850(40)	gas	PE	1

D ^2E C_{3v}

T^a = 39530(320) gas PE[1]

C ^2E C_{3v}

T^a = 33640(320) gas PE[1]

B $^2A_2$ C_{3v}

T^a = 29370(320) gas PE[1]

A $^2A_1$ C_{3v}

T^a = 16860(320) gas PE[1]

X ^2E C_{3v}

[a] From vertical ionization potentials.

References

[1] S. Cradock, E. A. V. Ebsworth, and R. A. Whiteford, J. Chem. Soc., Dalton Trans. 2401 (1973).

$SiCl_4^+$

D $^2A_1$ T_d

T_o = 48900(400) gas PE[1,2]

C $^2T_2$

T_o = 26620(160) gas PE[1,2]

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[3] to the C̃-X̃ transition of $SiCl_4^+$. The energy difference is attributed to structural relaxation in the argon matrix. The absorption can be destroyed by exposure of the sample to 290-1000 nm radiation.

B ^2E

T^a = 13880(400) gas PE[1,2]

A $^2T_2$

T_o = 7750(160) gas PE[1,2]

X $^2T_1$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		$SiCl_2$ a-stretch 717[b]		Ar	IR	3

[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).
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GeF_4^+

D̃ $^2A_1$ T_d

T^{ab} = 45300(1000) gas PE[2,4]

EF[6] D̃-C̃ 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 D̃-B̃ and D̃-Ã transitions of GeF_4^+, respectively.[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	GeF stretch	644.3	gas	EF	6

C̃ $^2T_2$ [c]

T_o^a = 20330(240) gas PE[1-4]

EF[6] D̃-C̃ 390-420 nm

D̃-C̃ band origin measured at 25064.0 in emission studies on a cooled beam.[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	GeF stretch	620.8	gas	EF	6
e	2	Deformation	82.8	gas	EF	6
t_2	4	Deformation	288.3	gas	EF	6

Spin-orbit splitting = -18.6[d] EF[6]

B ^2E

T^{ab} = 11210(320) gas PE[1-4]

A $^2T_2$

T^{ab} = 7020(320) gas PE[1-4]

X $^2T_1$

[a] First ionization potential taken to be 15.69(2) eV, as in Ref. 1.
[b] From vertical ionization potential.
[c] Distorted by Jahn-Teller interaction.
[d] Tentative value.

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$GeCl_4^+$

D $^2A_1$ T_d

T_o = 51070(400) gas PE[1,2]

C $^2T_2$ T_d

T_o = 21620(240) gas PE[1,2]

B ^2E

T^a = 9440(240) gas PE[1,2]

A $^2T_2$

T^a = 6130(320) gas PE[1,2]

X $^2T_1$

[a] From vertical ionization potential.

References

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F_3NO^+

F $^2A_1$ C_{3v}

T^{ab} = 62450(900) gas PE[2]

E ^2E C_{3v}

T_o^b = 52770(240) gas PE[2]

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

T_o^b = 24040(320) gas PE[2]

A,B $^2A_2$,^2E C_{3v}

T_o^b = 11860(560) gas PE[2]

X ^2E C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NO stretch	1025(25)	gas	PE	2

[a] From vertical ionization potential.
[b] The first ionization potential is taken as 13.36(1) eV, the value obtained in the PES study of Ref. 2. The difference between that value and the alternate value of 13.26(1) eV, obtained in the photoionization study of Ref. 1, does not correspond with the excitation of a whole number of vibrational quanta.

References

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F_3NS^+

C $^2A_2$? C_{3v}

T^a = 47200(320) gas PE[1]

B ^2E C_{3v}

T^a = 33480(320) gas PE[1]

A $^2A_1$ C_{3v}

T^a = 13310(320) gas PE[1]

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

[a] From vertical ionization potentials.

References

[1]D. O. Cowan, R. Gleiter, O. Glemser, and E. Heilbronner, Helv. Chim. Acta 55, 2418 (1972).

F_3PO^+

$\tilde{G}\ ^2A_1$ C_{3v}

T^a = 85800(1100) gas PE[1]

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

T_o = 61240(480) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		654(80)	gas	PE	1

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

T^a = 55190(400) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		718(50)	gas	PE	1

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

T_o = 45830(480) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		718(25)	gas	PE	1

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

$T^a \sim$ 39620 gas PE[1]

$\tilde{B}\ ^2A_2$ C_{3v}

T_o = 31630(720) gas PE[1]

$\tilde{A}\ ^2A_1$ C_{3v}

T_o = 19280(640) gas PE[1]

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

[a] From vertical ionization potential.

References

[1]P. J. Bassett and D. R. Lloyd, J. Chem. Soc., Dalton Trans. 248 (1972).

Cl_3PO^+

$\tilde{G}\ ^2A_1$ C_{3v}

T^a = 66080(320) gas PE[1,2]

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

T_o = 38490(320) gas PE[1-3]

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

T_o = 30180(320) gas PE[1-3]

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

T^a = 20090(320) gas PE[1-3]

$\tilde{C}\ ^2A_1$ C_{3v}

T^a = 17020(320) gas PE[1-3]

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

T^a = 12910(600) gas PE[1-3]

Spin-orbit splitting = 650(240) gas PE[2,3]

$\tilde{A}\ ^2A_2$ C_{3v}

T^a = 8230(320) gas PE[1-3]

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

[a] From vertical ionization potential.

References

[1]P. A. Cox, S. Evans, A. F. Orchard, N. V. Richardson, and P. J. Roberts, Faraday Discuss. Chem. Soc. 54, 26 (1972).
[2]J. C. Bünzli, D. C. Frost, and C. A. McDowell, J. Electron Spectrosc. Relat. Phenom. 1, 481 (1972/73).
[3]J. L. Berkosky, F. O. Ellison, T. H. Lee, and J. W. Rabalais, J. Chem. Phys. 59, 5342 (1973).

Br_3PO^+

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

T^a = 37280(320) gas PE[1-3]

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

T_o = 29210(320) gas PE[1-3]

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

T^a = 15000(500) gas PE[1-3]

$\tilde{C}\ ^2A_1$ C_{3v}

T^a = 13390(320) gas PE[1-3]

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

T^a = 8960(320) gas PE[1-3]

Spin-orbit splitting = 1940(320) gas PE[1-3]

$\tilde{A}\ ^2A_2$ C_{3v}

T^a = 5083(320) gas PE[1-3]

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

Spin-orbit splitting = 890(240) gas PE[1-3]

[a] From vertical ionization potential. The first ionization potential is taken as 10.75(2) eV, the onset of ionization to form Br_3PO^+ ($\tilde{X}\ ^2E_{3/2}$) determined by Ref. 2, and the positions of higher levels are calculated with respect to that energy level.

References

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[2] J. C. Bünzli, D. C. Frost, and C. A. McDowell, J. Electron Spectrosc. Relat. Phenom. 1, 481 (1972/73).
[3] J. L. Berkosky, F. O. Ellison, T. H. Lee, and J. W. Rabalais, J. Chem. Phys. 59, 5342 (1973).

F_3PS^+

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

T^a = 72450(320) gas PE[1]

$\tilde{F}\ ^2A_1$ C_{3v}

$T^a \sim$ 70300 gas PE[1]

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

T^a = 60110(500) gas PE[1]

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

T^a = 56160(320) gas PE[1]

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

T^a = 46960(500) gas PE[1]

$\tilde{B}\ ^2A_2$ C_{3v}

T^a = 42840(320) gas PE[1]

$\tilde{A}\ ^2A_1$ C_{3v}

T^a = 27350(320) gas PE[1]

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

[a] From vertical ionization potentials.

References

[1] S. Elbel and H. tom Dieck, J. Chem. Soc., Dalton Trans. 1757 (1976).

Cl_3PS^+

$\tilde{G}\ ^2A_1$ C_{3v}

T_o = 70270(320) gas PE[1-3]

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

T_o = 46230(320) gas PE[1-4]

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

T_o = 39620(320) gas PE[1-4]

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

T^a = 30340(320) gas PE[1-4]

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

$T^a \sim$ 24400 gas PE[1-4]

$\tilde{B}\ ^2A_1$ C_{3v}

$T^a \sim$ 22400 gas PE[1-4]

$\tilde{A}\ ^2A_2$ C_{3v}

T_o = 8390(320) gas PE[1-4]

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

[a] From vertical ionization potential.

References

[1] P. A. Cox, S. Evans, A. F. Orchard, N. V. Richardson, and P. J. Roberts, Faraday Discuss. Chem. Soc. 54, 26 (1972).
[2] J. C. Bünzli, D. C. Frost, and C. A. McDowell, J. Electron Spectrosc. Relat. Phenom. 1, 481 (1972/73).
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Br_3PS^+

F ^2E C_{3v}

T^a = 42520(320) gas PE[1-3]

E $^2A_1$ C_{3v}

T_o = 34450(320) gas PE[1-3]

D ^2E C_{3v}

T^a = 22510(320) gas PE[1-3]

C̃ $^2A_1$ C_{3v}

T^a = 19530(320) gas PE[1-3]

B̃ ^2E C_{3v}

T^a = 15170(320) gas PE[1-3]

Spin-orbit splitting = 1780(320) gas PE[1-3]

Ã $^2A_2$ C_{3v}

T^a = 12180(320) gas PE[1-3]

X̃ ^2E C_{3v}

[a] From vertical ionization potential.

References

[1]P. A. Cox, S. Evans, A. F. Orchard, N. V. Richardson, and P. J. Roberts, Faraday Discuss. Chem. Soc. 54, 26 (1972).
[2]J. C. Bünzli, D. C. Frost, and C. A. McDowell, J. Electron Spectrosc. Relat. Phenom. 1, 481 (1972/73).
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FSO_3

C̃ ^2E C_{3v} Structure: AB[3]

T_o = 19383.1 gas AB[1-3] C̃-X̃ 360-550 nm

19077(5) Ar AB[4] C̃-X̃ 420-525 nm

18986(5) N_2 AB[4] C̃-X̃ 420-525 nm

Overlapped by continuum beyond 460 nm.[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SO stretch	952.9	gas	AB	2
			947(10)	Ar	AB	4
			966(10)	N_2	AB	4
	2	SF stretch	800.5	gas	AB	2
			796(10)	Ar	AB	4
			820(10)	N_2	AB	4
	3	SO deform.	515.0	gas	AB	2
			512(10)	Ar	AB	4
			511(10)	N_2	AB	4
e	4	SO stretch	1114.5	gas	AB	2
	5	SO deform.	505.7	gas	AB	2
	6	SF wag	346.9	gas	AB	2

A = 66 gas AB[2]

A_o = 0.172; B_o = 0.158 AB[3] [a]

B̃ ^2E C_{3v}

gas AB[1-3] B̃-X̃ 570-1000 nm

Ã $^2A_1$ C_{3v}

gas AB[1-3] Ã-X̃ 1000-2000 nm

X̃ $^2A_2$ C_{3v} Structure: AB[1,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SO stretch	1055.5	gas	AB,LF	2,5
			1053	Ar	IR	4
	2	SF stretch	839.3	gas	AB,LF	2,5
			833	Ar	IR	4
	3	SO deform.	533.5	gas	AB,LF	2,5
			531	Ar	IR	4
e	4	SO stretch	1177.5	gas	AB,LF	2,5
			1177	Ar	IR	4
	5	SO deform.	604.1	gas	AB,LF	2,5
			601	Ar	IR	4
	6	SF wag	369.4	gas	AB,LF	2,5
			366	Ar	IR	4

A_o = 0.183; B_o = 0.158 AB^3

[a] For upper Jahn-Teller potential surface.

References

[1]G. W. King, D. P. Santry, and C. H. Warren, J. Mol. Spectrosc. 32, 108 (1969).
[2]G. W. King and C. H. Warren, J. Mol. Spectrosc. 32, 121 (1969).
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$FClO_3^+$

F $^2A_1$ C_{3v}

T^a = 67400(900) gas PE[1]

E ^2E C_{3v}

T_o = 54500(120) gas PE[1]

D ^2E C_{3v}

T^a = 33770(200) gas PE[1]

C ^2E C_{3v}

T_o = 19690(100) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ClO_3 stretch	790(40)	gas	PE	1

B $^2A_1$ C_{3v}

T^a = 10850(200) gas PE[1]

A ^2E C_{3v}

T_o = 5930(200) gas PE[1]

X $^2A_2$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ClO_3 stretch	900(40)	gas	PE	1
	3	ClO_3 "umbrella"	520(40)	gas	PE	1

References

[1]R. L. DeKock, D. R. Lloyd, I. H. Hillier, and V. R. Saunders, Proc. Roy. Soc. (London) A328, 401 (1972).

$F_2SO_2^+$

G $^2A_1$ C_{2v}

T_o = 53730(140) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	SF_2 stretch	855(30)	gas	PE	1,3
	3	SO_2 "scissors"	500(20)	gas	PE	1,3

F $^2B_2$ C_{2v}

T_o = 49500(140) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	SF_2 stretch	850(30)	gas	PE	1
	3	SO_2 "scissors"	485(40)	gas	PE	1

E $^2B_1$ C_{2v}

T_o = 40580(320) gas PE[1-3]

D $^2B_2$ C_{2v}

T_o = 29340(120) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SO_2 stretch	1135(16)	gas	PE	1-3
	2	SF_2 stretch	805(30)	gas	PE	1-3
	3	SO_2 "scissors"	510(20)	gas	PE	1-3

C $^2A_1$ C_{2v}

T_o = 17270(130) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SO_2 stretch	1025(30)	gas	PE	1-3

B $^2B_1$ C_{2v}

T_o = 14600(160) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4	SF_2 "scissors"	340(16)	gas	PE	1-3

Ã $^2A_2$ C_{2v}

T_o = 4280(240) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	SO_2 "scissors"	475(60)	gas	PE	1-3

X̃ $^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			370(40)	gas	PE	1

References

[1]R. L. DeKock, D. R. Lloyd, I. H. Hillier, and V. R. Saunders, Proc. Roy. Soc. (London) A328, 401 (1972).
[2]G. W. Mines, R. K. Thomas, and H. Thompson, Proc. Roy. Soc. (London) A329, 275 (1972).
[3]D. Chadwick, D. C. Frost, F. G. Herring, A. Katrib, C. A. McDowell, and R. A. N. McLean, Can. J. Chem. 51, 1893 (1973).

$FClSO^+_2$

T^a = 49900(1000) gas PE[1]

T^a = 33800(1000) gas PE[1]

T^a = 32030(320) gas PE[1]

T^a = 19610(320) gas PE[1]

T^a = 16300(320) gas PE[1]

T^a = 12340(320) gas PE[1]

T^a = 6050(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]G. W. Mines, R. K. Thomas, and H. Thompson, Proc. Roy. Soc. (London) A329, 275 (1972).

$Cl_2SO^+_2$

T^a = 48970(320) gas PE[1,2]

T^a = 44860(320) gas PE[1,2]

T_o = 39370(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SO_2 stretch	1170(40)	gas	PE	2
	2	SO_2 "scissors"	580(40)	gas	PE	2
	3	SCl_2 stretch	380(40)	gas	PE	2
	4	SCl_2 "scissors"	200(40)	gas	PE	2

T^a = 16540(1000) gas PE[1,2]

T^a = 13640(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			640(40)	gas	PE	2

T_o = 7660(1000) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			500(40)	gas	PE	2

[a] From vertical ionization potential.

References

[1]G. W. Mines, R. K. Thomas, and H. Thompson, Proc. Roy. Soc. (London) A329, 275 (1972).
[2]D. Chadwick, D. C. Frost, F. G. Herring, A. Katrib, C. A. McDowell, and R. A. N. McLean, Can. J. Chem. 51, 1893 (1973).

XeF^+_4

I $^2A_{2u}$ D_{4h}

$T^{ab} \sim$ 57200 gas PE[1]ESCA[4]

H ^2E_u D_{4h}

T^{ab} ∿ 43800 gas ESCA[4]

G $^2B_{2g}$ D_{4h}

T^{ab} = 29400(1000) gas PE[1]

F ^2E_g D_{4h}

T^{ab} ∿ 27000 gas PE[1]

E $^2B_{2g}$ D_{4h}

T^{ab} = 25300(1000) gas PE[1]

D ^2E_u D_{4h}

T^{ab} ∿ 22200 gas PE[1]

C $^2A_{2g}$ D_{4h}

T^{ab} = 20100(1000) gas PE[1]

B $^2B_{1g}$ D_{4h}

T^{ab} = 14600(1000) gas PE[1]

A $^2A_{1g}$ D_{4h}

T_o[a] = 5890(1000) gas PE[1]UV[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1	Sym. stretch	490(80)	gas	PE	1

X $^2A_{2u}$ D_{4h}

[a] The first ionization potential is taken as 12.65(10) eV, as in the photoionization study of Ref. 2.
[b] From vertical ionization potential.

References

[1]C. R. Brundle, G. R. Jones, and H. Basch, J. Chem. Phys. 55, 1098 (1971).
[2]J. Berkowitz, W. A. Chupka, P. M. Guyon, J. H. Holloway, and R. Spohr, J. Phys. Chem. 75, 1461 (1971).
[3]U. Nielsen and W. H. E. Schwarz, Chem. Phys. 13, 195 (1976).
[4]G. M. Bancroft, P.-Å. Malmquist, S. Svensson, E. Basilier, U. Gelius, and K. Siegbahn, Inorg. Chem. 17, 1595 (1978).

6.12. Six-Atomic Molecules

$H_2BNH_2^+$

D $^2A_1$ C_{2v}

T^a = 59100(1200) gas PE[1]

C $^2B_2$ C_{2v}

T^a = 51500(1200) gas PE[1]

B $^2A_1$ C_{2v}

T^a = 26800(1200) gas PE[1]

A $^2B_2$ C_{2v}

T^a = 10300(1200) gas PE[1]

X $^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		BN stretch	1100(80)	gas	PE	1

[a] From vertical ionization potential.

References

[1]N. P. C. Westwood and N. H. Werstiuk, J. Am. Chem. Soc. 108, 891 (1986).

$C_2H_4^+$

D $^2B_1$ D_2

T_o ∿ 67230 gas PE[1-3]

C $^2B_2$ D_2

T_o = 42140(350)[a] gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	2	CC stretch	1245(20)	gas	PE	1-3,6

B ^2A D_2

T_o = 31570(200)[a] gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	CH stretch	1900(100)	gas	PE	3

Ã $^2B_3$ D_2

T_o = 15600(200)[a] gas PE[2,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	CH stretch	2900(50)	gas	PE	1,3
	2		1150(100)	gas	PE	3
	3		800(100)	gas	PE	1,3

X̃ $^2B_3$ D_2 Structure: PE[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	2	CC stretch	1494(1)[b]	gas	PE	5,6
	3	CH_2 "scissors"	1261(3)[b]	gas	PE	5,6
	4	Torsion	∿220[c]	gas	PE	5,6

Barrier to inversion = 270(150).[6]

$C_2D_4^+$

D̃ $^2B_1$ D_2

T_o = ∿ 66740 gas PE[2,3]

C̃ $^2B_2$ D_2

T_o = 42050(100)[a] gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	2	CC stretch	1100(80)	gas	PE	2
	3	CD_2 "scissors"	930(40)	gas	PE	2,3

B̃ ^2A D_2

T_o = 31480(100)[a] gas PE[2,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a			1000(100)	gas	PE	3

Ã $^2B_3$ D_2

T_o = 15670(100)[a] gas PE[2,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	CD stretch	2640(100)	gas	PE	3
	2	CC stretch	900(100)	gas	PE	3

X̃ $^2B_3$ D_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	2	CC stretch	1332(8)	gas	PE	4,8
	3	CD_2 "scissors"	961(8)	gas	PE	4,8
	4	Torsion	23(10)[d]	gas	PE	8

[a] First ionization potential of C_2H_4 taken as 10.517(2) and of C_2D_4 as 10.528(2), from threshold PE study of Ref. 4.
[b] For reassignment see Refs. 7 and 8.
[c] $\frac{1}{2}(2\nu_4)$; evidence for appreciable anharmonicity.
[d] $2\nu_4$ = 269(7).[4,8]

References

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$NH_2BF_2^+$

Ã $^2A_1$ C_{2v}

T^a = 74200(1600) gas PE[2]

G̃ $^2B_2$ C_{2v}

T^a = 63900(1100) gas PE[2]

F̃ $^2A_1$ C_{2v}

T^a = 58500(1100) gas PE[1,2]

$E\ ^2B_1$ C_{2v}

T^a = 49700(1100) gas PE[2]

$D\ ^2B_2$ C_{2v}

T^a = 48400(1600) gas PE[1,2]

$B,C\ ^2B_2,^2A_2$ C_{2v}

T^a = 35700(1100) gas PE[1,2]

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

T^a = 32400(1100) gas PE[1,2]

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

[a] From vertical ionization potential.

References

[1]H. W. Kroto and D. McNaughton, J. Chem. Soc., Dalton Trans. 1767 (1985).
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$NH_2BCl_2^+$

$F\ ^2A_1$ C_{2v}

T^a = 38800(1100) gas PE[1]

$E\ ^2B_2$ C_{2v}

T^a = 26600(1600) gas PE[1]

$D\ ^2B_1$ C_{2v}

T^a = 23100(1100) gas PE[1]

$C\ ^2A_1$ C_{2v}

T^a = 12400(1100) gas PE[1]

$B\ ^2A_2$ C_{2v}

T^a = 9600(1100) gas PE[1]

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

T^a = 6500(1100) gas PE[1]

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

[a] From vertical ionization potential.

References

[1]C. A. Kingsmill, N. H. Werstiuk, and N. P. C. Westwood, J. Am. Chem. Soc. 109, 2870 (1987).

$NH_2BBr_2^+$

$F\ ^2A_1$ C_{2v}

T^a = 36600(1100) gas PE[1]

$E\ ^2B_2$ C_{2v}

T^a = 24200(1600) gas PE[1]

$D\ ^2B_1$ C_{2v}

T^a = 21200(1100) gas PE[1]

$C\ ^2A_1$ C_{2v}

T^a = 10200(1100) gas PE[1]

$B\ ^2A_2$ C_{2v}

T^a = 7100(1100) gas PE[1]

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

T^a = 5300(1100) gas PE[1]

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

[a] From vertical ionization potential.

References

[1]C. A. Kingsmill, N. H. Werstiuk, and N. P. C. Westwood, J. Am. Chem. Soc. 109, 2870 (1987).

$CH_2{=}SiH_2$

In an Ar or N_2 matrix, absorption maximum at 258 nm.[1-4] On irradiation at 254 nm, photoisomerizes to CH_3SiH.[2,4]

X C_{2v}

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	SiH s-stretch	2219	Ar	IR	1-3
		2214	N_2	IR	2,4
	CH_2 "scissors"	1350	Ar	IR	2,3
		1350	N_2	IR	2,4
	Si=C stretch	985	Ar	IR	1-3
		985	N_2	IR	1,2,4
	SiH_2 "scissors"	927	Ar	IR	1-3
		927	N_2	IR	2,4
b_1	CH_2 wag	741	Ar	IR	1-3
		747	N_2	IR	2,4

$\tilde{X}$---Continued

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	SiH a-stretch	2239	Ar	IR	1-3
		2235	N_2	IR	2,4
	CH_2 rock	817	Ar	IR	1-3
		817	N_2	IR	2,4

$CH_2{=}SiD_2$

In an Ar matrix, absorption maximum at 259 nm.[1,4]

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

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	SiD s-stretch	1600	Ar	IR	1,3
		1600	N_2	IR	4
	CH_2 "scissors"	1335	Ar	IR	3
		1352	N_2	IR	4
a_1	Si=C stretch	952	Ar	IR	1,3
		952	N_2	IR	4
b_1	CH_2 wag	719	Ar	IR	1,3
		725	N_2	IR	4
b_2	SiD a-stretch	1635	Ar	IR	1,3
		1635	N_2	IR	4
	CH_2 rock	759	Ar	IR	1,3
		760	N_2	IR	4
	SiD_2 rock	396	Ar	IR	1,3
		396	N_2	IR	4

References

[1]G. Maier, G. Mihm, and H. P. Reisenauer, Angew. Chem. 93, 615 (1981); Angew. Chem. Int. Ed. Engl. 20, 597 (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_3SiH

In an Ar matrix, absorption maximum at 480 nm. On irradiation in this spectral region, photoisomerizes to $CH_2{=}SiH_2$. An absorption band with similar behavior appears at 330 nm in N_2-matrix studies.[1,2]

$\tilde{X}$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		2004	Ar	IR	1,2
		1986	N_2	IR	1,2
		1978	N_2	IR	1,2
		1971	N_2	IR	1,2
		1935	Ar	IR	1,2

References

[1]H. P. Reisenauer, G. Mihm, and G. Maier, Angew. Chem. 94, 864 (1982); Angew. Chem. Int. Ed. Engl. 21, 854 (1982).
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CH_3OH^+

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

T_o = 49600(120) gas PE[1-3]

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

T_o = 38300(120) gas PE[1-3]

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

T_o = 29420(120) gas PE[1-3]

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

T_o = 10060(120) gas PE[1-3]

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

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	CH_3 "umbrella"	1372(80)	gas	PE	2,3
	CO stretch ?	895(80)	gas	PE	1-3

CD_3OD^+

X $^2A''$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		1030(30)	gas	PE	2
		763(30)	gas	PE	2

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CH_3SH^+

C $^2A''$ C_s

T^a = 49930(160) gas PE[1-3]

B $^2A'$ C_s

T^a = 34110(160) gas PE[1-3]

A $^2A'$ C_s

T^a = 21280(160) gas PE[1-3]

X $^2A''$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	CH_3 "umbrella"	1250(80)	gas	PE	2
	CS stretch	680(40)	gas	PE,PI	1,2,4

[a] From vertical ionization potential. The first ionization potential of CH_3SH is taken as 9.442 eV, as in the photoionization study of Ref. 4.

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SiH_3SH^+

C $^2A'$ C_s

T^a = 35820(320) gas PE[1]

B $^2A''$ C_s

T^a = 20400(1000) gas PE[1]

A $^2A'$ C_s

T^a = 14360(320) gas PE[1]

X $^2A''$ C_s

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, J. Chem. Soc., Faraday Trans. 2 68, 281 (1972).

GeH_3SH^+

C $^2A'$ C_s

T^a = 35420(320) gas PE[1]

B $^2A''$ C_s

T^a = 22700(1000) gas PE[1]

A $^2A'$ C_s

T^a = 13720(320) gas PE[1]

X $^2A''$ C_s

[a] From vertical ionization potentials.

References

[1]S. Cradock and R. A. Whiteford, J. Chem. Soc., Faraday Trans. 2 68, 281 (1972).

$N_2H_4^+$

D ^2A C_2

T^a = 59600(1000) gas PE[2]

C ^2B C_2

T^a = 54460(320) gas PE[1,2]

B ^2A C_2

T^a = 45990(320) gas PE[1,2]

$\tilde{A}\ ^2B^b$ C_2

T^a = 5890(320) gas PE[1,2]

$\tilde{X}\ ^2A^b$ C_2

[a] From vertical ionization potentials.
[b] Ref. 2 reverses these two assignments.

References

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$P_2H_4^+$

$\tilde{D},\tilde{E}\ ^2A,^2B$ C_2

T^a = 33730(320) gas PE[1]

$\tilde{C}\ ^2A$ C_2

T^a = 20090(320) gas PE[1]

$\tilde{B}$ C_2

$T^a \sim 14600$ gas PE[1]

$\tilde{A}\ ^2B$ C_2

T^a = 5570(320) gas PE[1]

$\tilde{X}\ ^2A$ C_2

[a] From vertical ionization potentials.

References

[1] S. Elbel, H. tom Dieck, G. Becker, and W. Ensslin, Inorg. Chem. 15, 1235 (1976).

BH_3CO^+

$\tilde{C}\ ^2A_1$ C_{3v}

T_o = 59220(320) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		1660(30)	gas	PE	1

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

T_o = 39940(320) gas PE[1]

$\tilde{A}\ ^2A_1$ C_{3v}

T_o = 20900(240) gas PE[1]

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

Spin-orbit splitting = 4760(320) gas PE[1]

References

[1] D. R. Lloyd and N. Lynaugh, J. Chem. Soc., Faraday Trans. 2 68, 947 (1972).

CH_2CCH

T_o = 30109[a] gas AB[1] 290-345 nm

Ar AB[2] 288-359 nm

All bands in the gas-phase spectrum are diffuse.

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	C-C stretch	961(10)	gas	AB	1
		965(10)	Ar	AB	2

$\tilde{X}$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CH stretch	3310	Ar	IR	2
	CCH bend	687	Ar	IR	2
	CCH OPLA bend	510(10)	gas	PE	3
		548	Ar	IR	2
	C_3 deformation	483	Ar	IR	2

CD_2CCD

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CD stretch	2548	Ar	IR	2
	CCD bend	553	Ar	IR	2

[a] Assignment of gas-phase band origin is tentative. The extension of the progression to 27886 in the argon-matrix study suggests that as many as two quanta of the C-C stretching vibration may be excited in the gas phase band at 30109.

References

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CH_3CN^+

$\tilde{C}\ ^2A_1$ C_{3v}

T_o = 38600(1000) gas PE[1,4]

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

T_o = 26630(320) gas PE[1,2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CH_3 "umbrella"	1440(80)	gas	PE	4
	4	C-C stretch	860(80)	gas	PE	4

Jahn-Teller splitting ∿ 4000 gas PE[4]

$\tilde{A}\ ^2A_1$ C_{3v}

T_o = 7580(320) gas PE[1,2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CH_3 "umbrella"	1290(80)	gas	PE	2-4

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C≡N stretch	2010(80)	gas	PE	1-4
	3	CH_3 "umbrella"	1430(80)	gas	PE	3,4
	4	C-C stretch	810(80)	gas	PE	2-4

CD_3CN^+

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

T_o = 23720(320) gas PE[2]

$\tilde{A}\ ^2A_1$ C_{3v}

T_o = 7340(320) gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CD_3 "umbrella"	970(80)	gas	PE	2,3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C≡N stretch	1990(80)	gas	PE	2,3
	3	CD_3 "umbrella"	1070(80)	gas	PE	3
	4	C-C stretch	810(80)	gas	PE	3

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CH_3NC^+

$\tilde{C}\ ^2A_1$ C_{3v}

T^a = 55900(1000) gas PE[3]

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

T_o = 34860(320) gas PE[2,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			∿770	gas	PE	2

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

T_o = 7830(320) gas PE[2,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	N≡C stretch	1870(100)	gas	PE	1-3
	3	CH_3 "umbrella"	1130(80)	gas	PE	1,2

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	N≡C stretch	2280(80)	gas	PE	1-3
	3	CH_3 "umbrella"	1410(80)	gas	PE	1-3

CD_3NC^+

$\tilde{B}\ ^2E$ C_{3v}

T^a = 39700(320) gas PE^2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			∿730	gas	PE	2

$\tilde{A}\ ^2E$ C_{3v}

T^a = 10090(320) gas PE^2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	N≡C stretch	1820(80)	gas	PE	2
	3	CD_3 "umbrella"	880(80)	gas	PE	2

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	N≡C stretch	2240(80)	gas	PE	2
	3	CD_3 "umbrella"	1030(80)	gas	PE	2

[a] From adiabatic ionization potential.

References

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CH_3CP^+

$\tilde{C}\ ^2A_1$ C_{3v}

T_o = 46070(880) gas PE^1

$\tilde{B}\ ^2E$ C_{3v}

T_o = 38800(1700) gas PE^1

$\tilde{A}\ ^2A_2$ C_{3v}

T_o = 18656(1) gas PE^1EF^2 $\tilde{A}$-$\tilde{X}$ 530-590 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1230(50)	gas	PE	1

$\tilde{X}\ ^2E$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CP stretch	1503(2)	gas	EF	2

A = -85(2) gas EF^2

References

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$CaOCH_3$

$\tilde{B}\ ^2A_1$ C_{3v}

T_o = 17674(5) gas $CL^1LF^{1,2}$ $\tilde{B}$-$\tilde{X}$ 525-590 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CO stretch	1150(5)	gas	LF	1
	4	CaO stretch	491(5)	gas	LF	1,2
e	8	CaOC bend	168(5)	gas	LF	1,2

$\tilde{A}\ ^2E$ C_{3v}

T_o = 15930(10) gas $CL^1LF^{1,2}$ $\tilde{A}$-$\tilde{X}$ 605-635 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CO stretch	1140(5)	gas	LF	1,2
	4	CaO stretch	500(10)	gas	LF	1,2
e	8	CaOC bend	145(5)	gas	LF	1

A = 68(5) gas LF^1

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CO stretch	1156(5)	gas	LF	2
	4	CaO stretch	488(5)	gas	LF	1,2
e	8	CaOC bend	144(5)	gas	LF	1,2

$CaOCD_3$

$\tilde{B}\ ^2A_1$ C_{3v}

T_o = 17674(5) gas LF[1] $\tilde{B}$-$\tilde{X}$ 528-600 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CO stretch	1156(5)	gas	LF	1
	4	CaO stretch	476(5)	gas	LF	1
e	8	CaOC bend	166(5)	gas	LF	1

$\tilde{A}\ ^2E$ C_{3v}

T_o = 15935(10) gas LF[1] $\tilde{A}$-$\tilde{X}$ 584-630 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CO stretch	1156(5)	gas	LF	1
	4	CaO stretch	480(5)	gas	LF	1
e	8	CaOC bend	140(5)	gas	LF	1

A = 72(5) gas LF[1]

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4	CaO stretch	467(5)	gas	LF	1
e	8	CaOC bend	142(5)	gas	LF	1

$SrOCH_3$

$\tilde{B}\ ^2A_1$ C_{3v}

T_o = 16069(5)[a] gas CL[1]LF[1,2] $\tilde{B}$-$\tilde{X}$ 603-622 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4	SrO stretch	420(5)	gas	LF	1
e	8	SrOC bend	154(15)	gas	LF	1

$\tilde{A}\ ^2E$ C_{3v}

T_o = 14658.872 gas CL[1]LF[1-3] $\tilde{A}$-$\tilde{X}$ 627-689 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CO stretch	1140(5)	gas	LF	1,3
	4	SrO stretch	418(5)	gas	LF	1-3

τ = 30(20) ns gas LF[1]

A = 267.5(3) gas LF[1-3]

A_o = 5.163; B_o = 0.085 LF[3]

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 deform.	1450(5)	gas	LF	3
	3	CO stretch	1138(5)	gas	LF	2,3
	4	SrO stretch	405(5)	gas	LF	2,3
e	8	SrOC bend	136(5)[b]	gas	LF	3

$A_o \sim 5.185$; B_o = 0.084 LF[3]

$SrOCD_3$

$\tilde{B}\ ^2A_1$ C_{3v}

T_o = 16069(5) gas LF[1] $\tilde{B}$-$\tilde{X}$ 604-622 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4	SrO stretch	417(5)	gas	LF	1
e	8	SrOC bend	157(15)	gas	LF	1

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$\tilde{A}\ ^2E$ C_{3v}

T_o = 14650(10) gas LF[1] $\tilde{A}$-$\tilde{X}$ 627-690 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CO stretch	1159(5)	gas	LF	1
	4	SrO stretch	401(5)	gas	LF	1

A = 274(5) gas LF[1]

[a] Ref. 2 gives 16098(5).
[b] $\frac{1}{2}(2\nu_8)$.

References

[1]R. F. Wormsbecher and R. D. Suenram, J. Mol. Spectrosc. 95, 391 (1982).
[2]C. R. Brazier, L. C. Ellingboe, S. Kinsey-Nielsen, and P. F. Bernath, J. Am. Chem. Soc. 108, 2126 (1986).
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$BaOCH_3$

$\tilde{B}\ ^2A_1$ C_{3v}

T_o = 12923(5) gas CL[1]LF[2]

$\tilde{A}\ ^2E$ C_{3v}

T_o = 11448(5) gas CL[1]LF[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4	BaO stretch	342(5)	gas	LF	2

A = 660(10) gas LF[2]

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4	BaO stretch	375(5)	gas	LF	2
e	8	BaOC bend	127[a]	gas	LF	2

[a] $\frac{1}{2}(2\nu_8)$.

References

[1]R. F. Wormsbecher and R. D. Suenram, J. Mol. Spectrosc. 95, 391 (1982).
[2]C. R. Brazier, L. C. Ellingboe, S. Kinsey-Nielsen, and P. F. Bernath, J. Am. Chem. Soc. 108, 2126 (1986).

CH_3CO

A broad, unstructured gas-phase absorption between 200 and 240 nm, with maximum near 215 nm, has been attributed[2,3] to CH_3CO.

$\tilde{A}$

A broad, unstructured gas-phase absorption with onset near 700 nm and maximum near 550 nm has been attributed[4] to CH_3CO. In an argon matrix,[5] the threshold for the photodecomposition of CH_3CO into CH_3 + CO lies near 600 nm.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch[a]	1875	Ar[b]	IR	5
			1842	Ar[b]	IR	1,5
		CH_3 deform.	1420	Ar[b]	IR	5
		CH_3 deform.	1329	Ar[b]	IR	1,5

CD_3CO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1855	Ar[b]	IR	5

[a] Fermi resonance with overtone or combination band.
[b] In Ref. 1, LiCl trapped in nearby site; in Ref. 5, HF trapped in nearby site.

References

[1]J. S. Shirk, Ph.D. Thesis, Univ. of California, Berkeley (1966); J. S. Shirk and G. C. Pimentel, J. Am. Chem. Soc. 90, 3349 (1968).
[2]H. Adachi, N. Basco, and D. G. L. James, Chem. Phys. Lett. 59, 502 (1978).
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CH_2CHO

$\tilde{B}\ ^2A''$ C_s

T_o = 28784.09(1) gas AB[1]LF[2,4,6] $\tilde{B}$-$\tilde{X}$ 300-405 nm

The failure to detect fluorescence on excitation above 30000 suggests[2] the onset of predissociation near 330 nm. In the argon matrix experiments,[5] the threshold for the photodecomposition of CH_2CHO to produce CH_3 + CO was observed between 280 and 300 nm.

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		1122	gas	LF	2,6
		917	gas	LF	2,6
	CCO bend	450	gas	LF	2,6

τ = 0.84(13) μs gas LF[2]AB[3]

A_o = 2.103(4); B_o = 0.344(1); C_o = 0.296(1) LF[6]

$\tilde{A}\ ^2A'$ C_s

T_o = 8006 gas AB[3] $\tilde{A}$-$\tilde{X}$ 1000-1250 nm

$\tilde{X}$ C_s Structure: MW[8,9]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	CH_2 "scissors"	1558	Ar[a]	IR	5
	C=O stretch	1540	gas	LF	2,6
		1542[b]	Ar[a]	IR	5
		1525			
	OCH deform.	1375	Ar[a]	IR	5
	CC stretch	1143	gas	LF,PD	2,6,7
	CCO bend	496[c]	gas	LF,PD	2,6,7
a"		765	Ar[ad]	IR	5
		723	Ar[ad]	IR	5
		692	Ar[ad]	IR	5
	Torsion	100[d]	gas	PD	7

A_o = 2.224; B_o = 0.382; C_o = 0.326 LF[6]MW[8]

CD_2CDO

$\tilde{B}\ ^2A''$ C_s

T_o = 28840 gas LF[2] $\tilde{B}$-$\tilde{X}$ 335-411 nm

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		980	gas	LF	2
		768	gas	LF	2

$\tilde{X}\ ^2A''$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	C=O stretch	1540	gas	LF	2
		1513	Ar[a]	IR	5
		1223	Ar[a]	IR	5
	CC stretch	1050	gas	LF	2
	CCO bend	445[c]	gas	LF	2

A_o = 1.442; B_o = 0.336; C_o = 0.272 MW[9]

[a] HF trapped in nearby site.
[b] Fermi resonance with overtone of 765-cm^{-1} fundamental.
[c] Ref. 2 attributed a band displaced by approximately 950 cm^{-1} in fluorescence spectrum of CH_2CHO, with a counterpart near 800 cm^{-1} in the fluorescence spectrum of CD_2CDO, to a H-deformation fundamental of a" symmetry. However, measurements of Ref. 6 for CH_2CHO support reassignment to the first overtone of the CCO bend, which has a rather large anharmonic constant.
[d] The tentative assignment[7] of the torsional fundamental at 100 cm^{-1} would require that one of these three argon-matrix absorptions not be a fundamental of a" symmetry. A possible alternate assignment of that peak would be to the CH_2 in-plane rocking vibration.

References

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CH_3NO^+

$\tilde{D},\tilde{E}\ ^2A',^2A''$ C_s

T^a = 58300(1200) gas PE[1,3-5]

$\tilde{C}\ ^2A'$ C_s

T^a = 49400(1200) gas PE[1,4,5]

$\tilde{B}\ ^2A''$ C_s

T^a = 37300(1200) gas PE[1-5]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	NO stretch	~1900	gas	PE	3

Ã $^2A'$ C_s

T^a = 33200 gas PE[1-5]

X̃ $^2A'$ C_s

[a] From vertical ionization potentials.

References

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H_2CNOH^+

F̃ $^2A'$ C_s

T^a = 62200(1000) gas PE[2]

Ẽ $^2A'$ C_s

T^a = 55800(1000) gas PE[2]

D̃ $^2A'$ C_s

T^a = 44500(1000) gas PE[2]

C̃ $^2A'$ C_s

T^a = 34290(320) gas PE[2,3]

B̃ $^2A''$ C_s

T^a = 29370(320) gas PE[1-3]

Ã $^2A'$ C_s

T^a = 4280(320) gas PE[1-3]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	CNO bend	444(80)	gas	PE	3

X̃ $^2A''$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	NO stretch	928(80)	gas	PE	3

[a] From vertical ionization potentials.

References

[1]A. Dargelos and C. Sandorfy, J. Chem. Phys. 67, 3011 (1977).
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$HCONH_2^+$

Ẽ $^2A'$ C_s

$T^a \sim 71600$ gas PE[1]

D̃ $^2A'$ C_s

T_o = 48650(320) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		1100(30)	gas	PE	1

C̃ $^2A''$ C_s

T_o = 36230(320) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		1050(30)	gas	PE	1

B̃ $^2A'$ C_s

T_o = 29290(320) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		1090(30)	gas	PE	1

Ã $^2A''$ C_s

T^a = 3150(320) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		640(30)	gas	PE	1

X $^2A'$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	CO stretch	1600(30)	gas	PE	1

[a] From vertical ionization potential.

References

[1]C. R. Brundle, D. W. Turner, M. B. Robin, and H. Basch, Chem. Phys. Lett. 3, 292 (1969).

$HCSNH_2^+$

G $^2A'$ C_s

T^a = 82400(1000) gas PE[2]

F $^2A'$ C_s

T^a = 72700(1000) gas PE[2]

E $^2A'$ C_s

T^a = 55110(320) gas PE[2]

D $^2A'$ C_s

T^a = 44100(600) gas PE[2]

C $^2A''$ C_s

T^a = 36390(320) gas PE[1,2]

B $^2A'$ C_s

T^a = 33400(320) gas PE[1,2]

A $^2A''$ C_s

T_o = 4110(320) gas PE[1,2]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		730(80)	gas	PE	1,2

X $^2A'$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		1460(80)	gas	PE	1,2

[a] From vertical ionization potential.

References

[1]G. W. Mines and H. W. Thompson, Spectrochim. Acta 31A, 137 (1975).
[2]K. Kimura, S. Katsumata, T. Ishiguro, A. Y. Hirakawa, and M. Tsuboi, Bull. Chem. Soc. Japan 49, 937 (1976).

$CH_2{=}CHF^+$

F $^2A'$ C_s

T_o = 76410(320) gas PE[2,3]

E $^2A'$ C_s

T^a = 61320(320) gas PE[1-3]

C,D $^2A''$,$^2A'$ C_s

T^a = 51560(320) gas PE[1-3]

B $^2A'$ C_s

T^a = 33810(320) gas PE[1-3]

A $^2A'$ C_s

T^a = 27670(320) gas PE[1-3]

X $^2A''$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	C=C stretch	1570(80)	gas	PE	1,2
	CF stretch	1300(80)	gas	PE	1,2
	HCF bend	500(80)	gas	PE	1,2

[a] From vertical ionization potential.

References

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$CH_2=CHCl^+$

F $^2A'$ C_s

T^a = 70600(1000) gas PE[1-3]

E $^2A'$ C_s

T^a = 50830(320) gas PE[1-3]

D $^2A'$ C_s

T^a = 43410(320) gas PE[1-3]

C $^2A'$ C_s

T^a = 28640(500) gas PE[1-3]

B $^2A''$ C_s

T^a = 25250(320) gas PE[1-3]

A $^2A'$ C_s

T_o = 13400(500) gas PE[1-3]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	CH_2 "scissors"	1130(80)	gas	PE	2,3
	HCCl bend	440(80)	gas	PE	2,3

X $^2A''$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	C=C stretch	1300(80)	gas	PE	1-3
	CCl stretch	820(80)	gas	PE	1-3
	HCCl bend	350(80)	gas	PE	1-3

[a] From vertical ionization potential.

References

[1]R. F. Lake and H. Thompson, Proc. Roy. Soc. (London) A315, 323 (1970).
[2]G. W. Mines and H. W. Thompson, Spectrochim. Acta A29, 1377 (1973).
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CH_2CHO^-

Dipole-Bound State C_s

T_o = 14712.74(5) gas PD[1,2]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	C-C stretch	1143	gas	PD	2
	CCO bend	499	gas	PD	2
a"	Torsion	102[a]	gas	PD	2

A_o = 2.219(3); B_o = 0.376; C_o = 0.321 PD[2]

X C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	CCO bend	525	gas	PD	2
a"	Torsion	∿375[b]	gas	PD	2

A_o = 2.493(1); B_o = 0.362; C_o = 0.316 PD[2]

CD_2CDO^-

Dipole-Bound State C_s

T_o = 14665.97(5) gas PD[1,2]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		1382(10)	gas	PD	1
		981(10)	gas	PD	1
	CCO bend	437(10)	gas	PD	1
a"	Torsion	∿80[a]	gas	PD	1

A_o = 1.419(3); B_o = 0.330; C_o = 0.268 PD[2]

X C_s

A_o = 1.554(1); B_o = 0.319; C_o = 0.264 PD[2]

[a] $\frac{1}{2}(2\nu_i)$.
[b] Tentative assignment.

References

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CH_2=SiHCl

In an Ar or N_2 matrix, an absorption maximum appears at 255 nm. On 254-nm irradiation, photoisomerization to CH_3SiCl occurs.[1,2]

X C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	SiH stretch	2230	Ar	IR	1,2
		2230	N_2	IR	1,2
		984	Ar	IR	1,2
		980	N_2	IR	1,2
		843	Ar	IR	1,2
		840	N_2	IR	1,2
		699	Ar	IR	1,2
		544	Ar	IR	1,2
		539	Ar	IR	1,2

References

[1]H. P. Reisenauer, G. Mihm, and G. Maier, Angew. Chem. 94, 864 (1982); Angew. Chem. Int. Ed. Engl. 21, 854 (1982).
[2]G. Maier, G. Mihm, H. P. Reisenauer, and D. Littmann, Chem. Ber. 117, 2369 (1984).

CH_3SiCl

In an Ar matrix, an absorption maximum appears at 407 nm. A similar band appears at 387 nm in a N_2 matrix. On irradiation of the sample in this absorption region, photoisomerization to CH_2=SiHCl occurs.[1,2]

X

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		1223	Ar	IR	1,2
		1220	N_2	IR	2
		485	Ar	IR	1,2
		480	Ar	IR	1,2

References

[1]H. P. Reisenauer, G. Mihm, and G. Maier, Angew. Chem. 94, 864 (1982); Angew. Chem. Int. Ed. Engl. 21, 854 (1982).
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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] to CH_3O_2 appears between 200 and 270 nm, with a maximum at ~235 nm. In an argon matrix, CH_3O_2 photolyzes on exposure to 254-nm radiation.[5]

Ã $^2A'$ C_s

T_0 = 7375(6) gas AB[2] Ã-X̃ 7375-9149 cm^{-1}

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	OO stretch	896(9)	gas	AB	2

X̃ $^2A''$ C_s

Vib. No. sym.		Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CH_3 deform.	1453(2)	Ar	IR	5
	4	CH_3 deform.	1440(2)	Ar	IR	5
	5	CH_3 rock	1183(2)	Ar	IR	5
	6	OO stretch	1112(2)	Ar	IR	5
	7	CO stretch	902(2)	Ar	IR	5
	8	COO bend	492(2)	Ar	IR	5
a"	9	CH_3 stretch	2968(2)	Ar	IR	5
	10	CH_3 deform.	1414(2)	Ar	IR	5
	11	CH_3 rock	~1120	Ar	IR	5

CD_3O_2

X̃ $^2A''$ C_s

Vib. No. sym.		Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		OO stretch	1146(2)	Ar	IR	5
		CD_3 deform.	1048(2)	Ar	IR	5
		CO stretch	821(2)	Ar	IR	5
		COO bend	445(2)	Ar	IR	5
a"	9	CD_3 stretch	2176(2)	Ar	IR	5
	10	CD_3 deform.	1078(2)	Ar	IR	5
	11	CD_3 rock	860(2)	Ar	IR	5

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[6]K. McAdam, B. Veyret, and R. Lesclaux, Chem. Phys. Lett. 133, 39 (1987).

CH_3OCl^+

F $^2A'$ C_s

T^a = 54140(560) gas PE[1]

D,E $^2A''$,$^2A'$ C_s

T^a = 45670(560) gas PE[1]

C $^2A'$ C_s

T^a = 25250(560) gas PE[1]

B $^2A''$ C_s

T^a = 21700(560) gas PE[1]

A $^2A'$ C_s

T^a = 10890(320) gas PE[1]

X $^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		OCl stretch	710(50)	gas	PE	1

[a] From vertical ionization potential.

References

[1]D. Colbourne, D. C. Frost, C. A. McDowell, and N. P. C. Westwood, J. Electron Spectrosc. Relat. Phenom. 23, 109 (1981).

$C_4H_2^+$

B

T_o = 51960(160) gas PE[2]

A $^2\Pi_u$ $D_{\infty h}$

T_o = 19722.59 gas EM[1]EF[7]LF[7] A-X 485-650 nm
19708(2) Ne LF[4] A-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 = -31.1(8) gas EM[1]LF[7]
-30(2) Ne LF[4]

B_o = 0.140 LF[7]

X $^2\Pi_g$ $D_{\infty h}$

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] 430.3[b]	gas	EM,LF	1,8
			432.5[b]	Ne	LF	4

A = -33.3(8) gas EM[1]LF[4]EF[7]

B_o = 0.147 EM[1]EF[7]

$C_4D_2^+$

B

T_o = 52930(160) gas PE[2]

A $^2\Pi_u$ $D_{\infty h}$

T_o = 19740.66 gas EM[1]LF[7]EF[7] A-X 485-640 nm
19727(2) Ne LF[4] A-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 = -30.8(2.0) gas LF[7]

B_o = 0.122 LF[7]

$\tilde{X}\ ^2\Pi_g$ $D_{\infty h}$

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 = -33.0(2.0) gas EF[7]

B_o = 0.128 EF[7]

[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

[1] J. H. Callomon, Can. J. Phys. 34, 1046 (1956).
[2] C. Baker and D. W. Turner, Proc. Roy. Soc. (London) A308, 19 (1968).
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[4] V. E. Bondybey and J. H. English, J. Chem. Phys. 71, 777 (1979).
[5] J. P. Maier and F. Thommen, J. Chem. Phys. 73, 5616 (1980).
[6] J. P. Maier, M. Ochsner, and F. Thommen, Faraday Discuss. Chem. Soc. 75, 77 (1983).
[7] R. Kuhn, J. P. Maier, and M. Ochsner, Mol. Phys. 59, 441 (1986).
[8] F. G. Celii, J. P. Maier, and M. Ochsner, J. Chem. Phys. 85, 6230 (1986).

$(HCO)_2^+$

$\tilde{E}$ C_{2h}

T_o[a] = 51000(700) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g			1410(80)	gas	PE	1
			990(80)	gas	PE	1

$\tilde{C},\tilde{D}$ C_{2h}

$T^{ab} \sim$ 44200 gas PE[1]

$\tilde{B}$ C_{2h}

T_o[a] = 26870(700) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2	CO stretch	1360(80)	gas	PE	1

$\tilde{A}$ C_{2h}

T_o[a] = 13470(700) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2	CO stretch	1610(80)	gas	PE	1
	4	CC stretch	970(80)	gas	PE	1
	5	Skel. deform.	400(80)	gas	PE	1

[a] The first ionization potential of $(HCO)_2$ is taken as 10.52(7) eV, the position of the maximum of the first photoelectron band.[2,3]
[b] From vertical ionization potential.

References

[1] D. W. Turner, C. Baker, A. D. Baker, and C. R. Brundle, "Molecular Photoelectron Spectroscopy," pp. 252-261. Wiley-Interscience, London, 1970.
[2] D. O. Cowan, R. Gleiter, J. A. Hashmall, E. Heilbronner, and V. Hornung, Angew. Chem. 83, 405 (1971); Angew Chem. Int. Ed. Engl. 10, 401 (1971).
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CH_2FCN^+

D $^2A'$ C_s

T^a = 18960(320) gas PE[1]

C $^2A''$ C_s

T^a = 15410(320) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		1450(80)	gas	PE	1
		810(80)	gas	PE	1

B $^2A'$ C_s

T^a = 6860(320) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		1050(80)	gas	PE	1

A $^2A'$ C_s

T^a = 4110(320) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		1450(80)	gas	PE	1

X $^2A''$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	C≡N stretch	2020(80)	gas	PE	1
		1210(80)	gas	PE	1
	C-C stretch	810(80)	gas	PE	1

[a] From vertical ionization potentials.

References

[1] R. Botter, Y. Gounelle, Y. Henry, J. Jullien, F. Menes, and D. Solgadi, J. Electron Spectrosc. Relat. Phenom. 10, 393 (1977).

CH_2ClCN^+

G C_s

T^a = 47840(320) gas PE[1]

F C_s

T^a = 40020(320) gas PE[1]

E C_s

T^a = 29930(320) gas PE[1]

D $^2A'$ C_s

T^a = 13230(320) gas PE[1,2]

C $^2A''$ C_s

T^a = 10250(320) gas PE[1,2]

B $^2A'$ C_s

T^a = 7910(320) gas PE[1,2]

A $^2A'$ C_s

T^a = 1210(320) gas PE[2]

X $^2A''$ C_s

[a] From vertical ionization potentials.

References

[1] R. F. Lake and H. Thompson, Proc. Roy. Soc. (London) A317, 187 (1970).
[2] R. Botter, Y. Gounelle, Y. Henry, J. Jullien, F. Menes, and D. Solgadi, J. Electron Spectrosc. Relat. Phenom. 10, 393 (1977).

CH_2NO_2

In an Ar matrix, threshold for photodecomposition into H_2CO + NO near 290 nm.[1]

X C_{2v}

Vib. No. sym.		Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s-stretch	3055	Ar[a]	IR	1,2
	2	CH_2 "scissors"	1419	Ar[a]	IR	1,2
	3	NO_2 s-stretch	1297	Ar[a]	IR	1,2
	4	CN stretch	986	Ar[a]	IR	1,2
	5	NO_2 "scissors"	693	Ar[a]	IR	1,2

X---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_1	7	CNO_2 OPLA[b]	719	Ar[a]	IR	1,2
	8	H_2CN OPLA[b]	606	Ar[a]	IR	1,2
b_2	9	CH_2 a-stretch	3200	Ar[a]	IR	1,2
	10	NO_2 a-stretch	1484[c] 1461	Ar[a]	IR	1,2
	11	CH_2 rock	1095	Ar[a]	IR	1,2
	12	NO_2 rock	~484[d]	Ar[a]	IR	1,2

CD_2NO_2

X C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	NO_2 s-stretch	1296	Ar[a]	IR	1,2
	4	CN stretch + CD_2 "scissors"	906	Ar[a]	IR	1,2
	5	NO_2 "scissors"	668	Ar[a]	IR	1,2
b_1	7	CNO_2 OPLA	694	Ar[a]	IR	1,2
b_2	10	NO_2 a-stretch	1460	Ar[a]	IR	1,2

[a] HF trapped in adjacent site.
[b] The two out-of-plane modes are strongly mixed.
[c] In Fermi resonance with ($\nu_4 + \nu_{12}$).
[d] Estimated from ($\nu_4 + \nu_{12}$).

References

[1]M. E. Jacox, J. Phys. Chem. 87, 3126 (1983).
[2]M. E. Jacox, J. Phys. Chem. 91, 5038 (1987).

$CH_2{=}CF_2^+$

G $^2B_2$ C_{2v}

T^a = 75920(320) gas PE[1-3]

E,F $^2A_1$,$^2B_1$ C_{2v}

T^a = 63820(320) gas PE[1-3]

C,D $^2B_2$,$^2A_2$ C_{2v}

T^a ~ 47000 gas PE[3]

B $^2A_1$ C_{2v}

T^a = 43890(320) gas PE[1-3]

A $^2B_2$ C_{2v}

T_o = 30420(320) gas PE[1-3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1050(80)	gas	PE	2

X $^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C=C stretch	1530(80)	gas	PE	1,2
	4	CF_2 s-stretch	700(80)	gas	PE	1,2

[a] From vertical ionization potential.

References

[1]R. F. Lake and H. Thompson, Proc. Roy. Soc. (London) A315, 323 (1970).
[2]J. A. Sell and A. Kupperman, J. Chem. Phys. 71, 4703 (1979).
[3]G. Bieri, W. von Niessen, L. Åsbrink, and A. Svensson, Chem. Phys. 60, 61 (1981).

c-CHF=CHF$^+$

F,G $^2A_1$,$^2A_2$ C_{2v}

T^a = 69150(320) gas PE[2,5]

D,E $^2B_2$,$^2B_1$ C_{2v}

T^a = 55110(320) gas PE[2,5]

F-atom detachment has been observed in this transition. PEPICO[3]

C $^2A_2$ C_{2v}

T^a = 47850(320) gas PE[2,5]

F-atom detachment has been observed in this transition. PEPICO[3]

B $^2B_2$ C_{2v}

T_o = 37680(160) gas PE[1,2,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH s-stretch	2610(80)	gas	PE	2
		CF s-stretch	1100(80)	gas	PE	2

$\tilde{A}\ ^2A_1$ C_{2v}

T_o = 28880(10) gas PE^1EF^1 $\tilde{A}$-$\tilde{X}$ 340-380 nm

The threshold for fragmentation into $HCCF^+$ + HF is near the onset of the transition. PEPICO[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CH deform.	1430(80)	gas	PE	1,2
	4	CF s-stretch	1020(80)	gas	PE	1,2
	5	CF deform.	260(10)	gas	EF,PE	1

τ_o = 320(30) ns gas EF^1PEFCO^4

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C=C stretch	1600(10)	gas	EF	1
	3	CH deform.	1330(10)	gas	EF	1
	4	CF stretch	1030(10)	gas	EF	1
	5	CF deform.	250(10)	gas	EF	1

[a] From vertical ionization potential.

References

[1] J. P. Maier, O. Marthaler, and G. Bieri, Chem. Phys. 44, 131 (1979).
[2] J. A. Sell and A. Kupperman, J. Chem. Phys. 71, 4703 (1979).
[3] J.-P. Stadelmann and J. Vogt, Int. J. Mass Spectrom. Ion Phys. 35, 83 (1980).
[4] J. P. Maier and F. Thommen, J. Chem. Soc., Faraday Trans. 2 77, 845 (1981).
[5] G. Bieri, W. von Niessen, L. Åsbrink, and A. Svensson, Chem. Phys. 60, 61 (1981).

t-CHF=CHF$^+$

$\tilde{F},\tilde{G}\ ^2A_g,^2B_u$ C_{2h}

T^a = 69060(320) gas $PE^{2,4}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g			920(80)	gas	PE	2
			450(80)	gas	PE	2

$\tilde{D},\tilde{E}\ ^2A_g,^2A_u$ C_{2h}

T^a = 54780(320) gas $PE^{2,4}$

F-atom detachment has been observed in this transition. PEPICO[3]

$\tilde{C}\ ^2B_g$ C_{2h}

T^a = 49780(320) gas $PE^{2,4}$

F-atom detachment has been observed in this transition. PEPICO[3]

$\tilde{B}\ ^2B_u$ C_{2h}

T_o = 39370(160) gas $PE^{1,2,4}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	CH s-stretch	2820(80)	gas	PE	2
		CF s-stretch	1180(80)	gas	PE	2

$\tilde{A}\ ^2A_g$ C_{2h}

T_o = 26630(160) gas $PE^{1,2,4}$

The threshold for fragmentation into $HCCF^+$ + HF is near the onset of the transition. PEPICO[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g		CF deform.	500(80)	gas	PE	2

$\tilde{X}\ ^2A_u$ C_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2	C=C stretch	1600(80)	gas	PE	2
	3	CH deform.	1230(80)	gas	PE	2
	4	CF s-stretch	850(80)	gas	PE	2
	5	CF deform.	550(80)	gas	PE	2

[a] From vertical ionization potential.

References

[1]J. P. Maier, O. Marthaler, and G. Bieri, Chem. Phys. 44, 131 (1979).
[2]J. A. Sell and A. Kupperman, J. Chem. Phys. 71, 4703 (1979).
[3]J.-P. Stadelmann and J. Vogt, Int. J. Mass Spectrom. Ion Phys. 35, 83 (1980).
[4]G. Bieri, W. von Niessen, L. Åsbrink, and A. Svensson, Chem. Phys. 60, 61 (1981).

$CH_2{=}CFCl^+$

F $^2A''$ C_s

T^a = 60190(320) gas PE[1]

E $^2A'$ C_s

T^a = 57280(320) gas PE[1]

D $^2A'$ C_s

T^a = 38160(320) gas PE[1]

C $^2A'$ C_s

T^a = 32600(320) gas PE[1]

B $^2A''$ C_s

T^a = 24200(320) gas PE[1]

A $^2A'$ C_s

T^a = 17670(320) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	CFCl deform.	460(80)	gas	PE	1

X $^2A''$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	C=C stretch	1250(80)	gas	PE	1
	CCl stretch	660(80)	gas	PE	1

[a] From vertical ionization potentials.

References

[1]A. W. Potts, J. M. Benson, I. Novak, and W. A. Svensson, Chem. Phys. 115, 253 (1987).

$CH_2{=}CCl_2^+$

H $^2A_1$ C_{2v}

T^a = 69710(320) gas PE[1-5]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		1290(80)	gas	PE	1

F,G $^2A_1$,$^2B_2$ C_{2v}

T^a = 51400(1000) gas PE[1-5]

E $^2B_1$ C_{2v}

T^a = 35580(320) gas PE[1-5]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		1010(80)	gas	PE	1

D $^2B_2$ C_{2v}

T^a = 32030(320) gas PE[1-5]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		930(100)	gas	PE	3,4

C $^2A_1$ C_{2v}

T^a = 21860(320) gas PE[1-5]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	CCl_2 "scissors"	320(40)	gas	PE	1,4

B $^2A_2$ C_{2v}

T_o = 17990(320) gas PE[1-5]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	CCl_2 "scissors"	270(40)	gas	PE	1,4

Ã $^2B_2$ C_{2v}

T_o = 13150(320) gas PE[1-5]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	CCl_2 "scissors"	270(40)	gas	PE	1,4

X̃ $^2B_1$ C_{2v}

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	C=C stretch	1290(80)	gas	PE	1-4
	CCl stretch	560(80)	gas	PE	1,3,4

[a] From vertical ionization potential.

References

[1]R. F. Lake and H. Thompson, Proc. Roy. Soc. (London) A315, 323 (1970).
[2]N. Jonathan, K. Ross, and V. Tomlinson, Int. J. Mass Spectrom. Ion Phys. 4, 51 (1970).
[3]K. Wittel and H. Bock, Chem. Ber. 107, 317 (1974).
[4]J. C. Bünzli, D. C. Frost, F. G. Herring, and C. A. McDowell, J. Electron Spectrosc. Relat. Phenom. 9, 289 (1976).
[5]W. von Niessen, L. Åsbrink, and G. Bieri, J. Electron Spectrosc. Relat. Phenom. 26, 173 (1982).

c−CHCl=CHCl$^+$

G̃ $^2A_1$ C_{2v}

T^a = 57700(1000) gas PE[1-4]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	CH s-stretch	1940(80)	gas	PE	1

F̃ $^2A_1$ C_{2v}

T^a ∿ 49600 gas PE[1-4]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	CCl s-stretch	600(80)	gas	PE	1

Ẽ $^2B_2$ C_{2v}

T^a ∿ 36700 gas PE[1-4]

D̃ $^2B_1$ C_{2v}

T^a ∿ 33500 gas PE[1-4]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	CCl s-stretch	640(80)	gas	PE	1,3

C̃ $^2A_2$ C_{2v}

T^a = 22750(500) gas PE[1-4]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	CCl s-stretch	640(80)	gas	PE	1-3

B̃ $^2A_1$ C_{2v}

T^a = 18960(320) gas PE[1-4]

Ã $^2B_2$ C_{2v}

T^a = 16100(1000) gas PE[1-4]

X̃ $^2B_1$ C_{2v}

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	C=C stretch	1370(80)	gas	PE	1,3
	CCl s-stretch	800(80)	gas	PE	1-3

[a] From vertical ionization potential.

References

[1]R. F. Lake and H. Thompson, Proc. Roy. Soc. (London) A315, 323 (1970).
[2]N. Jonathan, K. Ross, and V. Tomlinson, Int. J. Mass Spectrom. Ion Phys. 4, 51 (1970).
[3]K. Wittel and H. Bock, Chem. Ber. 107, 317 (1974).
[4]W. von Niessen, L. Åsbrink, and G. Bieri, J. Electron Spectrosc. Relat. Phenom. 26, 173 (1982).

t−CHCl=CHCl$^+$

F̃,G̃ ^2A_g,^2B_u C_{2h}

T^a ∿ 53000 gas PE[1-4]

Ẽ ^2A_g C_{2h}

T^a = 36790(320) gas PE[1-4]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g		880(80)	gas	PE	3

D ^2A_u C_{2h}

T^a = 33970(320) gas PE[1-4]

C ^2B_g C_{2h}

T^a = 24290(320) gas PE[1-4]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g		720(80)	gas	PE	3

B ^2B_u C_{2h}

$T^a \sim$ 19800 gas PE[1-4]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g		640(80)	gas	PE	3

A ^2A_g C_{2h}

T^a = 17910(500) gas PE[1-4]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g		600(80)	gas	PE	3

X ^2A_u C_{2h}

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	C=C stretch	1400(80)	gas	PE	1,3
	CCl s-stretch	850(80)	gas	PE	1-3
	CCl s-deform.	340(80)	gas	PE	11,3

[a] From vertical ionization potential.

References

[1] R. F. Lake and H. Thompson, Proc. Roy. Soc. (London) A315, 323 (1970).
[2] N. Jonathan, K. Ross, and V. Tomlinson, Int. J. Mass Spectrom. Ion Phys. 4, 51 (1970).
[3] K. Wittel and H. Bock, Chem. Ber. 107, 317 (1974).
[4] W. von Niessen, L. Åsbrink, and G. Bieri, J. Electron Spectrosc. Relat. Phenom. 26, 173 (1982).

NH_2NO_2

In an Ar or N_2 matrix, photolyzes with a threshold near 250 nm to produce N_2O, H_2O, c-$(NO)_2$, and H_2.[2]

X C_s Structure: MW[1]

Vib. No. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH_2 s-stretch	3359	Ar	IR	2
			3361	N_2	IR	2
	2	NH_2 "scissors"	1558	Ar	IR	2
			1581	N_2	IR	2
	3	NO_2 s-stretch	1350	Ar	IR	2
			1368	N_2	IR	2
	4	NN stretch	951	Ar	IR	2
	5	NO_2 wag	798	Ar	IR	2
			776	N_2	IR	2
	6	NO_2 bend	692	Ar	IR	2
			714	N_2	IR	2
	7	NH_2 wag	628	Ar	IR	2
			587	N_2	IR	2
a"	8	NH_2 a-stretch	3478	Ar	IR	2
			3474	N_2	IR	2
	9	NO_2 a-stretch	1613	Ar	IR	2
			1610	N_2	IR	2
	10	NH_2 twist	1227	Ar	IR	2
			1238	N_2	IR	2
	11	NO_2 rock	484	Ar	IR	2
a"	12	Torsion	402	Ar	IR	2
			434	N_2	IR	2

A_o = 0.422; B_o = 0.397; C_o = 0.206 gas MW[1]

ND_2NO_2

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO_2 s-stretch	2455	Ar	IR	2
			2458	N_2	IR	2
	2	NO_2 s-stretch	1352	Ar	IR	2
			1366	N_2	IR	2
	3	NO_2 "scissors"	1174	Ar	IR	2
	4	NN stretch	948	Ar	IR	2
	5	NO_2 wag	774	Ar	IR	2
			772	N_2	IR	2
	6	NO_2 bend	662	Ar	IR	2
			671	N_2	IR	2
	7	ND_2 wag	485	Ar	IR	2
			498	Ar	IR	2
a"	8	ND_2 a-stretch	2604	Ar	IR	2
			2603	N_2	IR	2
a"	9	NO_2 a-stretch	1588	Ar	IR	2
			1583	N_2	IR	2
	10	ND_2 twist	972	Ar	IR	2
			972	N_2	IR	2
	11	NO_2 rock	434	Ar	IR	2
	12	Torsion	287	Ar	IR	2
			318	N_2	IR	2

A_o = 0.405; B_o = 0.351; C_o = 0.190 gas MW[1]

References

[1]J. K. Tyler, J. Mol. Spectrosc. 11, 39 (1963).
[2]M. Nonella, R. P. Muller, and J. R. Huber, J. Mol. Spectrosc. 112, 142 (1985).

$CH_2{=}SiCl_2$

In an Ar matrix, absorption maximum at 246 nm.[1]

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1008	Ar	IR	1
			732	Ar	IR	1
			593	Ar	IR	1

References

[1]G. Maier, G. Mihm, and H. P. Reisenauer, Angew. Chem. 93, 615 (1981); Angew. Chem. Int. Ed. Engl. 20, 597 (1981).

$H(C{\equiv}C)_2F^+$

$\tilde{F}$ $^2\Sigma$ $C_{\infty v}$

T^a = 108100(1000) gas PE[1]

$\tilde{E}$ $^2\Sigma$ $C_{\infty v}$

T^a = 89600(1000) gas PE[1]

$\tilde{D}$ $^2\Sigma$ $C_{\infty v}$

T^a = 75800(1000) gas PE[1]

$\tilde{B},\tilde{C}$ $^2\Pi,^2\Sigma$ $C_{\infty v}$

T^a = 61300(1000) gas PE[1]

$\tilde{A}$ $^2\Pi$ $C_{\infty v}$

T_o = 20570(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	CF stretch	1370(80)	gas	PE	1
	4	C-C stretch	705(80)	gas	PE	1

$\tilde{X}$ $^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	C≡C stretch	2350(80)	gas	PE	1
	4	C-C stretch	685(80)	gas	PE	1

[a] From vertical ionization potential.

References

[1]G. Bieri, A. Schmelzer, L. Åsbrink, and M. Jonsson, Chem. Phys. 49, 213 (1980).

$H(C{\equiv}C)_2Cl^+$

$\tilde{D}$

$T_0 \leq 61700(560)$ gas PE[1]

$\tilde{C}$

$T_0 \leq 57280(320)$ gas PE[1]

$\tilde{B}\ ^2\Pi_{3/2}$ $C_{\infty v}$

$T_0 \leq 35100(320)$ gas PE[1]

$\tilde{A}\ ^2\Pi_{3/2}$ $C_{\infty v}$

$T_0 = 19715.0(1)$ gas $EF^{2,4}LF^4$ $\tilde{A}$-$\tilde{X}$ 445-652 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	C≡C s-stretch	2171(2)	gas	LF	4
	3	C≡C a-stretch	2101(2)	gas	LF	4
	4	C-C stretch	1088(1)	gas	EF,LF	3,4
	5	CCl stretch	523(1)	gas	EF,LF	2-4
Π	8	Skel. deform.	307(1)[a]	gas	EF,LF	3,4
	9	Skel. deform.	125(2)[a]	gas	LF	4

$\tau = 41(2)$ ns gas EF^2PEFCO^3

$A = -200(100)$ gas PE[1]

$\tilde{X}\ ^2\Pi_{3/2}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3101[b]	gas	EF	4
	2	C≡C stretch	2191(1)	gas	EF	2-4
	3	C≡C stretch	1920(1)	gas	EF	2-4
	4	C-C stretch	1184(1)	gas	EF	2-4
	5	CCl stretch	547(1)	gas	EF	2-4
Π	8	Skel. deform.	309(1)[a]	gas	EF	3,4
	9	Skel. deform.	124(1)[a]	gas	EF	4

$A = -200(100)$ gas PE[1]

[a] $\frac{1}{2}(2\nu_i)$.
[b] Tentative value.

References

[1] E. Heilbronner, V. Hornung, J. P. Maier, and E. Kloster-Jensen, J. Am. Chem. Soc. 96, 4252 (1974).
[2]J. P. Maier, O. Marthaler, and E. Kloster-Jensen, J. Electron Spectrosc. Relat. Phenom. 18, 251 (1980).
[3]J. P. Maier, O. Marthaler, L. Misev, and F. Thommen, J. Chem. Soc., Faraday Disc. 71, 181 (1981).
[4]D. Klapstein, J. P. Maier, L. Misev, and W. Zambach, Chem. Phys. 72, 101 (1982).

$H(C{\equiv}C)_2Br^+$

$\tilde{D}$

$T_0 \leq 59700(560)$ gas PE[1]

$\tilde{C}$

$T_0 \leq 52525(320)$ gas PE[1]

$\tilde{B}\ ^2\Pi$ $C_{\infty v}$

$T_0 \leq 29130(320)$ gas PE[1]

$A = -800(300)$ gas PE[1]

$\tilde{A}\ ^2\Pi_{3/2}$ $C_{\infty v}$

$T_0 = 18401.9(3)$ gas EF^3LF^3 $\tilde{A}$-$\tilde{X}$ 467-658 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	C≡C stretch	2138(2)	gas	LF	3
	3	C≡C stretch	2037(2)	gas	LF	3
	4	C-C stretch	918(2)	gas	PE,LF	2,3
	5	CBr stretch	409(1)	gas	EF,LF	2,3
Π	7	Skel. deform.	478(1)[a]	gas	EF,LF	3
	8	Skel. deform.	348(2)[a]	gas	LF	3
	9	Skel. deform.	111(2)[a]	gas	LF	3

$\tau = 27(3)$ ns gas EF^2

$A = -970(80)$ gas $PE^1EF^3LF^3$

$\tilde{X}\ ^2\Pi_{3/2}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3196[b]	gas	EF	3
	2	C≡C stretch	2155(1)	gas	EF	2,3
	3	C≡C stretch	1914(1)[c]	gas	EF	2,3
	4	C-C stretch	1115(1)	gas	EF	2,3
	5	CBr stretch	440(1)	gas	EF	2,3
Π	7	Skel. deform.	509(1)[a]	gas	EF	3
	8	Skel. deform.	370(1)[a]	gas	EF	3
	9	Skel. deform.	112(1)[a]	gas	EF	3

A = -650(80) gas EF^3LF^3

[a] $\frac{1}{2}(2\nu_i)$.
[b] Tentative assignment.
[c] 1906(1) in $\tilde{X}\ ^2\Pi_{1/2}$ state.

References

[1]E. Heilbronner, V. Hornung, J. P. Maier, and E. Kloster-Jensen, J. Am. Chem. Soc. 96, 4252 (1974).
[2]J. P. Maier, O. Marthaler, and E. Kloster-Jensen, J. Electron Spectrosc. Relat. Phenom. 18, 251 (1980).
[3]D. Klapstein, J. P. Maier, L. Misev, and W. Zambach, Chem. Phys. 72, 101 (1982).

$H(C{\equiv}C)_2I^+$

$\tilde{D}$

$T_o \leq 62600(560)$ gas PE[1]

$\tilde{B}\ ^2\Pi$ $C_{\infty v}$

$T_o \leq 27110(320)$ gas PE[1]

$\tilde{A}\ ^2\Pi$ $C_{\infty v}$

$T_o = 14600(320)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1050(80)	gas	PE	1

A = -2980(320) gas PE[1]

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2100(80)	gas	PE	1

A = -2020(320) gas PE[1]

References

[1]E. Heilbronner, V. Hornung, J. P. Maier, and E. Kloster-Jensen, J. Am. Chem. Soc. 96, 4252 (1974).

$CHF{=}CF_2^+$

$\tilde{H},\tilde{I}\ ^2A',^2A'$ C_s

$T^a = 80680(320)$ gas PE[1,2]

$\tilde{G}\ ^2A''$ C_s

$T^a = 68300(1000)$ gas PE[1,2]

$\tilde{F}\ ^2A'$ C_s

$T^a = 63900(320)$ gas PE[1,2]

$\tilde{D},\tilde{E}\ ^2A',^2A''$ C_s

$T^a = 52900(1000)$ gas PE[1,2]

$\tilde{C}\ ^2A''$ C_s

$T^a = 50500(1000)$ gas PE[1,2]

$\tilde{B}\ ^2A'$ C_s

$T^a = 46500(1000)$ gas PE[1,2]

$\tilde{A}\ ^2A'$ C_s

$T^a = 36150(320)$ gas PE[1,2]

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			600(80)	gas	PE	1

[a] From vertical ionization potential.

References

[1]J. A. Sell and A. Kupperman, J. Chem. Phys. 71, 4703 (1979).
[2]G. Bieri, W. von Niessen, L. Åsbrink, and A. Svensson, Chem. Phys. 60, 61 (1981).

$CHCl{=}CF_2^+$

G,H $^2A'$,$^2A''$ C_s

T^a = 65760(320) gas PE[1]

F $^2A'$ C_s

T^a = 49700(320) gas PE[1]

E $^2A''$ C_s

T^a = 46470(320) gas PE[1]

D $^2A'$ C_s

T^a = 40500(320) gas PE[1]

B,C $^2A''$,$^2A'$ C_s

T^a = 26380(320) gas PE[1]

A $^2A'$ C_s

T^a = 15570(320) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		1090(80)	gas	PE	1
		570(80)	gas	PE	1

X $^2A''$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	C=C stretch	1570(80)	gas	PE	1
	CCl stretch	930(80)	gas	PE	1
	CF_2 "scissors"	470(80)	gas	PE	1

[a] From vertical ionization potentials.

References

[1]A. W. Potts, J. M. Benson, I. Novak, and W. A. Svensson, Chem. Phys. 115, 253 (1987).

$CHCl{=}CCl_2^+$

J $^2A'$ C_s

T^a = 74310(320) gas PE[1,2]

I $^2A'$ C_s

T^a = 58740(320) gas PE[1,2]

H $^2A'$ C_s

T^a = 54950(320) gas PE[1,2]

G $^2A''$ C_s

T^a = 41870(320) gas PE[1,2]

F $^2A'$ C_s

T^a = 39620(320) gas PE[1,2]

E $^2A''$ C_s

T^a = 28000(320) gas PE[1,2]

D $^2A'$ C_s

T^a = 26060(320) gas PE[1,2]

C $^2A''$ C_s

T^a = 23600(1000) gas PE[2]

B $^2A'$ C_s

T^a = 21700(320) gas PE[1,2]

A $^2A'$ C_s

T^a = 18150(320) gas PE[1,2]

X $^2A''$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	C=C stretch	1390(80)	gas	PE	1
	Deformation	330(80)	gas	PE	1

[a] From vertical ionization potential.

References

[1]R. F. Lake and H. Thompson, Proc. Roy. Soc. (London) A315, 323 (1970).
[2]W. von Niessen, L. Åsbrink, and G. Bieri, J. Electron Spectrosc. Relat. Phenom. 26, 173 (1982).

$NCC{\equiv}CCN^+$

D $^2\Pi_u$ $D_{\infty h}$

T_o = 25500(160) gas PE[1,3]

$\tilde{C}\ ^2\Sigma_u^+$ $D_{\infty h}$

T_0 = 18720(160) gas PE[1,3]

$\tilde{B}\ ^2\Sigma_g^+$ $D_{\infty h}$

T_0 = 17430(160) gas PE[1,3]

$\tilde{A}\ ^2\Pi_g$ $D_{\infty h}$

T_0 = 16781(1) gas EF[2]LF[3] $\tilde{A}$-$\tilde{X}$ 528-720 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡N stretch	2151(3)	gas	LF	3
	2	C≡C stretch	2099(3)	gas	LF	3
	3	C-C stretch	696(3)	gas	LF	3

τ = 13(2) ns gas EF[2]PEFCO[3]

$\tilde{X}\ ^2\Pi_u$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡N stretch	2210(10)	gas	EF	2,3
	2	C≡C stretch	1930(10)	gas	EF	2,3
	3	C-C stretch	570(10)	gas	EF	2,3

References

[1]G. Bieri, E. Heilbronner, V. Hornung, E. Kloster-Jensen, J. P. Maier, F. Thommen, and W. Von Niessen, Chem. Phys. 36, 1 (1979).
[2]J. P. Maier, O. Marthaler, and F. Thommen, Chem. Phys. Lett. 60, 193 (1979).
[3]J. P. Maier, L. Misev, and F. Thommen, J. Phys. Chem. 86, 514 (1982).

$CO(CN)_2^+$

T^a = 43100(1000) gas PE[1]

T^a = 33400(1000) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CO stretch	1580(80)	gas	PE	1
		CC stretch	700(80)	gas	PE	1

T^a = 17990(320) gas PE[1]

T^a = 14930(320) gas PE[1]

T^a = 9680(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]R. K. Thomas and H. Thompson, Proc. Roy. Soc. (London) A327, 13 (1972).

$F(C{\equiv}C)_2F^+$

$\tilde{D}\ ^2\Sigma_g^+$ $D_{\infty h}$

T_0 = 72200(1200) gas PE[1]

$\tilde{C}\ ^2\Pi_{u,3/2}$ $D_{\infty h}$

T_0 = 63700(800) gas PE[1]

$\tilde{B}\ ^2\Pi_{g,3/2}$ $D_{\infty h}$

T_0 = 59700(800) gas PE[1]

$\tilde{A}\ ^2\Pi_{u,3/2}$ $D_{\infty h}$

T_0 = 21230(10) gas EF[2] $\tilde{A}$-$\tilde{X}$ 460-610 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2290(80)	gas	PE	2
	2	CF stretch	1450(80)	gas	PE	2
	3	C-C stretch	520(80)	gas	PE	2

τ = 28(3) ns gas PEFCO[2]

$\tilde{X}\ ^2\Pi_{g,3/2}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2320(10)	gas	EF	2
	2	CF stretch	1550(10)	gas	EF	2
	3	C-C stretch	520(10)	gas	EF	2
Π_g	7	Deformation	300(10)[a]	gas	EF	2

[a] $\frac{1}{2}(2\nu_7)$.

References

[1]G. Bieri, E. Heilbronner, J.-P. Stadelmann, J. Vogt, and W. von Niessen, J. Am. Chem. Soc. 99, 6832 (1977).
[2]M. Allan, J. P. Maier, O. Marthaler, and J.-P. Stadelmann, J. Chem. Phys. 70, 5271 (1979).

$Cl(C{\equiv}C)_2Cl^+$

E

$T_o \leq 64060(560)$ gas PE[1]

D

$T_o \leq 60600(560)$ gas PE[1]

C $^2\Pi_u$ $D_{\infty h}$

$T_o \leq 38730(320)$ gas PE[1]

B $^2\Pi_g$ $D_{\infty h}$

$T_o \leq 35580(320)$ gas PE[1]

A $^2\Pi_{u,3/2}$ $D_{\infty h}$

$T_o = 19081(0.5)$ gas EF^4LF^4 Ã-X̃ 460-690 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2125(2)	gas	LF	4
	2	C-C stretch	1179(1)	gas	EF,LF	3,4
	3	CCl stretch	373(1)	gas	EF,LF	3,4
Π_g	7	Skel. deform.	222(2)[a]	gas	LF	4
Π_u	9	Skel. deform.	78(2)[a]	gas	LF	4

$\tau_1 = 21(2)$ ns gas EF^2PEFCO^3

$\tau_2 \sim 0.5$ μs gas EF^2

$A \sim -230$ gas LF^4

X̃ $^2\Pi_{g,3/2}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C s-stretch	2214	gas	EF	2-4
	2	C-C stretch	1316	gas	EF	2-4
	3	CCl s-stretch	393	gas	EF	2-4
Σ_u^+	5	CCl a-stretch	657	gas	EF	4

$A \sim -180$ gas LF^4

[a] $\frac{1}{2}(2\nu_i)$.

References

[1] E. Heilbronner, V. Hornung, J. P. Maier, and E. Kloster-Jensen, J. Am. Chem. Soc. 96, 4252 (1974).
[2] M. Allan, E. Kloster-Jensen, J. P. Maier, and O. Marthaler, J. Electron Spectrosc. Relat. Phenom. 14, 359 (1978).
[3] J. P. Maier, O. Marthaler, L. Misev, and F. Thommen, J. Chem. Soc., Faraday Disc. 71, 181 (1981).
[4] D. Klapstein, J. P. Maier, and L. Misev, J. Chem. Phys. 78, 5393 (1983).

$Br(C{\equiv}C)_2Br^+$

E

$T_o \leq 56480(560)$ gas PE[1]

D

$T_o \leq 53650(560)$ gas PE[1]

C $^2\Pi_u$ $D_{\infty h}$

$T_o \leq 32840(320)$ gas PE[1]

$A = -730(320)$ gas PE[1]

B $^2\Pi_g$ $D_{\infty h}$

$T_o \leq 27670(320)$ gas PE[1]

$A = -1775(320)$ gas PE[1]

Ã $^2\Pi_{u,3/2}$ $D_{\infty h}$

$T_o = 16838(0.5)$ gas EF^3LF^3 Ã-X̃ 510-695 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2186(2)	gas	LF	3
	2	C-C stretch	1071(2)	gas	LF	3
	3	CBr stretch	242(1)	gas	EF,LF	3
Π_g	7	Skel. deform.	281[ab]	gas	LF	3
Π_u	9	Skel. deform.	62(2)[a]	gas	LF	3

$\tau_1 = 12(2)$ ns gas EF^2

$\tau_2 \sim 0.5$ μs gas EF^2

$A = -1450(80)$ gas $PE^{1,2}$

$\tilde{X}\ ^2\Pi_{g,3/2}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C s-stretch	2186	gas	EF	2,3
	2	C-C stretch	1225	gas	EF	2,3
	3	CBr s-stretch	252	gas	EF	2,3

A = -950(80) gas PE[1]LF[3]

[a] $\frac{1}{2}(2\nu_i)$.
[b] Tentative value.

References

[1]E. Heilbronner, V. Hornung, J. P. Maier, and E. Kloster-Jensen, J. Am. Chem. Soc. 96, 4252 (1974).
[2]M. Allan, E. Kloster-Jensen, J. P. Maier, and O. Marthaler, J. Electron Spectrosc. Relat. Phenom. 14, 359 (1978).
[3]D. Klapstein, J. P. Maier, and L. Misev, J. Chem. Phys. 78, 5393 (1983).

$I(C{\equiv}C)_2I^+$

$\tilde{E}$

$T_o \leq 49540(560)$ gas PE[1]

$\tilde{D}$

$T_o \leq 47120(560)$ gas PE[1]

$\tilde{C}\ ^2\Pi_u$ $D_{\infty h}$

$T_o \leq 30180(320)$ gas PE[1]

A = -890(320) gas PE[1]

$\tilde{B}\ ^2\Pi_g$ $D_{\infty h}$

$T_o \leq 21300(320)$ gas PE[1]

A = -3150(320) gas PE[1]

$\tilde{A}\ ^2\Pi_{u,3/2}$ $D_{\infty h}$

$T_o \sim 12013$ gas PE[1,3]

11973(2) Ne AB[3] $\tilde{A}$-$\tilde{X}$ 600-840 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2216(3)	Ne	AB	3
	2	C-C stretch	970(80)	gas	PE	1
	3	CI stretch	183(3)	Ne	AB	3

$\tilde{A}\ ^2\Pi_{u,3/2}$---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_g	7	Skel. deform.	≧190	Ne	AB	3

A = -4280(320) gas PE[1]

$\tilde{X}\ ^2\Pi_{u,3/2}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2100(80)	gas	PE	1

A = -2340(320) gas PE[1]

References

[1]E. Heilbronner, V. Hornung, J. P. Maier, and E. Kloster-Jensen, J. Am. Chem. Soc. 96, 4252 (1974).
[2]M. Allan, E. Kloster-Jensen, J. P. Maier, and O. Marthaler, J. Electron. Spectrosc. Relat. Phenom. 14, 359 (1978).
[3]S. Leutwyler, J. P. Maier, and U. Spittel, Chem. Phys. Lett. 96, 645 (1983).

$(SCN)_2^+$

$\tilde{J}\ ^2A$ C_2

$T^a = 58500(1000)$ gas PE[1]

$\tilde{I}\ ^2B$ C_2

$T^a = 43250(320)$ gas PE[1]

$\tilde{H}\ ^2A$ C_2

$T^a = 33480(320)$ gas PE[1]

$\tilde{G}\ ^2B$ C_2

$T^a = 25660(320)$ gas PE[1]

$\tilde{F}\ ^2A$ C_2

$T^a = 23480(320)$ gas PE[1]

$\tilde{E}\ ^2A$ C_2

$T^a = 21060(320)$ gas PE[1]

$\tilde{D}\ ^2B$ C_2

$T^a = 19690(320)$ gas PE[1]

$\tilde{C}\ ^2B$ C_2

T^a = 19040(320) gas PE[1]

$\tilde{B}\ ^2A$ C_2

T^a = 11050(320) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	CN stretch	1590(60)	gas	PE	1

$\tilde{A}\ ^2B$ C_2

T^a = 2180(320) gas PE[1]

$\tilde{X}\ ^2A$ C_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a			920(80)	gas	PE	1

[a] From vertical ionization potentials.

References

[1]D. C. Frost, C. Kirby, W. M. Lau, C. B. MacDonald, C. A. McDowell, and N. P. C. Westwood, Chem. Phys. Lett. 69, 1 (1980).

$S_3N_3^+$

T^a = 76500(1000) gas PE[1]

T^a = 45000(1000) gas PE[1]

T^a = 39400(1000) gas PE[1]

T^a = 34500(1000) gas PE[1]

T^a = 32100(1000) gas PE[1]

T^a = 20000(1000) gas PE[1]

$\tilde{X}\ ^3A_2'$ D_{3h}[b]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			870(50)	gas	PE	1
			630(50)	gas	PE	1

[a] From vertical ionization potentials.
[b] Calculations suggest that this state may experience Jahn-Teller distortion to give a $^3B_2$ state, of C_{2v} symmetry.

References

[1]W. M. Lau, N. P. C. Westwood, and M. H. Palmer, J. Am. Chem. Soc. 108, 3229 (1986).

$B_2F_4^+$

$\tilde{F}\ ^2E$ D_{2d}

T_o = 66890(560) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		BB stretch	600(60)	gas	PE	1

$\tilde{E}\ ^2E$ D_{2d}

T_o = 52280(720) gas PE[1]

$\tilde{D}\ ^2B_2$ D_{2d}

T_o = 40100(560) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		BB stretch	600(100)	gas	PE	1

$\tilde{A},\tilde{B},\tilde{C}\ ^2E,^2A_2,^2B_1$ D_{2d}

T_o = 26380(720) gas PE[1]

$\tilde{X}\ ^2A_1$ D_{2d}

References

[1]N. Lynaugh, D. R. Lloyd, M. F. Guest, M. B. Hall, and I. H. Hillier, J. Chem. Soc., Faraday Trans. 2 68, 2192 (1972).

$B_2Cl_4^+$

$\tilde{I}\ ^2A_1$ D_{2d}

T_o = 60350(400) gas PE[1]

$\tilde{H}\ ^2B_2$ D_{2d}

T_o = 49860(240) gas PE[1]

$\tilde{F},\tilde{G}\ ^2E,^2A_1$ D_{2d}

T_o = 32270(320) gas PE[1]

D,E $^2B_2$,^2E D_{2d}

T_o = 23560(320) gas PE[1]

A,B,C ^2E,$^2A_2$,$^2B_1$ D_{2d}

T_o = 8630(240) gas PE[1]

X $^2A_1$ D_{2d}

References

[1]N. Lynaugh, D. R. Lloyd, M. F. Guest, M. B. Hall, and I. H. Hillier, J. Chem. Soc., Faraday Trans. 2 68, 2192 (1972).

t-(FCO)$_2$

H

T^a = 52360(480) gas PE[1]

G ^2A_u C_2

T^a = 46880(320) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		560(40)	gas	PE	1

F ^2B_u C_2

T^a = 39130(480) gas PE[1]

E ^2B_g C_2

T^a = 30420(480) gas PE[1]

D C_2

T^a = 27030(480) gas PE[1]

C ^2A_u C_2

T_o = 24690(480) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		1130(40)	gas	PE	1

B ^2B_u C_2

T_o = 17190(480) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		1410(40)	gas	PE	1
		1280(40)	gas	PE	1

A ^2B_g C_2

T_o = 14040(320) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CO stretch	1600(30)	gas	PE	1
		380(30)	gas	PE	1

X ^2A_g C_2

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		570(30)	gas	PE	1
		300(30)	gas	PE	1

[a] From vertical ionization potential.

References

[1]D. C. Frost, C. A. McDowell, G. Pouzard, and N. P. C. Westwood, J. Electron Spectrosc. Relat. Phenom. 10, 273 (1977).

t-(ClCO)$_2$

K C_2

T^a = 67300(1200) gas PE[1]

J C_2

T^a = 61800(800) gas PE[1]

I C_2

T^a = 50430(560) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		1270(70)	gas	PE	1

A ^2A_u C_2

T^a = 48090(800) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		1400(70)	gas	PE	1

G C_2

T^a = 41390(800) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		1225(70)	gas	PE	1

F ^2B_g C_2

T_o = 31790(560) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CO stretch	1650(50)	gas	PE	1
		820(50)	gas	PE	1

E ^2B_u C_2

T^a = 21780(560) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CO stretch	1660(50)	gas	PE	1
		600(50)	gas	PE	1

D C_2

T^a = 17190(800) gas PE[1]

C C_2

T^a = 15980(800) gas PE[1]

B C_2

T^a = 13960(800) gas PE[1]

Ã C_2

T^a = 11860(800) gas PE[1]

X̃ ^2A_g C_2

[a] From vertical ionization potential.

References

[1] D. C. Frost, C. A. McDowell, G. Pouzard, and N. P. C. Westwood, J. Electron Spectrosc. Relat. Phenom. 10, 273 (1977).

$C_2F_4^+$

Ã,Ĩ $^2B_{3g}$,$^2B_{3u}$ D_{2h}

T_o = 73020(320) gas PE[1,4]

G̃ $^2B_{2g}$ D_{2h}

T^a = 65190(320) gas PE[2-4]

F̃ $^2B_{1u}$ D_{2h}

T_o = 59460(400) gas PE[1-4]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	CF s-stretch	740(80)	gas	PE	1
	CF_2 deform.	330(80)	gas	PE	1

B̃,C̃,D̃,Ẽ ^2A_g,$^2B_{2u}$,^2A_u,$^2B_{1g}$ D_{2h}

$T^a \sim$ 52000 gas PE[1-4]

Ã $^2B_{3g}$ D_{2h}

T^a = 46880(320) gas PE[1-4]

X̃ $^2B_{3u}$ D_{2h}

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	C=C stretch	1710(80)	gas	PE	1-3
	CF s-stretch	820(80)	gas	PE	1-3
		400(80)	gas	PE	2,3

[a] From vertical ionization potential.

References

[1] R. F. Lake and H. Thompson, Proc. Roy. Soc. (London) A315, 323 (1970).
[2] C. R. Brundle, M. B. Robin, N. A. Kuebler, and H. Basch, J. Am. Chem. Soc. 94, 1451 (1972).

[3]J. A. Sell and A. Kupperman, J. Chem. Phys. 71, 4703 (1979).
[4]G. Bieri, W. von Niessen, L. Åsbrink, and A. Svensson, Chem. Phys. 60, 61 (1981).

$CF_2=CFCl^+$

H $^2A'$ C_s

T^a = 72130(320) gas PE[3,4]

G $^2A''$ C_s

T^a = 64060(320) gas PE[1,3,4]

F $^2A'$ C_s

T^a = 57610(320) gas PE[1,3,4]

E $^2A''$ C_s

T^a = 55190(600) gas PE[1,3,4]

D $^2A'$ C_s

T^a = 51960(600) gas PE[1,3,4]

C $^2A'$ C_s

T^a = 42840(320) gas PE[1,3,4]

B $^2A''$ C_s

T^a = 30980(320) gas PE[1,3,4]

A $^2A'$ C_s

T^a = 25900(320) gas PE[1,3,4]

X $^2A''$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	C=C stretch	1590(80)	gas	PE	1,3,4
	CF stretch	1120(80)	gas	PE	1,3,4
	CCl stretch	680(80)	gas	PE	1,3,4
	CF_2 rock	330(80)	gas	PE	3,4

[a] From vertical ionization potential. The first ionization potential is taken as 9.76 eV, as in the spectroscopic study of Ref. 2.

References

[1]R. F. Lake and H. Thompson, Proc. Roy. Soc. (London) A315, 323 (1970).
[2]J. D. Scott and B. R. Russell, J. Am. Chem. Soc. 94, 2634 (1972).
[3]K. Wittel and H. Bock, Chem. Ber. 107, 317 (1974).
[4]A. W. Potts, J. M. Benson, I. Novak, and W. A. Svensson, Chem. Phys. 115, 253 (1987).

$CF_2=CCl_2^+$

I $^2A_1$ C_{2v}

T^a = 68820(400) gas PE[1-3]

F,G,H $^2A_1,^2B_2,^2A_2$ C_{2v}

T^a = 53250(320) gas PE[1-3]

E $^2B_2$ C_{2v}

T^a = 47200(320) gas PE[1-3]

D $^2B_1$ C_{2v}

T^a = 38570(320) gas PE[1-3]

C $^2A_1$ C_{2v}

T_o = 25660(320) gas PE[1-3]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	CCl_2 "scissors"	250(40)	gas	PE	1-3

B $^2A_2$ C_{2v}

T_o = 23240(320) gas PE[1-3]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	CF_2 s-stretch	1070(60)	gas	PE	1-3
		600(40)	gas	PE	2
	CCl_2 "scissors"	190(40)	gas	PE	1-3

A $^2B_2$ C_{2v}

T^a = 20000(400) gas PE[1-3]

X $^2B_1$ C_{2v}

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	C=C stretch	1540(40)	gas	PE	1-3
	CF_2 s-stretch	1160(80)	gas	PE	1-3
	CCl_2 s-stretch	530(80)	gas	PE	1-3

[a] From vertical ionization potential.

References

[1]R. F. Lake and H. Thompson, Proc. Roy. Soc. (London) A315, 323 (1970).
[2]J. C. Bünzli, D. C. Frost, F. G. Herring, and C. A. McDowell, J. Electron Spectrosc. Relat. Phenom. 9, 289 (1976).
[3]A. W. Potts, J. M. Benson, I. Novak, and W. A. Svensson, Chem. Phys. 115, 253 (1987).

$C_2Cl_4^+$

C $^2B_{1u}$ D_{2h}

T^a = 72370(320) gas PE[1,2]

J,K $^2B_{2u}$,^2A_g D_{2h}

$T^a \sim$ 59400 gas PE[1,2]

I $^2B_{3u}$ D_{2h}

T^a = 46470(320) gas PE[1,2]

H $^2B_{3g}$ D_{2h}

T^a = 43080(320) gas PE[1,2]

G $^2B_{2g}$ D_{2h}

T^a = 33400(320) gas PE[1,2]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g		460(80)	gas	PE	1

B,C,D,E,F ^2A_u,$^2B_{2u}$,$^2B_{1g}$,$^2B_{1u}$,^2A_g D_{2h}

$T^a \sim$ 23000-29500 gas PE[1,2]

A $^2B_{3g}$ D_{2h}

T^a = 16460(320) gas PE[1,2]

X $^2B_{3u}$ D_{2h}

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	C=C stretch	1320(80)	gas	PE	1

[a] From vertical ionization potential.

References

[1]R. F. Lake and H. Thompson, Proc. Roy. Soc. (London) A315, 323 (1970).
[2]W. von Niessen, L. Åsbrink, and G. Bieri, J. Electron Spectrosc. Relat. Phenom. 26, 173 (1982).

$N_2O_4^+$

G $^2B_{2g}$ D_{2h}

T^a = 58500(1200) gas PE[1-5]

F $^2B_{3g}$ D_{2h}

T^a = 45200(1600) gas PE[1-5]

E $^2B_{1u}$ D_{2h}

T^a = 33900(1600) gas PE[1-5]

C,D $^2B_{1g}$, $^2B_{3u}$ D_{2h}

T^a = 16700(1000) gas PE[1-5]

B ^2A_u D_{2h}

T^a = 13200(1000) gas PE[1-5]

A $^2B_{2g}$ D_{2h}

T^a = 7700(900) gas PE[1-5]

X ^2A_g D_{2h}

[a] From vertical ionization potentials.

References

[1]D. L. Ames and D. W. Turner, Proc. Roy. Soc. (London) A348, 175 (1976).
[2]D. C. Frost, C. A. McDowell, and N. P. C. Westwood, J. Electron Spectrosc. Relat. Phenom. 10, 293 (1977).
[3]T. H. Gan, J. B. Peel, and G. D. Willett, J. Chem. Soc., Faraday Trans. 2 73, 1459 (1977).
[4]K. Nomoto, Y. Achiba, and K. Kimura, Bull. Chem. Soc. Japan 52, 1614 (1979).
[5]D. P. Chong, D. C. Frost, W. M. Lau, and C. A. McDowell, Chem. Phys. Lett. 90, 332 (1982).

$N_2S_4^+$

H $^2A'$ C_s

T^a = 47680(320) gas PE[1]

G $^2A'$ C_s

$T^a \sim$ 44500 gas PE[1]

F $^2A''$ C_s

T^a = 37520(320) gas PE[1]

E $^2A'$ C_s

T^a = 31630(320) gas PE[1]

D $^2A''$ C_s

T^a = 28400(320) gas PE[1]

C $^2A'$ C_s

T^a = 20010(320) gas PE[1]

B $^2A''$ C_s

T^a = 17270(320) gas PE[1]

A $^2A'$ C_s

T^a = 6450(320) gas PE[1]

X $^2A''$ C_s

[a] From vertical ionization potentials.

References

[1]M. H. Palmer, W.-M. Lau, and N. P. C. Westwood, Z. Naturforsch. 37a, 1061 (1982).

PF_2NCO^+

F C_s

T^a = 67400(1000) gas PE[1]

E C_s

T^a = 53700(1000) gas PE[1]

D C_s

T^a = 44800(1000) gas PE[1]

C C_s

T^a = 38300(1000) gas PE[1]

B C_s

T^a = 17300(1000) gas PE[1]

A C_s

T^a = 9280(1000) gas PE[1]

[a] From vertical ionization potentials.

References

[1]S. Cradock and D. W. H. Rankin, J. Chem. Soc., Faraday Trans. 2 68, 940 (1972).

PF_2NCS^+

E C_s

T^a = 62900(1600) gas PE[1]

D C_s

T^a = 50000(1600) gas PE[1]

C C_s

T^a = 42800(1600) gas PE[1]

B C_s

T^a = 29900(1600) gas PE[1]

A C_s

T^a = 13700(1600) gas PE[1]

[a] From vertical ionization potentials.

References

[1]S. Cradock and D. W. H. Rankin, J. Chem. Soc., Faraday Trans. 2 68, 940 (1972).

CF_3NO^+

T^a = 73700(1000) gas PE[2]

T^a = 59200(1000) gas PE[2]

T^a = 56000(1000) gas PE[1,2]

T^a = 48700(1000) gas PE[1,2]

T^a = 41500(1000) gas PE[1,2]

T^a = 39000(1000) gas PE[2]

[a] From vertical ionization potentials.

References

[1]H. Bergmann, S. Elbel, and R. Demuth, J. Chem. Soc., Dalton Trans. 401 (1977).
[2]N. P. Ernsting, J. Pfab, J. C. Green, and J. Romelt, J. Chem. Soc., Faraday Trans. 2 76, 844 (1980).

CF_2ClNO^+

T^a = 68100(320) gas PE[1]

T^a = 50700(1000) gas PE[1]

T^a = 45100(1000) gas PE[1]

T^a = 36070(320) gas PE[1]

T^a = 17990(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]N. P. Ernsting, J. Pfab, J. C. Green, and J. Romelt, J. Chem. Soc., Faraday Trans. 2 76, 844 (1980).

$CFCl_2NO^+$

T^a = 63980(320) gas PE[1]

T^a = 47930(320) gas PE[1]

T^a = 43890(320) gas PE[1]

T^a = 33200(1000) gas PE[1]

T^a = 22910(320) gas PE[1]

T^a = 21540(320) gas PE[1]

T^a = 16940(320) gas PE[1]

T^a = 14040(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]N. P. Ernsting, J. Pfab, J. C. Green, and J. Romelt, J. Chem. Soc., Faraday Trans. 2 76, 844 (1980).

CCl_3NO^+

T^a = 58900(1000) gas PE[1]

T^a = 54100(1000) gas PE[1]

T^a = 43810(320) gas PE[1]

T^a = 42800(1000) gas PE[1]

T^a = 40740(320) gas PE[1]

T^a = 24200(1000) gas PE[1]

T^a = 22670(320) gas PE[1]

T^a = 16140(320) gas PE[1]

T^a = 12430(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]N. P. Ernsting, J. Pfab, J. C. Green, and J. Romelt, J. Chem. Soc., Faraday Trans. 2 76, 844 (1980).

CF_3OF^+

F C_s

T^a = 54500 gas PE[1]

E C_s

T^a = 43000 gas PE[1]

D C_s

T^a = 31000 gas PE[1]

C C_s

T^a = 24000 gas PE[1]

X $^2A''$ C_s

[a] From vertical ionization potentials.

References

[1]M. B. Robin and N. A. Kuebler, J. Electron Spectrosc. Relat. Phenom. 1, 13 (1972/73).

$P_2F_4^+$

B

T^a = 38400(1000) gas PE[1]

A

T^a = 22670(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1]S. Cradock and D. W. H. Rankin, J. Chem. Soc., Faraday Trans. 2 68, 940 (1972).

CF_3ClF

Threshold for photodecomposition in solid Ar, producing CF_4 + Cl, between 300 and 260 nm.[1]

$\tilde{X}$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CF stretch	1235	Ar	IR	1
	CF stretch	1224	Ar	IR	1
	CF stretch	1073	Ar	IR	1
	ClF stretch	633	Ar	IR	1

References

[1]M. E. Jacox, Chem. Phys. 51, 69 (1980).

CF_3BrF

Threshold for photodecomposition in solid Ar, producing CF_4 + Br, between 345 and 370 nm.[1]

$\tilde{X}$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CF stretch	1251	Ar	IR	1
	CF stretch	1225	Ar	IR	1
	CF stretch	1051	Ar	IR	1
	BrF stretch	588	Ar	IR	1
	CF_3 deform.	454	Ar	IR	1

References

[1]M. E. Jacox, Chem. Phys. 51, 69 (1980).

CF_3IF

Threshold for photodecomposition in solid Ar, producing CF_4 + I, at a wavelength longer than 490 nm.[1]

$\tilde{X}$ C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CF stretch	1223	Ar	IR	1
	CF stretch	1197	Ar	IR	1
	CF stretch	1052	Ar	IR	1
	CF_3 deform.	432	Ar	IR	1,2

References

[1]M. E. Jacox, Chem. Phys. 51, 69 (1980).
[2]M. E. Jacox, J. Chem. Phys. 83, 3255 (1985).

PF_5^+

T^a = 42440(320) gas PE[1]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'		702(40)	gas	PE	1

$T^a \sim 32000$ gas PE[1]

T^a = 28700(1000) gas PE[1]

T^a = 23320(320) gas PE[1,2]

T^a = 18150(320) gas PE[1,2]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1' 2	PF_2 ax. stretch	480(80)	gas	PE	2

T^a = 12830(500) gas PE[1,2]

T^a = 9760(500) gas PE[1,2]

T^a = 7420(320) gas PE[1,2]

[a] From vertical ionization potentials.

References

[1]P. A. Cox, S. Evans, A. F. Orchard, N. V. Richardson, and P. J. Roberts, Faraday Discuss. Chem. Soc. 54, 26 (1972).
[2]D. W. Goodman, M. J. R. Dewar, J.R. Schweiger, and A. H. Cowley, Chem. Phys. Lett. 21, 474 (1973).

PCl_5^+

T^a = 72800(1000) gas PE[1]

T^a = 43490(320) gas PE[1]

$T^a \sim 41300$ gas PE[1]

$T^a \sim 25200$ gas PE[1]

T^a = 23480(320) gas PE[1]

T^a = 19690(320) gas PE[1]

T^a = 12020(320) gas PE[1]

T^a = 8470(320) gas PE[1]

T^a = 6450(320) gas PE[1]

T^a = 1290(320) gas PE[1]

[a] From vertical ionization potentials.

References

[1] P. A. Cox, S. Evans, A. F. Orchard, N. V. Richardson, and P. J. Roberts, Faraday Discuss. Chem. Soc. 54, 26 (1972).

BrF_5^+

$I,J\ ^2A_1,^2E$ C_{4v}

T^a = 56480(560) gas PE[1]

$G,H\ ^2E,^2B_2$ C_{4v}

T_o = 30260(320) gas PE[1]

$E,F\ ^2A_1,^2B_1$ C_{4v}

T^a = 24690(320) gas PE[1]

$C,D\ ^2E,^2B_1$ C_{4v}

T^a = 20330(320) gas PE[1]

$A,B\ ^2A_2,^2E$ C_{4v}

T_o = 9520(320) gas PE[1]

$X\ ^2A_1$ C_{4v}

[a] From vertical ionization potential.

References

[1] R. L. DeKock, B. R. Higginson, and D. R. Lloyd, Faraday Discuss. Chem. Soc. 54, 84 (1972).

IF_5^+

$I,J\ ^2A_1,^2E$ C_{4v}

T_o = 47520(650) gas PE[1]

$G,H\ ^2E,^2B_2$ C_{4v}

T_o = 31870(560) gas PE[1]

$E,F\ ^2A_1,^2B_1$ C_{4v}

T^a = 26460(320) gas PE[1]

$C,D\ ^2E,^2B_1$ C_{4v}

T^a = 24040(400) gas PE[1]

$A,B\ ^2A_2,^2E$ C_{4v}

T_o = 14200(500) gas PE[1]

$X\ ^2A_1$ C_{4v}

[a] From vertical ionization potential.

References

[1] R. L. DeKock, B. R. Higginson, and D. R. Lloyd, Faraday Discuss. Chem. Soc. 54, 84 (1972).

$XeOF_4^+$

T^a = 57300(800) gas PE[1]

T^a = 50000(800) gas PE[1]

T^a = 39100(800) gas PE[1]

T^a = 27400(800) gas PE[1]

T^a = 23000(800) gas PE[1]

T^a = 17800(800) gas PE[1]

T^a = 12100(800) gas PE[1]

[a] From vertical ionization potentials.

References

[1] C. R. Brundle and G. R. Jones, J. Electron Spectrosc. Relat. Phenom. 1, 403 (1972/73).

7. Index

8. Acknowledgment

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9. References

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