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

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A summary is presented of recently published, critically evaluated experimental vibrational and electronic energy level data for neutral and ionic transient molecules and high temperature species possessing from three to sixteen atoms. Although the emphasis is on species with lifetimes too short for study using conventional sampling techniques, there has been selective extension of the compilation to include data for isolated molecules of inorganic species such as the heavy-metal oxides, which are important in a wide variety of industrial chemical systems. Radiative lifetimes and the principal rotational constants are included. Observations in the gas phase, in molecular beams, and in rare-gas and diatomic molecule matrices are evaluated. The types of measurement surveyed include conventional and laser-based absorption and emission techniques, laser absorption with mass analysis, and photoelectron spectroscopy. Not counting isotopic species, 904 molecules are surveyed, and 2696 distinct references are given. © *1998 American Institute of Physics and American Chemical Society.* [S0047-2689(98)00102-0]

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

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1. Introduction

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

In the early studies of complex chemical processes, it was necessary to postulate mechanisms involving such transient intermediates, present in concentrations too small for direct detection. Conventional end product analysis aids in the se-

lection of suitable mechanisms, but generally does not yield a complete description of the system. Consequently, the improvement of industrial chemical processes often is achieved by semiempirical experimentation. The determination of the detailed chemical mechanism would, in turn, permit the development of rational strategies for removing undesired products and enhancing the yield of the desired species.

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

For many years, the most important source of vibrational and electronic energy level data for small polyatomic reaction intermediates was the compilation of spectroscopic data for small polyatomic molecules (3–12 atoms) given by Herzberg.[1] To meet the need for an updated, critically evaluated compilation, a series of publications[2–4] have appeared in this journal, culminating in the publication in 1994 of a monograph[5] which presented evaluated spectral data for more than 1550 small polyatomic transient molecules. Vibrational fundamentals in the ground and excited electronic states and radiative lifetimes were included. To aid in spectral identification, the principal rotational constants were also given to three decimal places. These tables have provided the basis for a personal computer software database (Vibrational and Electronic Energy Levels of Small Polyatomic Transient Molecules, National Institute of Standards and Technology Standard Reference Database 26), designed to supplement the published compilation by providing a capability for rapid searches by molecule or wave number.

The rapid growth in the scientific literature concerned with the spectroscopic study of transient molecules and with their detection in chemical reaction systems continues. Since the October 1993 cutoff in the data evaluation for the 1994 monograph,[5] substantive new spectroscopic data have been published for many species included in it, and the first data have become available for several hundred other molecules. There has been especially great progress in the spectroscopic characterization of transient species produced by the reaction of metal atoms with oxygen and other small molecules. This paper attempts to provide a comprehensive, critically evaluated summary of these new data on the vibrational and electronic energy levels of small polyatomic transient molecules, in order to support further research and new technologies such as those of plasma processing and chemical vapor deposition.

2. Scope of Review

This review provides a critical evaluation of the vibrational and electronic spectral data available in mid-1997 for approximately 900 small polyatomic transient molecules. Of these, about 570 were not represented in the 1994 monograph; the remainder are molecules included in that monograph for which new data have become available. Despite this rapid progress, many gaps remain in our knowledge of the energy levels of the species represented, and many new and potentially important transient molecules are still to be discovered.

Data have been selectively included for some molecules which are important in environmental and industrial chemical reaction systems but which can be studied only with difficulty using conventional sampling techniques because of the ease with which they decompose, rearrange, or polymerize. Also included are data derived from spectra of many high-temperature species, such as metal oxides, studied in molecular beams and in rare-gas matrices.

3. Types of Measurement

Studies in the gas phase offer the potential for the most precise, detailed measurements. Because of the high chemical reactivity of transient molecules, it is difficult to obtain gas-phase infrared spectra of them. The well known advantages of Fourier transform infrared measurements, coupled with sophisticated digital data handling procedures, have permitted the acquisition of gas-phase survey spectra for a number of transient molecules. Diode lasers and other laser-based techniques with limited tunability have been used to obtain high resolution spectra of individual vibrational transitions of these species.

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

As in the earlier compilations, spectral data obtained in rare gas and small covalent molecule matrices are included. The application of matrix isolation sampling for the stabilization and spectroscopic study of uncharged reaction intermediates has recently been reviewed.[6] Because nitrogen and the rare gases are transparent through the entire infrared spectral region, matrix isolation measurements provide a potentially valuable survey tool. In these matrices, infrared absorptions are typically sharp, with half band widths between 0.1 and 1 cm^{-1}. Rotational structure is, with few exceptions, quenched. Multiple trapping sites occur, often resulting in

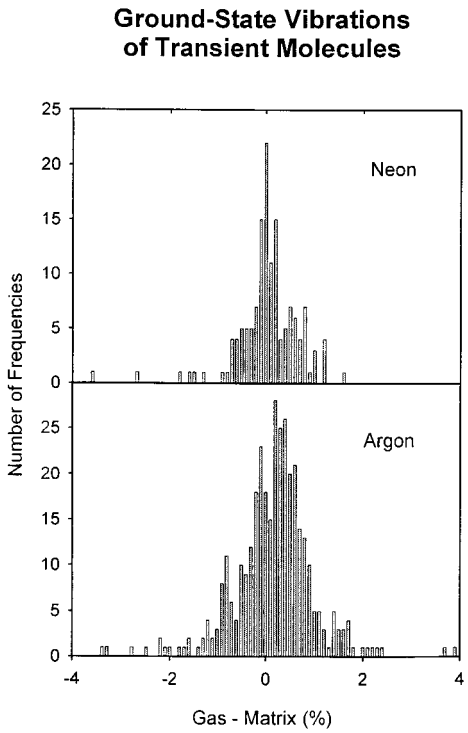

FIG. 1. Comparison of ground-state vibrational frequencies reported for transient molecules (2–16 atoms) in neon and argon matrices with corresponding values obtained from gas-phase measurements.

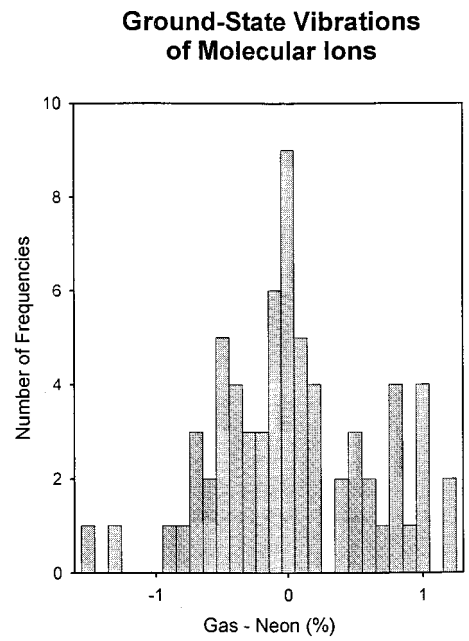

FIG. 2. Comparison of ground-state vibrational frequencies reported for molecular ions (2–16 atoms) in a neon matrix with corresponding values obtained from gas-phase measurements.

the appearance of several absorption maxima—usually one or two of which predominate—over a range of a few cm^{-1}.

Matrix shifts for covalently bonded molecules trapped in solid neon or argon often are quite small. A comparison[7] of the positions of the ground-state vibrational fundamentals of over two hundred diatomic molecules observed in the gas phase and in nitrogen and rare-gas matrices has shown that, typically, the smallest matrix shift occurs for neon matrix observations, with successively greater matrix shifts for the heavier rare gases and for nitrogen. Except for very weakly bonded molecules and for the alkali metal and Group IIIa halides, matrix shifts of most diatomic molecules isolated in solid argon are smaller than 2%. Similar conclusions resulted from a comparison of neon- and argon-matrix shifts for the ground-state vibrational fundamentals of larger molecules.[8] The generalization that matrix interactions are minimal for neon and that they increase as the mass of the rare gas is increased and become even more important for nitrogen and most other small molecule matrices is supported by experimental observations on larger molecules, as well. Figure 1 compares the observed matrix shifts for the ground-state fundamental vibrations of transient molecules trapped in solid neon and argon. For neon matrices, the maximum in the distribution lies near 0.0%, and for argon matrices, near 0.2%. For both neon and argon matrices, fewer than one-tenth of the matrix shifts are greater than 1%.

For molecular ions, neon is the matrix of choice. Polarization and charge-transfer interactions become successively more important for molecules isolated in the heavier rare gases. Charge delocalization sometimes also occurs for ionic species trapped in the rare gases.[9,10] The anomalously large matrix shift for ν_3 of $ClHCl^-$ may be attributed to this phenomenon. As is shown in Fig. 2, data for small cation species trapped in solid neon are consistent with the matrix shift generalizations given above. Only twelve comparisons are available for molecular cations observed both in the gas phase and trapped in solid argon. The absolute values of five of the observed matrix shifts are greater than 1%. For several other vibrations of molecular ions which have been observed in both neon and argon matrices but not in the gas phase, there are deviations greater than 1% between the neon- and argon-matrix frequencies. Very few comparisons are possible for molecular anions. A number of these species have been generated in rare-gas (usually argon) matrices by charge transfer between a precursor molecule and an alkali metal atom. Recent studies of such species as CO_2^- and SO_2^- generated instead by photoionization and/or Penning ionization and trapped in solid neon indicate that shifts on the order of 50 cm^{-1} may be attributed to the relatively strong interaction of the anion with the nearby alkali metal cation. On the other hand, when the uncharged molecule has a relatively large electron affinity, as is true for C_2 and for NO_2, charge transfer occurs at a relatively great separation, and a substantial fraction of the anion population may be trapped in sites in which interaction with the alkali metal cation is minimal.

Matrix shifts for vibrations associated with ionic bonds are often considerably larger than those associated with uncharged molecules or with intramolecular vibrations of mo-

lecular ions. Criteria for inclusion of data for species which include an ionic bond are exemplified by the selection process for the heavy-metal oxides. Often the stable dioxide structures include an $M^+O_2^-$ species with significant covalent bond character for the attachment of M^+, as evidenced by a substantial shift in the O_2^- stretching fundamental as M^+ is varied. Such species are included in the compilation. On the other hand, there is little evidence for substantial metal-atom participation in the vibrations characteristic of the O_3^- moiety of $M^+O_3^-$. Accordingly, spectral data are given for O_3^-, but not for $M^+O_3^-$.

Data are beginning to appear for molecules trapped in a hydrogen matrix. Insufficient information is available for generalization on the magnitude of matrix shifts in this medium. For the few species heretofore studied, including several transient molecules present in this compilation, the matrix shifts have been comparable to those in a neon matrix.

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

Because of the prevalence of electronic emission spectra and the sensitivity, rapid time response, and cumulative detection capability of the photographic plate in the visible and ultraviolet spectral regions, the study of the electronic spectra of gas-phase reaction intermediates has a comparatively long history. Flash photolysis has permitted the preparation of relatively high concentrations of transient species. Many electronic band systems of gas-phase transient molecules have been discovered through flash photolysis studies. More recently, a wide variety of laser-based techniques have also been used for electronic spectral observations, often with exceptionally high detection sensitivity. The spatial configuration of the laser beam makes possible crossed molecular beam-laser beam studies, providing an extremely powerful tool for studies of the energy levels of molecules in molecular beams. Laser-based techniques show great promise for application in the development of diagnostics for chemical reaction intermediates in the environment, the laboratory, and the industrial plant. Laser studies may be broadly classified according to whether the interaction of the molecule with the laser beam(s) is followed by photon or mass detection. Photon-based observations are amenable to remote sensing applications. Because pulsed lasers offer an exceptionally wide range of time specificity, they are very useful for determining radiative lifetimes and rates of elementary chemical reactions.

Much valuable information on the energy levels of molecular cations has been obtained from photoelectron spectroscopy. These tables include selective coverage of the voluminous literature on photoelectron spectroscopic measurements. The number of stable molecules which possess more than six atoms for which photoelectron spectra have been reported is too great to permit the inclusion of low-to-moderate resolution photoelectron spectral data for molecular cations with more than six atoms. Those who need such data for larger molecules may find the reviews by Turner *et al.*,[11] Rabalais,[12] and Kimura *et al.*[13] helpful. Several criteria are important in determining whether a given reference should be included in the present work. The first of these is resolution. In the few instances in which high resolution photoelectron data are available, these data are heavily weighted. Where direct spectroscopic observation is possible, the measurements generally are of considerably higher precision than are the photoelectron data, which are then omitted from the tables. A second criterion is the availability of adiabatic ionization potentials. In order to obtain information on the positions of electronic transitions from photoelectron spectral data, it is necessary to subtract the first ionization potential from the energy of the photoelectron band. Where there is little change in the molecular geometry in the transition, the difference between the vertical ionization potentials gives a reasonable approximation to the position of the electronic transition. However, this is not the general case. Therefore, priority is given to papers which include adiabatic ionization potentials.

For most photoelectron spectroscopic transitions, structure has not been resolved. Many of these states are dissociative. Further information on the dissociation products can be obtained from values of the appearance potentials for various products in photoionization studies on the parent molecule. Such studies are beyond the scope of this review. The tables of ionization and appearance potentials by Lias and co-workers[14,15] constitute a valuable source of information on the appearance potentials of photofragments.

The range of tunability of visible and ultraviolet lasers, like that of infrared lasers, is limited. Therefore, a preliminary survey using conventional gas-phase and/or matrix-isolation spectroscopic studies is often desirable. A comparison of the positions of the electronic band origins of diatomic molecules in the gas phase and in rare-gas and nitrogen matrices has been published.[16] As in the determination of ground-state vibrational energy levels, neon is the matrix material of choice, with a sharp maximum at 0.0% in the distribution of matrix deviations for valence transitions of covalently bonded molecules. In argon-matrix observations, most such band origins are shifted by less than 2% from the gas-phase values. At the somewhat higher temperatures often used for electronic spectral observations in matrices of the heavier rare gases or of nitrogen, relatively broad phonon bands become prominent. The blue shift of the phonon maximum from the zero-phonon line in absorption measurements, and the red shift in emission measurements, typically amount to approximately 1 to 1.5%. Rydberg transitions of molecules in matrices often are greatly broadened and experience much larger shifts. Further details of the

behavior of electronic transitions of matrix-isolated molecules have previously been discussed.[3,6,16]

The radiative lifetime of a relatively large molecule isolated in a rare-gas matrix is frequently related to the radiative lifetime in the gas phase by a simple refractive index correction.[17] In a neon matrix, such a correction typically decreases the radiative lifetime by about 15%. For such molecules, often intramolecular mechanisms for nonradiative energy transfer are available both in the gas phase and in the matrix. On the other hand, the density of excited states is much lower for small molecules, and matrix shifts may alter perturbation interactions between strongly coupled electronic states, providing a path for nonradiative deactivation. In this circumstance, fluorescence which is prominent in the gas phase may even be completely quenched in the matrix.

4. Guide to the Compilation

The goal of this paper is to extend the previously published compilation[5] of critically evaluated vibrational and electronic spectroscopic data for small polyatomic transient molecules. The literature has been surveyed through June 1997; only limited addition of more recent data has been possible. Unfortunately, with a few exceptions it is not possible to include data for stable molecules. However, the spectra of many of these species are relatively well established, and sources of data such as the tables of Herzberg[1] and Shimanouchi[18] remain extremely useful. In obtaining spectral identifications with the help of the present compilation, it is crucial that the possible contribution of the absorptions or emissions by a stable molecule also be considered.

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

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

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

br	bridged
cyc	cyclic. If parentheses follow, only the atoms enclosed in them are included in the ring.
c	*cis*
t	*trans*

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

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

The heading for each electronic state gives its symmetry, the point group to which the molecule belongs in that electronic state, and, where available, references to the determination of a quantitative molecular structure. For C_{2v} molecules, there is potential ambiguity in the definition of the molecular symmetry axes. The convention in which the x axis is chosen perpendicular to the plane of the molecule, recommended by the Joint Commission for Spectroscopy of IAU and IUPAP,[19] has been adopted. Often this has required the interchange of published assignments of energy levels with B_1 and B_2 symmetry.

Most authors of papers on photoelectron spectroscopy have proposed assignments for the various photoelectron bands, using arguments based on molecular orbital theory and often on semiempirical or *ab initio* calculations. These assignments have been included in the present tables. Where

several conflicting assignments have been given in the literature, an attempt has been made to choose the most satisfactory one. Generally, the assignments of photoelectron spectra have been made with the presumption that the point group to which the molecular cation belongs is the same in all of its excited states. Structural data for these excited states are extremely rare. Therefore, the molecular point group which has been adopted in the analysis of the photoelectron spectrum is given in these tables. In practice, it is likely that there is some variation in excited-state molecular symmetries. Thus, a bent molecular ion may become linear in some of its excited states. For highly symmetric species, Jahn–Teller distortion may reduce the molecular symmetry.

The energy of the electronic transition follows the state designation and symmetry information. Where possible, T_0, the energy separation between the electronic energy level of interest and the ground electronic, vibrational, and rotational states of the molecule, is given. However, where only low resolution data or photoelectron data are available, often only band maxima have been given in the literature. With photoelectron data, T_0 is derived by subtracting the value of the first ionization potential from that of the higher ionization potential which corresponds to the state of interest. When data for the first adiabatic ionization potential are available, the footnote phrase ''from vertical ionization potential'' implies that the first adiabatic ionization potential is known but that the higher ionization potential is measured to the peak maximum; the phrase ''from vertical ionization potentials'' implies that the energy difference between the higher and the first absorption maximum was used. If the first photoelectron transition has a gradual onset, a better value of the first ionization potential may have been obtained from photoionization data or from the extrapolation of Rydberg series in the spectrum of the parent molecule. Supplementary sources of data for the first ionization potential are cited in the tables. However, if the difference between the first adiabatic ionization potential obtained in the photoelectron spectrum and that obtained in other measurements amounts to only 10 or 20 meV, the photoelectron spectroscopic value is used, because of the advantage of a consistent set of measurements. Where threshold energies differ by one quantum in a vibrational progression, a best value for the ionization potential is chosen which coincides with the most probable position of the vibrationally unexcited transition. Because of inherent uncertainties in the determination of higher ionization potentials in many photoelectron spectral measurements, photoelectron peaks above about 18 eV are often omitted. Except where otherwise indicated, the units of all quantities in these tables are cm^{-1}. Error estimates are those of the authors of the original literature. The numbers in parentheses give these estimated errors in relation to the last digits of the electronic or vibrational frequency (e.g., $1234.567(89) \equiv 1234.567 \pm 0.089$). Where the error includes a decimal point, the decimal point is retained inside the parentheses. When the uncertainty is not explicitly indicated, the value is given to the estimated number of significant figures. As in the tables of Herzberg,[1] T_0 values are given to the center of multiplet structure. For doublet states, the two components differ by $\pm A$ (the spin-orbit splitting constant), and the energy difference is measured from the average of the two bands, whereas for triplet states the three components fall at 0, $\pm A$ with respect to the position from which the band energy is measured. This convention is also followed here unless specific states (e.g., $^2\Pi_{3/2}$) are given. In matrix isolation absorption and many laser excitation studies only the lowest component of the ground electronic state is accessible. Except for transitions with relatively small values of A, this is also likely to be true for studies using cooled molecular beams. Often these latter studies give T_0 values from the lowest energy component with a precision better than that to which A is known.

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

The format of the vibrational tables is similar to that used in the earlier compilations. The vibrational numbering convention is that used by Herzberg.[1] Within a given symmetry species, vibrations are numbered starting with the highest frequency. The same convention is followed for deuterated species. Therefore, a given type of vibration may be numbered differently for the deuterated than for the unsubstituted molecule. For triatomic molecules, the bending vibration is always designated as ν_2. For aromatic molecules, an alternate vibrational numbering scheme developed by Wilson[19] has often been used in the literature. Where both the Herzberg and the Wilson numbering schemes have been used for the published data, the Herzberg numbering is adopted, and the Wilson numbering is sometimes shown in parentheses. For a few species, only the Wilson numbering has been used. To avoid confusion, this is retained in the present tables, and the use of the Wilson numbering is indicated in a footnote. Where possible, the values of $\Delta G(\frac{1}{2})$, the separation between the $v=0$ and $v=1$ levels for the vibration of interest, have been used. The expression of uncertainties is similar to that described for electronic band origins. Where vibrational frequencies have been determined with a precision greater than two decimal places, the tabulated values have been rounded off. If a bending fundamental is split by Renner–Teller interaction, the position of the unperturbed fundamental is given. Where specific components of such a split fundamental have been studied, they may also be listed, with the transition designated in a footnote. For a more complete treatment of the Renner effect and definitions of the

parameters included in many of these footnotes, see the discussion by Herzberg[1] and the references cited for the molecule of interest. A few of the species in these tables possess out-of-plane vibrations which have resolved inversion splitting structure. For these, the specific component for which the vibrational frequency is reported is designated in a footnote. Relative intensities of vibrational bands are dependent on the technique used for the measurement. When possible, the relative intensities of *ground-state infrared absorptions* are included. It is not feasible to give the corresponding relative intensities for other types of observation. Relative intensity abbreviations include:

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

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

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

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

5. Abbreviations

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

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

6. Acknowledgment

This work was supported by the Standard Reference Data Program of the National Institute of Standards and Technology.

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8. Tables

8.1. H_3^+, H_3, and Triatomic Dihydrides

H_3^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Ring breathing	3178.18[a]	gas	IR,PI LD,EM	10,12,13 19,22
e'	2	Deformation	2521.42[a]	gas	LD,IR	1,4,15,22

B_0=43.510; C_0=20.698 LD[1,4]DL[4]IR[10]EM[22]

H_2D^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Ring breathing	2992.51	gas	LD	3,6,11
	2	Deformation	2205.87	gas	LD,DL	7
b_2	3	Deformation	2335.45	gas	LD,DL	7

A_0=43.438(2); B_0=29.134; C_0=16.601 LD,MW[6,7,11]

D_2H^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Ring breathing	2736.98	gas	LD	5,11,14
	2	Deformation	1968.17	gas	DL	8,14
b_2	3	Deformation	2078.43	gas	DL	8,14

A_0=36.199; B_0=21.869; C_0=13.070 LD[5,11,14]DL[8,14]

D_3^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Ring breathing	2300.84[a]	gas	EM,DL	21
e'	2	Deformation	1834.67[a]	gas	IB,DL	2,9

B_0=21.810; C_0=10.533 DL[9,21]EM[21]

[a]Hot bands arising from ν_1 and ν_2 of H_3^+ have been observed,[16,19] as have been the first[17] and second[18,20] overtones of ν_2. Several of the corresponding hot bands and overtones of D_3^+ have also been reported.[21]

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H_3

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

$3d\ ^2A_1'$ D_{3h} Structure: EM[8]
T_0^a=18511 gas EM[8]PF[26] $3d-2p^2A_2''$ 568–615 nm
EM[8] $3d-3p^2E'$ 3891–4456 cm^{-1}
B_0=42.99; C_0=22.735 EM[8]

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

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

B_0=42.99; C_0=22.735 EM[8]

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

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

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

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

B_0=44.19; C_0=22.676 EM[6]

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

2p $^2A_2''$ D_{3h} Structure: EM[6]
T_0^a=993 gas EM[3,6] $3s^2A_1'-2p^2A_2''$ 592–615 nm
EM[8] $3d-2p^2A_2''$ 568–615 nm

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

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

2s $^2A_1'$[c] D_{3h} Structure: EM[3]
gas EM[2,3] $3p^2A_2''-2s^2A_1'$ 556–574 nm
gas EM[4] $3p^2E'-2s^2A_1'$ 708–736 nm
B_0=46.82; C_0=23.41 EM[3]

H_2D

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

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

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

D_2H

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

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

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

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

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

D_3

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

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

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

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

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

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

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

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

τ=17.5(2.0) ns gas EM[9,21]

B_0=21.15; C_0=10.59 EM[6]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Ring breathing	2353.3	gas	PI	29
e'	2	Deformation	1900.9	gas	PI	29

B_0=22.112; C_0=11.056 EM[6]

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

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

$B_0=23.09$; $C_0=11.544(6)$ $EM^{3,21}$

[a]Measured with respect to lowest bound state, $2s\ ^2A_1'$. Structure observed[1] in the dissociation spectrum of H_2 has been reinterpreted[5] as arising from the predissociation of H_3 ($2s\ ^2A_1'$) into $H+H_2$. Unstructured emission observed[11] between 190 and 280 nm, with a maximum near 230 nm, upon charge transfer between K and H_3^+ or D_3^+ has been attributed to transitions originating in bound Rydberg states of H_3 or D_3 and terminating in the dissociative ground-state continuum. When charge transfer with Cs was studied,[28] emission between 200 and 400 nm was detected for all four isotopic species of H_3. A double maximum for D_3 was interpreted as arising from emission to both sheets of the ground-state potential surface. Photofragment spectroscopy[14] has placed the $2p\ ^2A_2''$ state 5.563(20) eV above the ground-state $H+H_2$ dissociation limit.

[b]Observed for $N=1$ rotational level.

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

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BeH_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	697.9	Ar	IR	1
Σ_u^+	3	Asym. stretch	2159.1	Ar	IR	1

BeD_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	531.9	Ar	IR	1
Σ_u^+	3	Asym. stretch	1674.0	Ar	IR	1

Reference

[1] T. J. Tague, Jr. and L. Andrews, J. Am. Chem. Soc. **115**, 12111 (1993).

MgH_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	439.8	Ar	IR	2
			430	Kr	IR	1
			417	Xe	IR	1
Σ_u^+	3	Asym. stretch	1571.9	Ar	IR	2
			1558	Kr	IR	1
			1569	Xe	IR	1
			1544			

MgD_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	309	Kr	IR	1
			300	Xe	IR	1
Σ_u^+	3	Asym. stretch	1163.2	Ar	IR	2
			1153	Kr	IR	1
			1160	Xe	IR	1
			1144			

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TiH_2

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

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

TiD_2

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

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

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ZrH_2

$\tilde{X}$ $^3A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	ZrH_2 a-stretch	1518.6	Ar	IR	1

ZrD_2

$\tilde{X}$ $^3A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	ZrD_2 a-stretch	1092.5	Ar	IR	1

Reference

[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. **99**, 15004 (1995).

HfH_2

$\tilde{X}$ $^3A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	HfH_2 a-stretch	1629.1	Ar	IR	1
			1622.4			

HfD_2

$\tilde{X}$ $^3A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	HfD_2 a-stretch	1166.7	Ar	IR	1
			1161.0			

Reference

[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. **99**, 15004 (1995).

FeH_2

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

$\tilde{X}$ $^5\Delta$ $D_{\infty h}$ Structure: LMR[5]

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	1674.72	gas	LMR	5
			1660.8	Ar	IR	2,4
			1647	Kr	IR	1,2
			1636	Xe	IR	1,2

$B_0=3.013$ LMR[5]

FeD_2

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

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

$\tilde{X}$ $^5\Delta$ $D_{\infty h}$

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	1204.2	Ar	IR	2,4
			1195	Kr	IR	2
			1188	Xe	IR	1

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CoH_2

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

$T_0 \cong 2600$ gas PE[1]

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

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	Bend	380	Ar	IR	2
	3	CoH a-stretch	1684.5	Ar	IR	2,3
			1647	Kr	IR	2

CoD_2

$T_0 \cong 2600$ gas PE[1]

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

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	3	CoD a-stretch	1223.4	Ar	IR	2,3
			1215	Kr	IR	2

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NiH_2

$T_0 \cong 1600$ gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	2200T	gas	PE	1
			2007	Ar	IR	2
			1985	Kr	IR	2
	2	Bend	771	Ar	IR	2
b_2	3	Asym. stretch	1969	Ar	IR	2
			1947	Kr	IR	2

NiD_2

$T_0 \cong 1600$ gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1445	Ar	IR	2
			1430	Kr	IR	2
	2	Bend	602	Ar	IR	2
b_2	3	Asym. stretch	1426	Ar	IR	2
			1411	Kr	IR	2

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PtH_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2349T	Ar	IR	1
			2314T	Kr	IR	1
			2168T	Ar	IR	1
			2158T	Kr	IR	1

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ZnH_2

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

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

ZnD_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	454.4	Ar	IR	2
Σ_u^+	3	ZnD_2 a-stretch	1357.2	Ar	IR	1,2
			1350.9	Kr	IR	1

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CdH_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	604.6	Ar	IR	1
			601.7			
Σ_u^+	3	CdH_2 a-stretch	1753.5	Ar	IR	1

CdD_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	434.2	Ar	IR	1
			432.5			
Σ_u^+	3	CdD_2 a-stretch	1264.4	Ar	IR	1

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NbH_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1611m	Ar	IR	1
	2	Bend	519ms	Ar	IR	1
b_2	3	Asym. stretch	1569s	Ar	IR	1

NbD_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1154m	Ar	IR	1
	2	Bend	373ms	Ar	IR	1
b_2	3	Asym. stretch	1128s	Ar	IR	1

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HgH_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	773.0	Ar	IR	1
			771.1			
			769.7			
			769.2	Kr	IR	1
			772.5	H_2	IR	1
			781.0	N_2	IR	2
Σ_u^+	3	Asym. stretch	1895.8	Ar	IR	1
			1895.4			
			1893.1	Kr	IR	1
			1891.2			
			1889.2			
			1902.7	H_2	IR	1
			1943.7	N_2	IR	2

HgD_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	555.2	Ar	IR	1
			553.3			
			555.8	D_2	IR	1
			553.3			
			561.3	N_2	IR	2
Σ_u^+	3	Asym. stretch	1365.4	Ar	IR	1
			1363.6			
			1362.8			
			1368.5	D_2	IR	1
			1395.6	N_2	IR	2

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ThH_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1480.1	Ar	IR	1
b_2	3	Asym. stretch	1455.6	Ar	IR	1

ThD_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1055.6	Ar	IR	1
b_2	3	Asym. stretch	1040.3	Ar	IR	1

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UH_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1406.1	Ar	IR	1
			1399.0			
			1392.2			
b_2	3	Asym. stretch	1370.7	Ar	IR	1
			1365.3			
			1360.6			

UD_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1003.5	Ar	IR	1
			998.3			
			992.5			
b_2	3	Asym. stretch	978.7	Ar	IR	1
			975.7			
			972.5			

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AlH_2

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

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

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

B_0 $(cm^{-1}) = 3.57$ AB[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	AlH s-stretch	1770.0m	Ar	IR	3–5
			1766vw	Kr	IR	2
	2	Bend	766.4m	Ar	IR	4,5
			760m	Kr	IR	2
b_2	3	AlH a-stretch	1806.6vs	Ar	IR	3–5
			1799w	Kr	IR	2

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

AlD_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	AlD s-stretch	1278.9	Ar	IR	3,4
			1275vw	Kr	IR	2
	2	Bend	554.1	Ar	IR	4
			560m	Kr	IR	2
b_2	3	AlD a-stretch	1325.0	Ar	IR	3,4
			1320w	Kr	IR	2

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GaH_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1727.6wm	Ar	IR	1,2
			1730.8	Kr	IR	1
	2	Bend	740.1wm	Ar	IR	2
b_2	3	Asym. stretch	1799.2vs	Ar	IR	1,2
			1796.4	Kr	IR	1

GaD_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1244.7	Ar	IR	1,2
			1244.2wm	Kr	IR	1
	2	Bend	528	Ar	IR	2
b_2	3	Asym. stretch	1303.3	Ar	IR	1,2
			1302.4s	Kr	IR	1

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InH_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1548.6wm	Ar	IR	1
	2	Bend	607.4wm	Ar	IR	1
b_2	3	Asym. stretch	1615.6vs	Ar	IR	1

InD_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1115.3	Ar	IR	1
	2	Bend	429.1	Ar	IR	1
b_2	3	Asym. stretch	1165.8	Ar	IR	1

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SiH_2^+

$\tilde{A}$ $^2B_1$(Π)

gas PF[1,2] $\tilde{A}-\tilde{X}$ 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

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

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

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

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

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

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

$\tilde{b}$ $^1B_1$[b] C_{2v} Structure: AB[3,29]
$T_0 = 10255(20)$ gas AB[1,3,27,44]LMR[21]LF[33,38,40,42,43] $\tilde{b}-\tilde{a}$ 465–920 nm

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

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

$\tilde{a}$ $^1A_1$[b] C_{2v} Structure: AB[3,29,31]
$T_0 = 3147(5)$ gas AB[1,3,27,28,44]LMR[21,26,30]PE[23,24]LF[32,38,40,42,43,45]SEP[32,34] $\tilde{b}-\tilde{a}$ 465–920 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s-stretch	2806.01(7)	gas	LF,LD,IR	10,20,31,40
	2	Bend	1352.6	gas	AB,LF	3,27,28,40
b_2	3	CH_2 a-stretch	2864.97(2)	gas	LD,IR	20,31

$\tau \cong 18$ s[c]
$A_0 = 20.118(2)$; $B_0 = 11.205(2)$; $C_0 = 7.069(2)$ AB[3,27,28]
Barrier to linearity = 8600(400) LF[45]

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

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

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

CD_2

4p C_{2v}
$T_0 = 74228$ gas MPI[37]

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

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

3d $^3A_2$ C_{2v} Structure: AB[7]
$T_0 = 70591.7$ gas AB[1]MPI[36] $3d\,^3A_2-\tilde{X}$ 141.6 nm
$B_0 = 3.595$ AB[1]

3p C_{2v}
$T_0 = 64082$ gas MPI[37]

$\tilde{b}$ $^1B_1$[b] C_{2v}
gas LF[13,41] $\tilde{b}-\tilde{a}$ 510–610 nm
$\tau(0,16,0) = 6.0(7)\,\mu s$ LF[13]

$\tilde{a}$ $^1A_1$[b] C_{2v}
$T_0 = 3140(50)$ gas PE[23]LF[41]SEP[41] $\tilde{b}-\tilde{a}$ 510–610 nm

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

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

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

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

$A_0 = 37.787$; $\frac{1}{2}(B+C)_0 = 3.962$; $\frac{1}{2}(B-C)_0 = 0.267$ LMR[18,22]MW[46]

[a] Value given for $^{13}CH_2$.
[b] The $\tilde{a}$ $^1A_1$ and $\tilde{b}$ $^1B_1$ states are perturbed by strong Renner–Teller interaction.[13,14,29,44] They are also strongly perturbed by interaction with the $\tilde{X}$ $^3B_1$ state.[27,28,35]
[c] Calculated value.[21]
[d] From analysis of perturbations involving combination bands.[31]

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SiH_2

$\tilde{A}\ ^1B_1$ [a] C_{2v} Structure: AB[1,2]
$T_0 = 15530.4(5)$ gas AB[1,2]LF[10,11,13] $\tilde{A}-\tilde{X}$ 480–650 nm
Onset of predissociation into Si (^1D) + H_2 near 21450.[11]

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

$\tau_0 = 1.10(17)\,\mu s$ gas LF[6,7,11]
$A_0 = 17.75$;[b] $B_0 = 4.9$;[b] $C_0 \cong 2.8$[b] AB[2]
Barrier to linearity $\cong 8000$[3]

$\tilde{a}\ ^3B_1$ C_{2v}
$T_0 = 7340(240)$[c] gas PI[8]
Barrier to predissociation into Si (^3S) + H_2 between 17070 and 17690.[11]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1978.51[d]	gas	LF	10,13,15
			1964[d]	Ar	IR	5
	2	Bend	999.03	gas	AB,LF	2,4,9,13
					DL	15
			995	Ar	IR	5
b_2	3	Asym. stretch	1954[e]	gas	LF	10,13,15
			1973	Ar	IR	5

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

SiD_2

$\tilde{A}\ ^1B_1$ [a] C_{2v}
$T_0 = 15539.875(2)$ gas LF[11,14] $\tilde{A}-\tilde{X}$ 463–652 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	618.55	gas	AB,LF	1,11,14

$A_0 = 9.629$; $B_0 = 2.456$; $C_0 = 1.926$ LF[14]
$\tau_0 = 0.93(38)\,\mu s$ gas LF[11]

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

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

$A_0 = 4.334$; $B_0 = 3.519$; $C_0 = 1.919$ LF[14]

[a] The $\tilde{A}\ ^1B_1$ and $\tilde{X}\ ^1A_1$ states are perturbed by strong Renner–Teller interaction.[3] The combined effects of Renner–Teller and spin-orbit interaction have been considered in detail by Ref. 12.
[b] Extrapolated values.[2]
[c] Possibly 6290(240).[8]
[d] In Fermi resonance with $2\nu_2$, observed for SiH_2 at 2005.7 (gas) and 1993 (Ar) and for SiD_2 at 1445 (Ar).
[e] $\frac{1}{2}(2\nu_3)$.
[f] ω.

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GeH_2

$\tilde{A}\ ^1B_1$ C_{2v} Structure: LF[4]

$T_0=16325.54(2)$ gas LF[2–4] $\tilde{A}-\tilde{X}$ 489–750 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1798.4	gas	LF	4
	2	Bend	783.0	gas	LF	2–4

$\tau_0=2.29(7)\,\mu s$ gas LF[3,4]

$A_0=16.415(21)$; $B_0=4.518(3)$; $C_0=3.460(4)$ LF[4]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		GeH stretch	1887wm	Ar	IR	1
		GeH stretch	1864wm	Ar	IR	1
a_1	2	Bend	913	gas	LF	2
			920wm	Ar	IR	1

$A_0=6.998(15)$; $B_0=6.531(8)$; $C_0=3.332(3)$ LF[4]

GeD_2

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

$T_0=16323$ gas LF[2,3] $\tilde{A}-\tilde{X}$ 535–700 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	563	gas	LF	2,3

$\tau_0=2.5(5)\,\mu s$ gas LF[3]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1338ms			
		GeD stretch	1329vs	Ar	IR	1
			1325vs			
a_1	2	Bend	659	gas	LF	2
			658m	Ar	IR	1

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NH_2^+

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

$T_0 \leqslant 20490(160)$[a] gas PE[1]

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

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

$T_0=10530(80)$ gas PI[2]

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

$\tilde{X}\ ^3B_1$ $D_{\infty h}$[b] Structure: LD[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	439T	gas	LD	4
Σ_u^+	3	Asym. stretch	3359.94	gas	LD	3,4

$B_0=7.959$ LD[4]

ND_2^+

$\tilde{a}\ ^1A_1$ 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

$\tilde{X}\ ^3B_1$ $D_{\infty h}$[b]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	330(30)H	gas	PE	1

[a]Corrected for revision[2] of first adiabatic ionization potential of NH_2.
[b]Quasilinear; barrier to linearity $<\frac{1}{2}\nu_2$.[4]

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NH_2

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

$\tilde{A}\ ^2A_1(\Pi_u)$ [a] C_{2v} Structure: AB[1,4]
$T_0 = 11122.6$ gas AB[1,8,22]LF[6,21,25,26]EM[25] $\tilde{A}-\tilde{X}$ 342–2700 nm
Ne,Ar,Kr,Xe[b] AB[2,3,5,27] $\tilde{A}-\tilde{X}$ 344–880 nm
N_2[b] AB[5] $\tilde{A}-\tilde{X}$ 480–620 nm

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

$\tau_{090\Sigma} = 10.0(1.7)\,\mu s$ gas LF[7]
$\tau_{080\Pi} = 10(3)\,\mu s$ 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.
$B_0 = 8.78$ AB[1]
Barrier to linearity = 730[14]

$\tilde{X}\ ^2B_1$ [a] C_{2v} Structure: AB[1]IR[29]

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

$A_0 = 23.693$; $B_0 = 12.952$; $C_0 = 8.173$ AB[1,8]LMR[13] IR[20,29] MW[28]
Barrier to linearity = 12024[14]

ND_2

$\tilde{A}\ ^2A_1(\Pi_u)$ [a] C_{2v}
gas AB[1] $\tilde{A}-\tilde{X}$ 500–680 nm
Ar AB[27] $\tilde{A}-\tilde{X}$ 380–825 nm

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

$B_0 = 4.41$ AB[1]

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

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

$A_0 = 13.342$; $B_0 = 6.488$; $C_0 = 4.290$ AB[1,18] LMR[11]MW[24]IR[29]

[a]The $\tilde{A}\ ^2A_1$ and $\tilde{X}\ ^2B_1$ states are perturbed by strong Renner–Teller interaction.
[b]A detailed comparison of the argon-matrix data with gas-phase data has been given in Refs. 22 and 27. Rotational structure is resolved in the rare-gas matrices. In nitrogen,[5] bands are very broad and red-shifted by approximately 400 cm^{-1}, with no evidence for rotational structure.
[c]Assigned[5] in matrix studies to ν_3. Gas-phase observation of ν_1 at 3219.37 cm^{-1} and demonstration[16] that ν_1 is more intense than ν_3 dictate reassignment to ν_1.

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PH_2

$\tilde{A}\ ^2A_1$ [a] C_{2v} Structure: AB^4
T_0=18276.569 gas $AB^{1,4,6}EM^{2,3,5}LF^{22,23}$ $\tilde{A}-\tilde{X}$ 360–880 nm
18215(4) Ar $AB^{13,19}$ $\tilde{A}-\tilde{X}$ 405–550 nm

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

τ=4(1)μs gas $LF^{11,20}EM^{12}$
A_0=20.414(5); B_0=5.607; C_0=4.293 $AB^{4,6}EM^5LF^{22,23}$
Barrier to linearity= 6840[7]

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

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

A_0=9.132; B_0=8.084; C_0=4.214 $AB^{4,16}LMR^{8,14,15}MW^{17,18}LF^{22}$
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
			797w	Ar	IR	13

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

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

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H_2O^+

$\tilde{B}\ ^2B_2$ C_{2v}
T_0=36757(12) gas PE^9

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

$\tilde{A}\ ^2A_1(\Pi_u)$ [b] $D_{\infty h}$ Structure: $PE^{4,7}EM^7$
T_{070}=13409.3 gas $EM^{1,5,17}AB^{14}$ $\tilde{A}-\tilde{X}$ 400–750 nm

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

τ=10.5(1.0)μs gas EF^6
B_{070}=8.57 EM^5

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

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

A_0=29.036(2); B_0=12.423; C_0=8.469 $LMR^8LD^{11}DL^{12}CC^{15}$
Barrier to linearity $\leqslant$9187[7,17]

D_2O^+

$\tilde{B}\ ^2B_2$ C_{2v}
T_0= 37430(50) gas PE[2,4]
38498(12) gas PE[9]

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

$\tilde{A}\ ^2A_1(\Pi_u)$ [b] $D_{\infty h}$
T_{050}[c]=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
			2326.7	Ne	IR	16
	2	Bend	1044.27(5)	gas	EM	10
			1040.5	Ne	IR	16
b_2	3	Asym. stretch	2392.7	Ne	IR	16

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

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

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H_2S^+

$\tilde{B}\ ^2B_2$ C_{2v}
T_0=34770(160) gas PE[2]

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

$\tilde{A}\ ^2A_1$ [a] C_{2v} Structure: EF[3]
T_0=18518 gas EF[1,3]PE[2,5,6] $\tilde{A}-\tilde{X}$ 400–500 nm
Predissociated above 23300 into H_2+S^+.[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	2600T	gas	PE	6
	2	Bend	950(5)	gas	PE	2,5,6

τ=4.2(4)μs gas EF[4]
B_{020}=5.03 EF[3]
Barrier to linearity ≅4600[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	2490(5)	gas	PE	6
	2	Bend	1159.0	gas	EF,PE	3,6

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

D_2S^+

$\tilde{A}\ ^2A_1$ C_{2v}
T_0=18574 gas EF[3] $\tilde{A}-\tilde{X}$ 400–500 nm
B_{030}=2.46 EF[3]

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

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

A_0=5.37(2); B_0=4.32(1); C_0=2.34(2) EF[3]
[a]The $\tilde{A}\ ^2A_1$ and $\tilde{X}\ ^2B_1$ states are perturbed by strong Renner–Teller interaction.

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HXeH

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	700.8	Xe	IR	1
Σ_u^+	3	Asym. stretch	1180.6 1165.9	Xe	IR	1,2

DXeD

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	513.5wT	Xe	IR	1
Σ_u^+	3	Asym. stretch	856.2 845.8	Xe	IR	1

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8.2. Triatomic Monohydrides

Li_2H

$\tilde{B}'$

gas MPI[3] $\tilde{B}'-\tilde{X}$ 360–380 nm

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

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

A_0=6.87; B_0=0.455; C_0=0.427 MPI[1,2]

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

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BeBeH

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BeH stretch	2013.7	Ar	IR	1
Π	2	Bend	540.0	Ar	IR	1

BeBeD

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BeD stretch	1504.2	Ar	IR	1

Reference

[1] T. J. Tague, Jr. and L. Andrews, J. Am. Chem. Soc. **115**, 12111 (1993).

ZnZnH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	ZnH stretch	1657.6	Ar	IR	1

ZnZnD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ZnD stretch	1198.6	Ar	IR	1

Reference

[1] T. M. Greene, W. Brown, L. Andrews, A. J. Downs, G. V. Chertihin, N. Runeberg, and P. Pyykkö, J. Phys. Chem. **99**, 7925 (1995).

CdCdH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CdH stretch	1521.0	Ar	IR	1

CdCdD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CdD stretch	1098.0	Ar	IR	1

Reference

[1] T. M. Greene, W. Brown, L. Andrews, A. J. Downs, G. V. Chertihin, N. Runeberg, and P. Pyykkö, J. Phys. Chem. **99**, 7925 (1995).

TiCH

$\tilde{A}\ ^2\Pi$ $C_{\infty v}$
gas LF[1] $\tilde{A}-\tilde{X}$ 620–725 nm

$\tilde{X}\ ^2\Sigma^+$ $C_{\infty v}$ Structure: LF[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	578(5)	gas	LF	1
Σ^+	3	TiC stretch	855(5)	gas	LF	1

B_0=0.486 LF[1]

TiCD

$\tilde{A}\ ^2\Pi$ $C_{\infty v}$
gas LF[1] $\tilde{A}-\tilde{X}$ 620–725 nm

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	442(5)	gas	LF	1
Σ^+	3	TiC stretch	815(5)	gas	LF	1

B_0=0.416 LF[1]

Reference

[1] M. Barnes, A. J. Merer, and G. F. Metha, J. Mol. Spectrosc. **181**, 168 (1997).

VCH

$\tilde{A}$
gas LF[1] $\tilde{A}-\tilde{X}$ 600–810 nm

$\tilde{X}\ ^3\Delta_1$ $C_{\infty v}$ Structure: LF[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	564	gas	LF	1
Σ^+	3	VC stretch	838	gas	LF	1

Spin-orbit splitting=139 gas LF[1]
B_0=0.494 LF[1]

VCD

$\tilde{A}$
gas LF[1] $\tilde{A}-\tilde{X}$ 600–810 nm

$\tilde{X}\ ^3\Delta_1$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	442	gas	LF	1
Σ^+	3	VC stretch	813	gas	LF	1

B_0=0.422 LF[1]

Reference

[1] M. Barnes, P. G. Hajigeorgiou, R. Kasrai, A. J. Merer, and G. F. Metha, J. Am. Chem. Soc. **117**, 2096 (1995).

WCH

$\tilde{C}\ ^2\Phi_{5/2}$ $C_{\infty v}$
T_0=14109.7 gas LF[1] $\tilde{C}-\tilde{X}$ 652–709 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	554	gas	LF	1
Σ^+	3	WC stretch	862	gas	LF	1

B_0=0.392 LF[1]

$\tilde{B}\ ^2\Pi_{1/2}$ $C_{\infty v}$
T_0=13391.7 gas LF[1] $\tilde{B}-\tilde{X}$ 680–747 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	505	gas	LF	1
Σ^+	3	WC stretch	819	gas	LF	1

B_0=0.392 LF[1]

$\tilde{A}\ ^2\Delta_{3/2}$ $C_{\infty v}$ Structure: LF[1]
T_0=12090.3 gas LF[1] $\tilde{A}-\tilde{X}$ 749–827 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	489	gas	LF	1
Σ^+	3	WC stretch	936	gas	LF	1

B_0=0.395 LF[1]

$\tilde{a}\ ^4\Sigma^-$ $C_{\infty v}$
T_0=813 gas LF[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	612(5)	gas	LF	1
Σ^+	3	WC stretch	971(5)	gas	LF	1

B_0=0.41T LF[1]

$\tilde{X}\ ^2\Delta_{3/2}$ $C_{\infty v}$ Structure: LF[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	660(5)	gas	LF	1
Σ^+	3	WC stretch	1006(5)	gas	LF	1

B_0=0.408 LF[1]

WCD

$\tilde{C}\ ^2\Phi_{5/2}$ $C_{\infty v}$
T_0=14079.8 gas LF[1] $\tilde{C}-\tilde{X}$ 652–710 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	576	gas	LF	1
Σ^+	3	WC stretch	670T	gas	LF	1

B_0=0.336 LF[1]

$\tilde{B}\ ^2\Pi_{1/2}$ $C_{\infty v}$
T_0=13416.4 gas LF[1] $\tilde{B}-\tilde{X}$ 680–746 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	450	gas	LF	1
Σ^+	3	WC stretch	809	gas	LF	1

B_0=0.328(2) LF[1]

$\tilde{A}\ ^2\Delta_{3/2}$ $C_{\infty v}$
T_0=12122.4 gas LF[1] $\tilde{A}-\tilde{X}$ 749–825 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	376	gas	LF	1
Σ^+	3	WC stretch	896	gas	LF	1

B_0=0.337 LF[1]

$\tilde{a}\ ^4\Sigma^-$ $C_{\infty v}$
T_0=834 gas LF[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	451(5)	gas	LF	1
Σ^+	3	WC stretch	930(5)	gas	LF	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	501(5)	gas	LF	1
Σ^+	3	WC stretch	953(5)	gas	LF	1

B_0=0.347 LF[1]

Reference

[1] M. Barnes, D. A. Gillett, A. J. Merer, and G. F. Metha, J. Chem. Phys. **105**, 6168 (1996).

ScNH

$\tilde{A}\ ^2\Pi$ $C_{\infty v}$
T_0=15023.033 gas LF[1]
A=102.23 gas LF[1]
B_0 = 0.424 LF[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	511(5)	gas	LF	1
Σ^+	3	ScN stretch	935(5)	gas	LF	1

B_0=0.441 LF[1]

ScND

$\tilde{A}\ ^2\Pi_{1/2}$ $C_{\infty v}$
T_0=14952 gas LF[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	391(5)	gas	LF	1
Σ^+	3	ScN stretch	877(5)	gas	LF	1

Reference

[1] T. C. Steimle, J. Xin, A. J. Marr, and S. Beaton, J. Chem. Phys. **106**, 9084 (1997).

BeOH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BeO stretch	1245.5T	Ar	IR	1

Reference

[1] C. A. Thompson and L. Andrews, J. Phys. Chem. **100**, 12214 (1996).

MgOH

$\tilde{X}\ ^2\Sigma^+$ $C_{\infty v}$ Structure: MW[1,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	188(2)H	gas	LF	2
Σ^+	3	MgO stretch	750(3)	gas	LF	2

B_0=0.494 MW[1]

MgOD

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	130(2)H	gas	LF	2

B_0=0.448 MW[1,3]

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CaOH

$\tilde{G}$ $^2\Pi$ $C_{\infty v}$
T_0=32630.2 gas DR[22]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	311	gas	DR	22

B_0=0.347 DR[22]

$\tilde{F}$ C_s
T_0=30215 gas LF,MPI[21]

$\tilde{E}$ $^2\Sigma^+$ $C_{\infty v}$
T_0=29879 gas LF,MPI[21] $\tilde{E}-\tilde{X}$ 326–335 nm

$\tilde{D}$ $^2\Sigma^+$ $C_{\infty v}$ Structure: LF[21]
T_0=28153 gas LF,MPI[21] $\tilde{D}-\tilde{X}$ 335–355 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	412(2)	gas	LF,MPI	21
Σ$^+$	3	CaO stretch	674.0(1.5)	gas	LF,MPI	21

B_0=0.364 LF[21]

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

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

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

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

$\tilde{A}$ $^2\Pi$ $C_{\infty v}$ Structure: LF[3,20]
T_0=15998.122 gas CL^{2}LF[3,6,8,10,13,16,17,20] $\tilde{A}-\tilde{X}$ 600–650 nm
Absorption maximum at 16096(15) in a krypton matrix.[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	361.36[a]	gas	LF	13,16,18
Σ$^+$	3	CaO stretch	630.68[a]	gas	LF	13

A=66.818 gas LF[3,6,17]
$\varepsilon\omega_2$=−36.26 gas LF[13,16,18]
B_0=0.341 LF[3,6]

$\tilde{X}$ $^2\Sigma^+$ $C_{\infty v}$ Structure: LF[3,7,20]MW[19]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ$^+$	1	OH stretch	3778	gas	LF	21
Π	2	Bend	352.93	gas	LF	11,12,16 18
Σ$^+$	3	CaO stretch	609.02	gas	LF	3,11

B_0=0.334 LF[3,4,6,12,16]MW[9]MODR[15]

CaOD

$\tilde{G}$ $^2\Pi$ $C_{\infty v}$
T_0=32628.3 gas DR[22]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	267	gas	DR	22

B_0=0.327 DR[22]

$\tilde{C}$ $^2\Delta$ $C_{\infty v}$
T_0=21907.128 gas LF[12,14] $\tilde{C}-\tilde{X}$ 440–470 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	235.38	gas	LF	12
Σ$^+$	3	CaO stretch	549	gas	LF	12

A_0=11.494 gas LF[12]
B_0=0.294 LF[12]

$\tilde{B}$ $^2\Sigma^+$ $C_{\infty v}$
T_0=18013.894(4) gas LF[7]
B_0=0.307 LF[7]

$\tilde{A}$ $^2\Pi$ $C_{\infty v}$
T_0=15995.016 gas LF[3,8,17,20]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	273.33	gas	LF	18
Σ$^+$	3	CaO stretch	623(2)[b]	gas	LF	3

A_0=66.762 LF[17]
$\varepsilon\omega_2$=−26.96 LF[18]
B_0=0.309 LF[3,17]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ$^+$	1	OD stretch	2790	gas	LF	21
Π	2	Bend	266.84	gas	LF	11,12,18
Σ$^+$	3	CaO stretch	604.90	gas	LF	3,11

B_0=0.303 LF[3,7,8,12,17]MW[19]

[a] The Fermi resonance between ν_3 and $2\nu_2$ is analyzed by Ref. 13.
[b] $\omega_1+\frac{1}{2}x_{13}$.

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CaSH

$\tilde{C}\ ^2A'$ C_s
T_0=16082 gas LF^1 $\tilde{C}-\tilde{X}$ 597–647 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CaS stretch	312	gas	LF	1

$\tilde{B}\ ^2A''$ C_s
T_0=15859.4638(15) gas LF^1LS^3 $\tilde{B}-\tilde{X}$ 607–659 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CaS stretch	320	gas	LF	1

A_0=10.434; B_0=0.143; C_0=0.141 LS^3

$\tilde{A}\ ^2A'$ C_s Structure: LF^2
T_0=15380.2847(2) gas $LF^{1,2}$ $\tilde{A}-\tilde{X}$ 626–679 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CaS stretch	318	gas	LF	1

A_0=9.091; B_0=0.147; C_0=0.145 LF^2

$\tilde{X}\ ^2A'$ C_s Structure: LF^2MW^4

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CaS stretch	326	gas	LF	1

A_0=9.694; B_0=0.142; C_0=0.140 LF^2MW^4

CaSD

$\tilde{X}\ ^2A'$ C_s
A_0=4.987; B_0=0.139; C_0=0.135 MW^4

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SrOH

$\tilde{B}\ ^2\Sigma^+$ $C_{\infty v}$ Structure: LF^3
T_0=16377.505(1) gas $CL^2LF^{3,7,11}$ $\tilde{B}-\tilde{X}$ 580–611 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	400.84	gas	LF	3,11
Σ^+	3	SrO stretch	533.7	gas	LF	15

B_0=0.252 LF^3

$\tilde{A}\ ^2\Pi$ $C_{\infty v}$
T_0=14674.332(2) gas $CL^2LF^{6,7,12,13}$ $\tilde{A}-\tilde{X}$ 645–695 nm
Absorption maximum at 14598(15) in a krypton matrix.[4] An incompletely resolved absorption at 14777(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.
Π	2	Bend	381.36	gas	LF	12
Σ^+	3	SrO stretch	542.6	gas	LF	6,13

A=263.93 gas $LF^{6,13}$
ε=−0.0791 gas LF^{12}
B_0=0.254 gas LF^6

$\tilde{X}\ ^2\Sigma^+$ $C_{\infty v}$ Structure: LF^3MW^9

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	OH stretch	3766(10)	gas	LF	8
Π	2	Bend	363.69	gas	LF	3,6,11
Σ^+	3	SrO stretch	526.99	gas	LF	3,6,13
			479.3	Ar	IR	5

B_0=0.249 $LF^{3,6,10}MW^{9,10}$

SrOD

$\tilde{B}\ ^2\Sigma^+$ $C_{\infty v}$ Structure: LF^3
T_0=16366.0983 gas $LF^{3,14}$ $\tilde{B}-\tilde{X}$ 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	523.65	gas	LF	3,14

B_0=0.228 $LF^{3,14}$

$\tilde{X}\ ^2\Sigma^+$ $C_{\infty v}$ 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
			470.6	Ar	IR	5

B_0=0.225 LF[3,14]MW[9]

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ZnOH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		^{64}ZnO stretch	649.6	Ar	IR	1,2

ZnOD

$\tilde{X}$

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

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HNB

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NH stretch	3693.7	Ar	IR	1,2
Π	2	Bend	432.5	Ar	IR	2
Σ^+	3	NB stretch	1829.6	Ar	IR	2

DNB

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	ND stretch	2777.4	Ar	IR	1,2
	3	NB stretch	1776.1	Ar	IR	2

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HBS^+

$\tilde{B}\ ^2\Sigma^+$ $C_{\infty v}$
T_0=38000(1000) gas PE[2,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BH stretch	2190(100)	gas	PE	2,3

$\tilde{A}\ ^2\Sigma^+$ $C_{\infty v}$ Structure: PE[2,3,6]
T_0=19827 gas EM[1]EF[4] $\tilde{A}-\tilde{X}$ 479–635 nm

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

$\tau \geqslant$2300(200) ns gas EF[5]
B_0=0.615[a] EM[1]

$\tilde{X}\ ^2\Pi_{3/2}$ $C_{\infty v}$ Structure: PE[2,3,6]

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

$A_{010}=-321.4$, $\varepsilon\omega_2=-45(1)$.[4]
B_0 = 0.576[a] EM[1]

DBS$^+$

$\tilde{A}$ $^2\Sigma^+$ $C_{\infty v}$
T_0=19913 gas EF[4] $\tilde{A}$–$\tilde{X}$ 462–646 nm

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

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

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

[a]From analysis of bands originally attributed to BS and reassigned by Ref. 4 to HBS$^+$.
[b]975.9(4) in $\tilde{X}$ $^2\Pi_{1/2}$ state.
[c]937.4(4) in $\tilde{X}$ $^2\Pi_{1/2}$ state.

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HCC

3$p\sigma$ Rydberg state[a] $C_{\infty v}$
T_0=72100(1300) gas MPI[34]

T_0=51387(25)T Ar AB[8] 195–160 nm

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

$\tilde{B}$ $^2A_1'$? C_s
gas LF[35,36,40]EM[39] $\tilde{B}$–$\tilde{X}$ 250–313 nm

Approximately 20 emission bands of HCC have been assigned to transitions between a few common upper-state energy levels and HCC ($\tilde{X}$) with appreciable bending excitation. Analysis of these bands has yielded accurate vibrational and rotational constants for several highly excited ground-state vibrational levels. However, a definitive assignment of the upper-state energy levels has not been achieved.
$\tau \cong$ 120 ns gas LF[36]

$T_0 \leqslant$29360 Ar AB[2,8]
An absorption band system between 340 and 246 nm, with band spacings of approximately 2700, 1300 and 840 cm^{-1}, which has been observed on vacuum UV photolysis of C_2H_2 in an argon matrix, is tentatively attributed to HCC.

$\tilde{A}$ $^2\Pi$ $C_{\infty v}$
T_0^c=3692.61 gas CC[10,14]PE[32]
3685.8 Ne AB[38]
3732 Ar AB[21,38]

In neon and argon matrices, a complicated absorption band system of HCC extends from approximately 3600 to 9000.[21,38] This band system is extensively perturbed by high vibrational levels of the ground state. A few of the individual bands have been observed in the gas phase by color-center laser absorption,[10,14,29] by high resolution emission spectroscopy,[24] or by time-resolved emission spectroscopy.[30] Because of the extensive perturbations and because of the high energy input in the gas-phase studies, high ground-state vibrational levels are prominent both in the gas phase[10,14,19,26,27,32,37,40–42] and in neon and argon matrices.[20,21,38]
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.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	CC stretch	1706.2T	Ne	AB	38

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3298.85T	gas	CC	29
Π	2	Bend	371.60[d]	gas	DL	26,27
Σ^+	3	CC stretch	1840.57	gas	DL	23
			1835.5	Ne	IR	38
			1846.2m	Ar	IR	1,3,20,21

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

DCC

3$p\sigma$ Rydberg state[a] $C_{\infty v}$
T_0=72100(1300) gas MPI[34]

T_0=51493(25)T Ar AB[8] 194–170 nm

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

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

$\tilde{A}$ $^2\Pi$ $C_{\infty v}$
T_0<3800 Ar AB[21]
A complicated absorption band system extends to approximately 9700 in neon and argon-matrix studies of DCC.[21,38] As for HCC, the band system is extensively perturbed by high vibrational levels of the ground state. A few

of the bands, some of which arise from excited ground-state vibrational energy levels, have been studied in the gas phase using infrared laser absorption.[22,29,33]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2537.1	Ne	IR	38
Σ^+	3	CC stretch	1743.18	gas	DL	25
			1739.6	Ne	IR	38
			1746.3m	Ar	IR	1,3,20,21

B_0=1.203 MW[16]

[a]Tentative assignment.
[b]Observed band spacing; $2\nu_2$ if upper state is linear.
[c]The $\tilde{A}(000)$ band of HCC is strongly perturbed by high vibrational energy levels of the ground state which possess $^2\Pi$ vibronic symmetry. Accordingly, there is extensive mixing of the $^2\Pi$ vibronic levels in this spectral region, and designation of the band origin is approximate.[10,14,38,41]
[d]Derived from $(\nu_2+\nu_3)-[(\nu_2+\nu_3)-\nu_2]$. The detailed assignment of $(\nu_2+\nu_3)$ is given in Ref. 27 and that of $(\nu_2+\nu_3)-\nu_2$ in Ref. 26.

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AlOH

$\tilde{B}$

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

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

$\tilde{A}$

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

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

$\tilde{X}\ ^1\Sigma^+$ $C_{\infty v}$ Structure: MW[5]

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

B_0=0.525 MW[5]

AlOD

$\tilde{B}$

T_0=41706 gas MPI[4]

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

$\tilde{A}$

T_0=40025 gas MPI[4]

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

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

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

B_0=0.473 MW[5]

[a]ω.

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InOH

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

β $^3A''$ [a] C_s Structure: LF[3]

T_0=27188.00 gas LF[3] 345–377 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	829.6(4)	gas	LF	3
	3	InO stretch	496.9	gas	LF	3

$\tau>2.3\mu$s gas LF[3]
A=20.13; $\frac{1}{2}(B+C)$=0.273 LF[3]

α $^3A'$ [a] C_s Structure: LF[3]

T_0=26914.34 gas LF[3] 345–377 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	820.41(3)	gas	LF	3

$\tau>2.3$ μs gas LF[3]
A=26.70(3); $\frac{1}{2}(B+C)$=0.271 LF[3]

$\tilde{X}$ $^1A'$ C_s Structure: LF[3]MW[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	378(2)	gas	LF	3
			421.8	Ar	IR	1
	3	InO stretch	542(5)	gas	LF	3
			522.8	Ar	IR	1

A_0=42.049; B_0+C_0=0.535; B_0-C_0=0.002 LF[3]MW[5]

InOD

β $^3A''$ [a] C_s

T_0=27130.97 gas LF[3] 345–377 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	609.2(3)	gas	LF	3
	3	InO stretch	491.9(2)	gas	LF	3

A=11.20; $\frac{1}{2}(B+C)$=0.255 LF[3]

α $^3A'$ [a] C_s

T_0=26862.42 gas LF[3] 345–377 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	604.1(2)	gas	LF	3
	3	InO stretch	489.5(2)	gas	LF	3

A=13.73(7); $\frac{1}{2}(B+C)$=0.252 LF[3]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	301(5)	gas	LF	3
	3	InO stretch	524(9)	gas	LF	3
			595.7	Ar	IR	1

A_0=20.637; B_0+C_0=0.490 LF[3]MW[5]

[a]Components of the $\tilde{a}$ $^3\Pi$ state, split by strong Renner–Teller interaction.[4]

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HSiN

In an argon matrix, absorption maxima at 42000, 38800, 37600, and 28600 (238, 258, 266, and 350 nm) have been assigned[1] to HSiN.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	SiH stretch	2152.2m	Ar	IR	1
Σ^+	3	SiN stretch	1162.2s	Ar	IR	1

DSiN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	SiD stretch	1580.5wm	Ar	IR	1
Σ^+	3	SiN stretch	1145.4s	Ar	IR	1

Reference

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HCO^+

$\tilde{X}$ $C_{\infty v}$ Structure: MW[2–4,15]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3088.74	gas	LD,CC	5,6,16,17
Π	2	Bend	829.72	gas	DL	10,11
Σ^+	3	CO stretch	2183.95	gas	DL	7,8,14

B_0=1.488 MW[2–4]

DCO^+

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

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

B_0=1.201 MW[2–4]

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HCS^+

$\tilde{X}$ $C_{\infty v}$ Structure: MW[6]

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

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

DCS^+

B_0=0.601 MW[6]

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HNC

$\tilde{A}$ [a]

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

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

$\tilde{X}$ $C_{\infty v}$ Structure: MW[4,5,9,12]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NH stretch	3652.66	gas	IR,EM	3,6,8,11
			3643.1	Ne	IR	10
			3620s	Ar	IR	2
			3583s N_2	Ar	IR	1,2
			3567s	N_2	IR	2
Π	2	Bend	464.24	gas	IR	8
			477s	Ar	IR	2
			535s N_2	Ar	IR	1
			559s	N_2	IR	2
Σ^+	3	NC stretch	2023.86	gas	IR	8
			2025.4	Ne	IR	10
			2029w	Ar	IR	2
			2032w N_2	Ar	IR	1
			2035w	N_2	IR	2

B_0=1.512 MW[4]IR[8]

DNC

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	ND stretch	2787.07	gas	IR	3,6
			2780.7	Ne	IR	10
			2769s	Ar	IR	2
			2733s N_2	Ar	IR	1
			2728s	N_2	IR	2
Π	2	Bend	374s	Ar	IR	2
			413s N_2	Ar	IR	1
			432s	N_2	IR	2
Σ^+	3	NC stretch	1938.7	Ne	IR	10
			1940w	Ar	IR	2
			1940w N_2	Ar	IR	1
			1937w	N_2	IR	2

B_0=1.273 MW[4]

[a]Tentative identification.

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HNSi

In an argon matrix, has a weak absorption maximum near 40000 (250 nm).[5]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NH stretch	3588.44	gas	EM	2,4
			3583	Ar	IR	1,5
Π	2	Bend	523	Ar	IR	1,5
Σ^+	3	NSi stretch	1198	Ar	IR	1,5

B_0 = 0.634 gas EM[2,4]MW[3]

DNSi

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

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

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HCO

4*p* $^2\Pi(A'')$ C_s
T_0=64073.5 gas DR[40,42]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	863.8(5)	gas	DR	40,42

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

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

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

$\tilde{B}\ ^2A'$ C_s Structure: MPI,LF[40]

T_0=38695.48 gas EM[6]LF[25,30,33,35,36,39,43]MPI[29]SEP[30,35] $\tilde{B}-\tilde{X}$ 235–475 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

Lifetime measurements[32,35,37,38] give evidence for predissociation. Large decrease in fluorescence quantum yield above 41465.[33]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	2596.4(2)	gas	EM,LF	6,25,30,33
					MPI	29
			2570(29)	Ar	AB	5,11
			2570(29)	CO	AB	5
	2	Mixed	1380.9(2)	gas	LF,MPI	25,29,30
						33
			1375(35)	Ar	AB	5,11
			1375(35)	CO	AB	5
	3	Mixed	1065.9(2)	gas	LF,MPI	25,29,30
						33
			1035(35)	Ar	AB	5,11
			1035(35)	CO	AB	5

A_0=15.976; $\frac{1}{2}(B_0+C_0)$=1.151; $\frac{1}{4}(B_0-C_0)$=0.021 LF[35,43]
τ_0=89(2) ns gas LF[27,32,35,37,38]

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

T_0=9297(3) gas AB[1,3,8]LF[24,26]DM[31]CR[41] $\tilde{A}-\tilde{X}$ 460–860 nm

Bands with K′>0 are diffuse.

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

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

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

Vibrational term energies up to 20777 have been reported by Ref. 36.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	2434.48	gas	LF,PE	17,18,25
					DL,LD	22,26
					IR	23
			2483m	Ar	IR	5
			2488m	CO	IR	4
	2	Bend	1080.76	gas	UV,LS	1,3,8
					LMR	9,10
					LF	25,26
			1087s	Ar	IR	5
			1090s	CO	IR	2,4
	3	CO stretch	1868.17	gas	IR	12,23
					LMR	13,25
			1863vs	Ar	IR	5
			1861vs	CO	IR	2,4

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

DCO

$4p\ ^2\Pi(A'')$ C_s

T_0=64033.3 gas DR[40,42]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	677.3(5)	gas	DR	40,42

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

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

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

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

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

T_0=38628.4(2.0) gas MPI[29]LF[34,40] $\tilde{B}-\tilde{X}$ 250–450 nm
38568(70) Ar AB[5] $\tilde{B}-\tilde{X}$ 200–260 nm
38569(35) CO AB[5] $\tilde{B}-\tilde{X}$ 204–260 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CD stretch	1944.2(2.0)	gas	MPI,LF	29,40,42
	2	Mixed	1212.9(2.5)	gas	MPI,LF	29,40,42
			1150(35)	Ar	AB	5
			1150(35)	CO	AB	5
	3	Mixed	922.1(1.6)	gas	MPI,LF	29,40,42
			925(35)	Ar	AB	5
			925(35)	CO	AB	5

A_0=9.172; B_0=1.093; C_0=0.974 LF[40]

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

T_0=9162(3) gas UV[1,3,8]LF[24,26] $\tilde{A}-\tilde{X}$ 460–860 nm

Bands with K′>0 are diffuse.

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

B_0=1.10 UV[1,3,8]

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

Vibrational term energies up to 18186 have been reported by Ref. 42.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CD stretch	1909.77	gas	LMR,LF,SEP	14,26,40,42
			1926s	Ar	IR	5
			1937s	CO	IR	4
	2	Bend	846.5	gas	UV,LF,SEP	1,3,8,26,40,42
			850s	Ar	IR	5
			852s	CO	IR	2,4
	3	CO stretch	1794.59	gas	LMR,LF,SEP	14,26,40,42
			1803m	Ar	IR	5
			1800m	CO	IR	2,4

A_0=14.734; B_0=1.281; C_0=1.171 UV[1,3,8]MW[21]
[a]ω_2.

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HCF

$\tilde{E}\ ^1A'(3p)$ C_s
T_0=62154(2) gas MPI[15]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	1128(4)	gas	MPI	15
	3	CF stretch	1614(4)	gas	MPI	15

$\tilde{A}\ ^1A''$ C_s Structure: AB^1LF[5,6]
T_0=17277.47 gas AB^1CL^3LF[5,10] $\tilde{A}-\tilde{X}$ 429–635 nm
17320(15) Ar AB^2 $\tilde{A}-\tilde{X}$ 469–546 nm

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

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

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

$\tilde{a}\ ^3A''$ C_s
T_0=5210(140) gas $PE^{12,14}$

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

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

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

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

DCF

$\tilde{E}\ ^1A'(3p)$ C_s
T_0=62175(2) gas MPI[15]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CD stretch	2095(5)	gas	MPI	15
	2	Bend	872(3)	gas	MPI	15
	3	CF stretch	1582(4)	gas	MPI	15

$\tilde{A}\ ^1A''$ C_s
T_0=17293.426(3) gas CL^3LF^6 $\tilde{A}-\tilde{X}$ 460–585 nm

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

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

$\tilde{a}\ ^3A'$ C_s
T_0 <5140(700) gas PE^{12}

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

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

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

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

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HCCl

$\tilde{A}\ ^1A''$ C_s Structure: AB^8
T_0=12280.411(2) gas $AB^{1,8,9}LF^{4,7}$ $\tilde{A}-\tilde{X}$ 550–820 nm
Ar AB^2 $\tilde{A}-\tilde{X}$ 570–750 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	873.0	gas	AB	1,9
			855(50)	Ar	AB	2
	3	CCl stretch	987.4	gas	AB	9

Barrier to linearity=2250[1]
B_0=0.609 AB^8

$\tilde{a}\ ^3A''$ C_s
T_0=1470(880) gas $PE^{5,6}$

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

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	1201wm	Ar	IR	2
	3	CCl stretch	811.60	gas	DL	10
			815s	Ar	IR	2

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

DCCl

$\tilde{A}\ ^1A''$ C_s
T_0=12274 gas AB^1 $\tilde{A}-\tilde{X}$ 550–820 nm

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

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

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

A_0=8.75; B_0=0.557; C_0=0.525 AB^1

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HCBr

$\tilde{A}\ ^1A''$ C_s Structure: AB^4
T_{020}=12786.06 gas LF^3AB^4 $\tilde{A}-\tilde{X}$ 550–785 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	840T	gas	LF	3
	3	CBr stretch	783T	gas	LF	3

Barrier to linearity≤1600.
B_0=0.437 AB^4

$\tilde{a}\ ^3A''$ C_s
T_0=910(770) gas PE[1,2]

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

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

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

B_0=0.422 AB[4]

DCBr

$\tilde{A}\ ^1A''$ C_s
gas LF[3] $\tilde{A}-\tilde{X}$ 550–600 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	620T	gas	LF	3
	3	CBr stretch	769T	gas	LF	3

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HSiF

$\tilde{A}\ ^1A''$ C_s Structure: LF[3-6]
T_0=23260.02 gas LF[2-6] $\tilde{A}-\tilde{X}$ 390–470 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SiH stretch	1547	gas	LF	5,6
	2	Bend	558	gas	LF	2,5,6
	3	SiF stretch	857	gas	LF	5,6

τ_0=175(6) ns gas LF[2,5]
A_0=9.319; B_0=0.549; C_0=0.516 LF[3–5]
Barrier to linearity=9130(20) LF[5]

$\tilde{X}\ ^1A'$ C_s Structure: LF[3,4,6]

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

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

DSiF

$\tilde{A}\ ^1A''$ C_s
T_0=23338.723(6) gas LF[6] $\tilde{A}-\tilde{X}$ 383–453 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SiD stretch	1174.3	gas	LF	6
	2	Bend	424.8	gas	LF	6
	3	SiF stretch	854.4	gas	LF	6

A_0=5.086; B_0=0.518; C_0=0.467 LF[6]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SiD stretch	1387m	Ar	IR	1
	2	Bend	641.5	gas	LF	6
			638w	Ar	IR	1
	3	SiF stretch	833m	Ar	IR	1

A_0=3.997; B_0=0.549; C_0=0.481 LF[6]

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HSiCl

$\tilde{A}\ ^1A''$ C_s Structure: UV[1]LF[2]
T_0=20717.77 gas UV[1]LF[2] $\tilde{A}-\tilde{X}$ 410–600 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SiH stretch	1747.1	gas	LF	2
	2	Bend	563.9	gas	UV,LF	1,2
	3	SiCl stretch	532.3	gas	UV,LF	1,2

τ_0=432(20) ns gas LF[2]
A_0=9.840(2); B_0=0.247; C_0=0.240 UV[1]LF[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SiH stretch	1968.8(2)	gas	LF	2
	2	Bend	805.9(2)	gas	UV,LF	1,2
	3	SiCl stretch	522.8	gas	UV,LF	1,2

A_0=7.587; B_0=0.246; C_0=0.238 UV[1]LF[2]

DSiCl

$\tilde{A}\ ^1A''$ C_s
T_0=20773.43 gas UV^1LF^2 $\tilde{A}-\tilde{X}$ 410–600 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SiD stretch	1300.8	gas	LF	2
	2	Bend	408.6	gas	UV,LF	1,2
	3	SiCl stretch	543.2	gas	LF	2

τ_0=437(20) ns gas LF^2
A_0=5.269; B_0=0.235; C_0=0.224 UV^1LF^2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SiD stretch	1434.4	gas	LF	2
	2	Bend	592.3(3)	gas	LF	2
	3	SiCl stretch	518.1(2)	gas	LF	2

A_0=3.970; B_0=0.240; C_0=0.226 UV^1LF^2

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HSiBr

$\tilde{A}\ ^1A''$ C_s Structure: UV^1LF^2
T_0=19902.851(7) gas UV^1LF^2 $\tilde{A}-\tilde{X}$ 429–620 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SiH stretch	1787.0	gas	LF	2
	2	Bend	535.3	gas	UV,LF	1,2
	3	SiBr stretch	416.5	gas	UV,LF	1,2

A_0=9.897(2); B_0=0.159; C_0=0.155 UV^1LF^2
τ_0 = 598(18) ns gas LF^2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SiH stretch	1976.2(3)	gas	LF	2
	2	Bend	771.9(2)	gas	UV,LF	1,2
	3	SiBr stretch	412.4(2)	gas	UV,LF	1,2

A_0=7.576(8); B_0=0.158; C_0=0.155 UV^1LF^2

DSiBr

$\tilde{A}\ ^1A''$ C_s
T_0=19953.677(5) gas LF^2 $\tilde{A}-\tilde{X}$ 464–502 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SiD stretch	1325.6	gas	LF	2
	2	Bend	375.9	gas	LF	2
	3	SiBr stretch	434.3	gas	LF	2

τ_0=586(21) ns gas LF^2
A_0=5.274(3); B_0=0.151; C_0=0.146 LF^2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SiD stretch	1439.5	gas	LF	2
	3	SiBr stretch	408.0	gas	LF	2

A_0=3.956(3); B_0=0.153; C_0=0.148 LF^2

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HNO

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

$\tilde{A}\ ^1A''$ C_s Structure: $AB^{1,4}$
T_0=13154.37 gas $AB^{1,4,25}LF^{13,21}CL^{24}CR^{26}$ $\tilde{A}-\tilde{X}$ 544–770 nm
13118(2) Ar $AB^{2,3}$ $\tilde{A}-\tilde{X}$ 590–762 nm
Onset of predissociation at 16450(10). LF^{13}

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

τ=25(4) μs $LF^{12,14,23}$
A_0=22.161; B_0=1.327; C_0=1.241 $AB^{1,4,25}MODR^{11,17}$

$\tilde{a}\ ^3A''$ C_s
T_0=6280(160) gas PE^{15}

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

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

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

A_0=18.476; B_0=1.411; C_0=1.306 $AB^{1,25}MW^{7,19}IR^{10,16,22}$

DNO

T_0=48400 gas AB[5] 196–206 nm
Diffuse bands.

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

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

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

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

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

A_0=10.524; B_0=1.292; C_0=1.146 AB[1]MW[6,19]IR[10,16]

[a]Refined value from unpublished Fourier transform spectra.

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HSO^+

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1150(160)	gas	PI	1

Reference

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HNF

$\tilde{A}$ $^2A'$ C_s Structure: AB[3]LF[5,8]
T_0=20141.26(1) gas AB[1,3]CL[4]LF[5,7] $\tilde{A}$–$\tilde{X}$ 380–650 nm
20140(20) Ar AB[2] $\tilde{A}$–$\tilde{X}$ 395–497 nm
Onset of predissociation into NH+F identified at 23800(500) gas LF[5]PF[6]

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

τ_0=3.6 μs gas LF[5]
A_0=27.570(5); B_0=1.033; C_0=0.992 AB[3]

$\tilde{X}$ $^2A''$ C_s Structure: AB[3]LF[5,8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH stretch	3167(6)	gas	LF	7
	2	Bend	1439(3)	gas	CL,LF	4,7
			1432m	Ar	IR	2
	3	NF stretch	1020(8)	gas	LF	7
			1000s	Ar	IR	2

A_0=17.688(8); B_0=1.039; C_0=0.978 AB[3]

DNF

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

T_0=20169.10 gas LF[5,7,8] $\tilde{A}-\tilde{X}$ 400–500 nm

20220 Ar AB[2] $\tilde{A}-\tilde{X}$ 413–495 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	837.4(8)[a]	gas	LF	5
			798[b]	Ar	AB	2
	3	NF stretch	1124[c]	gas	LF	5

τ_0=3.5(2) μs gas LF[5]

A_0=15.665(6); $\frac{1}{2}(B_0+C_0)$=0.900; $\frac{1}{4}(B_0-C_0)$=0.015 LF[8]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ND stretch	2339(4)	gas	LF	7
	2	Bend	1075(3)	gas	LF	7
			1069[d]	Ar	IR	2
	3	NF stretch	1007(7)	gas	LF	7
			1000s	Ar	IR	2

A_0=9.49; $\frac{1}{2}(B_0+C_0)$=0.929; $\frac{1}{4}(B_0-C_0)$=0.023 LF[8]

[a]$\omega_2+0.5\ x_{12}$.
[b]Average value.
[c]$\omega_3+2x_{33}+0.5x_{13}$.
[d]Overlapped by NF_2 absorption.

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HO_2

Broad, unstructured gas-phase absorption between 200 and 280 nm, with maximum near 205 nm.[2,3,5,6,37]

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

T_0=7029.684(2) gas AB[9,15]EM[10,16,19,20,35] $\tilde{A}-\tilde{X}$ 1.13–2.12 μm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	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_0=20.486; B_0=1.021; C_0=0.968 EM[16,20,35]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3436.20	gas	LD	26
			3415.1	Ne	IR	36
			3412.5s[a]	Ar	IR	1,4,7
			3400	O_2	IR	32
	2	Bend	1391.75	gas	DL,IR	24,39
			1397.8	Ne	IR	36
			1388.5vs[a]	Ar	IR	1,4,7
			1392	O_2	IR	32
	3	OO stretch	1097.63	gas	LMR	18,29
					DL,IR	29,38,39
			1100.3	Ne	IR	36
			1101.1s[a]	Ar	IR	1,4,7
			1109	O_2	IR	32

A_0=20.356; B_0=1.118; C_0=1.056 LMR[8,11,12,18]MW[13,17,25]EM[16]IR[40]

DO_2

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

T_0=7041.1(1) gas AB[9]EM[10,19,21] $\tilde{A}-\tilde{X}$ 1.13–2.12 μm

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

A_0=11.147(7); B_0=0.970; C_0=0.887 EM[21]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2549.22	gas	LD,DL	31
			2529.2	Ne	IR	36
			2529.5m[a]	Ar	IR	1,4,7
			2521	O_2	IR	32
	2	Bend	1020.16	gas	LMR,DL	22,33
			1027.3	Ne	IR	36
			1019.9s[a]	Ar	IR	1,4,7
			1024	O_2	IR	32
	3	OO stretch	1121.47	gas	LMR, DL	22,33
			1124.7	Ne	IR	36
			1122.9vw[a]	Ar	IR	7

A_0=11.194; B_0=1.056; C_0=0.961 MW[14,27,34]EM[21]LMR[22,23,34]ESR[23]

[a]Refined value from unpublished Fourier transform spectra.

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HSO

$\tilde{A}\ ^2A'$ C_s Structure: LF[2,3]
T_0=14367 gas CL[1] $\tilde{A}-\tilde{X}$ 520–960 nm

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

τ_0=81(10) μs gas LF[6,9]
Values decrease as v_3' increases.
A_{003}=9.735; B_{003}=0.565; C_{003}=0.527 LF[2]

$\tilde{X}\ ^2A''$ C_s Structure: LF[2,3]MW[4]

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

A_0=9.990; B_0=0.684; C_0=0.638 LF[2]MW[4]

DSO

$\tilde{A}\ ^2A'$ C_s
T_0=14371 gas CL[1]LF[8] $\tilde{A}-\tilde{X}$ 520–960 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	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]
$A_0{}^b$=4.969(7); $B_0{}^b$=0.566; $C_0{}^b$=0.507 LF[7,8]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	770(10)	gas	CL	1
	3	SO stretch	1029(15)	gas	CL	1

A_0=5.295; B_0=0.662; C_0=0.586 LF[3]MW[4]

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

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HS_2

gas AB[1–3] 297–380 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SH stretch	2500T	gas	AB	3
	2	Bend	900T	gas	AB	3
	3	SS stretch	600T	gas	AB	3

$\tilde{A}\ ^2A'$ C_s
T_0=7255(7) gas CL[4] $\tilde{A}-\tilde{X}$ 950–2100 nm

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

A_0=9.7(5) CL[4]

$\tilde{X}\ ^2A''$ C_s Structure: MW[5]

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_0=9.906; B_0=0.267; C_0=0.259 MW[5]LMR[6]

DS_2

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

T_0=7264(15) gas CL[4] $\tilde{A}$–$\tilde{X}$ 950–2100 nm

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

A_0=5.184; B_0=0.260; C_0=0.247 MW[5]

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$HOBr^+$

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

T_0=6500(80) gas PI[1]TPE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	OBr stretch	670T	gas	PI,TPE	1,2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	OBr stretch	730(20)	gas	PI,TPE	1,2

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HOI^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	OI stretch	702(60)	gas	PI	1

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HOCl

$\tilde{X}$ C_s Structure: IR[2,14]MW[4,12]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3609.48	gas	IR	2,6,7,11,15
			3581	Ar	IR	3
	2	Bend	1238.62	gas	IR	1,5,6,8,9 11,13
			1239	Ar	IR	3
	3	OCl stretch	724.36	gas	IR	5,6,8,11,13
			728	Ar	IR	3

A_0=20.464; B_0=0.504; C_0=0.491 IR[2,11,15,16]MW[4,10]

DOCl

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2665.58	gas	IR	1,2,11,14
			2647	Ar	IR	3
	2	Bend	909.63	gas	IR	1,11,14
			911	Ar	IR	3
	3	OCl stretch	723.25	gas	IR	11,14
			728	Ar	IR	3

A_0=11.052; B_0=0.477; C_0=0.456 IR[2,14]MW[4,12]

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HOBr

In the gas phase, a prominent absorption maximum near 280 nm (35700) has been assigned[6,8] to HOBr.

In the gas phase, an absorption maximum near 350 nm (28600), with onset near 400 nm, has been assigned[6,8] to HOBr.

In the gas phase, a maximum in the production of OH near 440 nm (22700) is believed to arise from excitation of HOBr to a dissociative triplet state.[9]

$\tilde{X}$ C_s Structure: MW^3IR^7

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3614.90	gas	IR	2,7
			3590	Ar	IR	1
	2	Bend	1162.57	gas	IR	4
			1164	Ar	IR	1
	3	OBr stretch	620.2	gas	IR	2,4,5
			626.0	Ar	IR	1

A_0=20.470; B_0=0.353; C_0=0.346 MW^3IR^7

DOBr

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2652	Ar	IR	1
	2	Bend	854	Ar	IR	1
	3	OBr stretch	621.8	Ar	IR	1

A_0=11.027; B_0=0.331; C_0=0.321 MW^3

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HOI

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3625.84	gas	IR	2,3
			3597m	N_2	IR	1
	2	Bend	1069.8	gas	IR	2
			1075	Ar	IR	1
			1103m	N_2	IR	1
	3	OI stretch	577	Ar	IR	1
			575m	N_2	IR	1

A_0=20.935; B_0=0.279; C_0=0.275 EM^3

DOI

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2653	N_2	IR	1
	2	Bend	808	N_2	IR	1
	3	OI stretch	571	N_2	IR	1

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FHF^-

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

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

B_0=0.334 DL^5

FDF^-

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	588T	gas	DL	6
Π_u	2	Bend	928.73	gas	DL	6
			880m Cs	Ar	IR	1,2
Σ_u^+	3	Asym. stretch	934.19	gas	DL	6
			965s	Ar	IR	3,4
			969vs Cs	Ar	IR	1,2

B_e=0.342 DL^6

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$ClHCl^-$

An absorption maximum which appeared at 287 nm in argon-matrix studies[2] of the 122-nm photolysis of Ar:HCl or Ar:H_2O:Cl_2 samples and in argon-matrix studies[6] of the electron bombardment of Ar:HCl samples has been assigned to an electronic transition of $ClHCl^-$.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	263.4[b]	Ne	IR	8
			259.3[a,b]	Ar	IR	1–3,7
			252.8[b]	Kr	IR	7
			248.8[b]	Xe	IR	7
Σ_u^+	3	Asym. stretch	722.90	gas	DL	5
			737.9	Ne	IR	8
			728.9			
			695.6s[a]	Ar	IR	1–3,7
			662.8	Kr	IR	7
			644.1	Xe	IR	7

B_0=0.0974 DL[5]

$ClDCl^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	267[a,b]	Ar	IR	1–3
			255.3[b]	Kr	IR	7
Σ_u^+	3	Asym. stretch	496.2	Ne	IR	8
			489.3			
			463[a]	Ar	IR	1–3
			437.7	Kr	IR	7

[a]Attributed by Ref. 1 to the uncharged species. Reassigned to the anion by Ref. 2, and Ref. 3 demonstrated that the absorptions did not appear when the atoms were present but a supplementary high energy source suitable for inducing photoionization or electron transfer was not. The increase in the rate of isotopic exchange in the $^{37}Cl+H^{35}Cl$ reaction for vibrationally excited HCl[4] indicates that there is a potential barrier, rather than a minimum, for the ClHCl neutral species.
[b]$(\nu_1+\nu_3)-\nu_3$.

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$BrHBr^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	165.1[b]	Ne	IR	4
			163.1[b]			
			162.6[b]			
			164[a,b]	Ar	IR	1,2
			158.5[b]	Kr	IR	3
			151.9[b]	Xe	IR	3
Σ_u^+	3	Asym. stretch	752.9	Ne	IR	4
			745.4			
			741.2			
			728s[a]	Ar	IR	1,2
			686.6	Kr	IR	3
			645.6	Xe	IR	3

$BrDBr^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	163.9[b]	Ne	IR	4
			160.8[b]			
			170[a,b]	Ar	IR	1,2
			163.8[b]	Kr	IR	3
			157.9[b]	Xe	IR	3
Σ_u^+	3	Asym. stretch	516.5	Ne	IR	4
			510.7			
			507.6			
			498s[a]	Ar	IR	1,2
			465.5	Kr	IR	3
			434.6	Xe	IR	3

[a]Attributed in Ref. 1 to the uncharged species. Reassigned to the anion by Ref. 2. See $ClHCl^-$.
[b]$(\nu_1+\nu_3)-\nu_3$.

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IHI^-

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	115.2[b]	Ne	IR	4
			114.8[b]			
			121[a,b]	Ar	IR	1,2
			116.7[b]	Kr	IR	3
			109.0[b]	Xe	IR	3
Σ_u^+	3	Asym. stretch	671.8	Ne	IR	4
			653.3			
			644.7			
			682m[a]	Ar	IR	1,2
			647.4	Kr	IR	3
			580.8	Xe	IR	3

IDI^-

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	124[a,b]	Ar	IR	1,2
Σ_u^+	3	Asym. stretch	470m[a]	Ar	IR	1,2

[a]Attributed in Ref. 1 to the uncharged species. Reassigned by Ref. 2 to the anion. See $ClHCl^-$.
[b]$(\nu_1+\nu_3)-\nu_3$.

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HKrCl

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	HKr stretch	1476vs	Kr	IR	1
Π	2	Bend	544w	Kr	IR	1

DKrCl

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	DKr stretch	1106s	Kr	IR	1

Reference

[1]M. Pettersson, J. Lundell, and M. Räsänen, J. Chem. Phys. **102**, 6423 (1995).

HXeCl

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	HXe stretch	1664	Kr	IR	1
			1649	Xe	IR	1

DXeCl

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	DXe stretch	1198	Xe	IR	1

Reference

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HXeBr

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	HXe stretch	1524	Kr	IR	1
			1504vs	Xe	IR	1
Π	2	Bend	489w	Xe	IR	1

DXeBr

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	DXe stretch	1100s	Xe	IR	1

Reference

[1]M. Pettersson, J. Lundell, and M. Räsänen, J. Chem. Phys. **102**, 6423 (1995).

HXeI

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	HXe stretch	1193vs	Xe	IR	1
Π	2	Bend	450w	Xe	IR	1

DXeI

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	DXe stretch	893vs	Xe	IR	1

Reference

[1] M. Pettersson, J. Lundell, and M. Räsänen, J. Chem. Phys. **102**, 6423 (1995).

HAr_2^+ [a]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	237[b]	Ar	IR	5
Σ_u^+	3	Asym. stretch	905wm[c]	Ar	IR	1,2,4,5

DAr_2^+ [a]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	644s[c]	Ar	IR	1–5

[a]May be complexed with two or four additional Ar atoms.[2]
[b]$(\nu_1+\nu_3)-\nu_3$.
[c]Assigned in Ref. 1 to vibration of uncharged H (or D) atoms trapped in the Ar lattice. Reassigned by Ref. 2 to the cation. Peak at 644 cm^{-1} was prominent in deuteron radiolysis experiments.[3] Ref. 4 demonstrated that the absorptions did not appear when H or D atoms were present but a supplementary high energy source suitable for inducing photoionization or electron transfer was not.

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HKr_2^+ [a]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	155[b]	Kr	IR	4
Σ_u^+	3	Asym. stretch	853m[c]	Kr	IR	1–4

DKr_2^+ [a]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	165[b]	Kr	IR	4
Σ_u^+	3	Asym. stretch	606m[c]	Kr	IR	1,4

[a]May be complexed with two or four additional Kr atoms.[2]
[b]$(\nu_1+\nu_3)-\nu_3$.
[c]Assigned in Ref. 1 to vibration of uncharged H (or D) atoms trapped in the Kr lattice. Reassigned by Ref. 2 to the cation. Ref. 3 demonstrated that the 852 cm^{-1} absorption did not appear when H atoms were present but a supplementary high energy source suitable for inducing photoionization or electron transfer was not.

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8.3. Triatomic Nonhydrides

Li_3

$\tilde{C}$ $^2E''$ D_{3h}[a]
T_0=21541 gas MPI[3] $\tilde{C}-\tilde{X}$ 450–472 nm
B=0.57 MPI[4]

$\tilde{A}$ $^2E'$ D_{3h}[a]
T_0=14583 gas MPI[2,3,5] $\tilde{A}-\tilde{X}$ 660–706 nm

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

Structure in the $\tilde{A}$ state is characterized[2] by a radial frequency ω_0=191 and linear and quadratic Jahn–Teller parameters k=0.77 and g=0.15.
B=0.57 MPI[4]

$\tilde{X}$ $^2E'$ D_{3h}[a] Structure: MPI[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	302	gas	MPI	3
			303	Xe	Ra	1

Barrier to pseudorotation=26; pseudorotation frequency=34 MPI[3]
B=0.584 MPI[4]

[a]Subject to dynamic Jahn–Teller distortion.

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Na_3

$\tilde{D}\ ^2E''(^2A_2)$ $D_{3h}(C_{2v})$[a]
gas MPI[4,5,14,19]DPI[12]PE[14] $\tilde{D}-\tilde{X}$ 410–440 nm
Fragments into Na_2 + Na in less than 1 ps.[19]

$\tilde{C}\ ^2E''(^2A_2)$ $D_{3h}(C_{2v})$[a]
T_0=20813 gas MPI[2,4,6]DPI[8,12] $\tilde{C}-\tilde{X}$ 467–481 nm
Higher vibrational bands are predissociated.[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	135	gas	MPI,PF	8

Extensive vibronic structure has been tentatively assigned[8] to energy levels derived from excitation of ν_2 (e′), perturbed by dynamic Jahn–Teller interaction.
τ_0=7(3) ns gas MPI[7]
τ_{frag}=1.12 ns for the lowest vibrational level. MPI[25]

$\tilde{B}''\ ^2B_2$
T^b=19200 gas DPI[12]

$\tilde{B}\ ^2A_1'$ D_{3h}[a] Structure: MPI[24]
T_0=16124.63 gas MPI[1–6,17,20–24]DPI[12]TPE[18] $\tilde{B}-\tilde{X}$ 550–625 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			128	gas	MPI,TPE	1,3,18
			105	gas	MPI,TPE	18
			74	gas	MPI,TPE	18

$\tau_{\tilde{B}}$(16255)=14(5) ns gas MPI[7]
$\tau_{\tilde{B}'}$ (17418)=7(3) ns gas MPI[7]
A_0=0.082(2); B_0=0.138(4); C_0=0.051 MPI[22,24]
Vibronic pseudorotation occurs,[3] with a beat structure period of approximately 3 ps.[17,20,21]

$\tilde{A}\ ^2E''(^2A_2)$ $D_{3h}(C_{2v})$[a] Structure: MPI[15,16]
T_0=14894.769(4) gas MPI[1,2,4–6,11,13,15,16,26]DPI[12] $\tilde{A}-\tilde{X}$ 658–675 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	150	gas	MPI	11
	2	Bend	127	gas	MPI	4,6,11,26
	3	Asym. stretch	47	gas	MPI	4,6,11

Vibronic structure assigned in Ref. 11. First three bands are partially localized; pseudorotation barrier=196.
τ_0=60(10) ns gas MPI[7]
A_0=0.166; B_0=0.085; C_0=0.056 MPI[15,16]

$\tilde{A}'\ ^2A_1$ D_{3h}
T^b=13500 gas DPI[12]

$\tilde{X}\ ^2E'(^2B_2)$ $D_{3h}(C_{2v})$[a] Structure: MPI[15,16]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	139	gas	MPI,SEP	4,6,9,10
	2	Bend	49.5	gas	MPI,SEP	4,6,9,10
	3	Asym. stretch	87	gas	MPI,SEP	6,9,10

A_0=0.177; B_0=0.085; C_0=0.057 MPI[15,16,22]

[a]Distorted by Jahn–Teller interaction.
[b]Band maximum.

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Cu_3

$\tilde{B}$

In the ion depletion study of Ref. 10, a weak, broad band with maximum near 20600 (485 nm) has been attributed to the $\tilde{B}-\tilde{X}$ transition of Cu_3.

$\tilde{A}$

$^2A_1'$ D_{3h}

T_0=18524 gas DPI[3,8,10]LF[5,6]AB[9] $\tilde{A}-\tilde{X}$ 522–567 nm

In an argon matrix, an absorption maximum at 18760 (533 nm) has been assigned[1] to Cu_3.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	146.4(5)	gas	DPI,LF AB	3,5,8 9
e'	2	Deformation	243	gas	DPI LF,AB	3,8 5,9

τ_0=35(5) ns gas MPI[3]LF[5]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	269.5 354T	gas Ar	LF Ra	5,7 2,4

[a]Distorted by Jahn–Teller interaction.

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[7] J. W. Zwanziger, R. L. Whetten, and E. R. Grant, J. Phys. Chem. **90**, 3298 (1986).
[8] M. D. Morse, Chem. Phys. Lett. **133**, 8 (1987).
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[10] M. B. Knickelbein, J. Chem. Phys. **100**, 4729 (1994).

Ag_3

In an argon matrix study with mass selection,[8] an absorption maximum at 31150 (321 nm) behaves appropriately for assignment to Ag_3, as does an emission maximum at 26700 (374 nm). In a similar krypton matrix study,[6] the corresponding absorption maximum lies at 30200 (331 nm), and there is an emission maximum at 26200 (381 nm).

In the krypton-matrix mass selection study,[6] there is also a less prominent absorption maximum near 27500 (364 nm).

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

T_0=26969.0 gas MPI[4,5,9]LF[7] $^2E''-\tilde{X}$ 365–385 nm

In an argon matrix study with mass selection,[8] an absorption maximum at 25900 (386 nm) behaves appropriately for assignment to Ag_3. In a similar krypton matrix study,[6] the absorption maximum appears at 24900 (402 nm).

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	158.2	gas	MPI,LF	4,5,7,9
e'	2	Deformation	96	gas	MPI,LF	4,5,7,9

τ<80 ns gas LF[7]

In argon, krypton, and xenon matrices, an absorption maximum near 23700 (422 nm) has been attributed[2,3,6] to Ag_3.

$^2A_1'$? D_{3h}

T_0=19809(2) gas EM[10] 495–505 nm

In an argon matrix study with mass selection,[8] an absorption maximum at 20300 (492 nm) and an emission maximum at 16100 (622 nm) behave appropriately for assignment to Ag_3. In a krypton matrix study with mass selection,[6] absorption maxima at 21830 (458 nm) and 19500 (514 nm) and emission maxima at 17900 (560 nm) and 16000 (626 nm) also behave appropriately for assignment to Ag_3.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	107[b]	gas	EM	10
e'	2	Deformation	94[b]	gas	EM	10

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	121	gas	LF	7,9
e'	2	Deformation	99 60HT	gas Kr	LF Ra	7,9 1

[a]Distorted by Jahn–Teller interaction.
[b] $^{107}Ag_2{}^{109}Ag$.

References

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[8] S. Fedrigo, W. Harbich, and J. Buttet, J. Chem. Phys. **99**, 5712 (1993).
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[10] T. Okazaki, Y. Saito, A. Kasuya, and Y. Nishina, J. Chem. Phys. **104**, 812 (1996).

Au_3

In an argon matrix study with mass selection,[4] absorption maxima at 43300 (231 nm), 38800 (258 nm), 35100 (285 nm), and 33100 (302 nm) behave appropriately for assignment to Au_3. An absorption maximum at 34200 (292 nm) reported in an earlier study[1] without mass selection may corre-

spond to the 285 nm maximum. In a krypton matrix study with mass selection,[3] the four absorption maxima appear at 42900 (233 nm), 39200 (255 nm), 35500 (282 nm), and 32500 (308 nm).

In an argon matrix study with mass selection,[4] an absorption maximum at 27000 (370 nm) behaves appropriately for assignment to Au_3. This absorption maximum experiences a relatively large shift, to 28600 (349 nm), in the corresponding krypton matrix study.[3]

In an argon matrix study with mass selection,[4] absorption maxima at 21900 (457 nm) and 19600 (511 nm) behave appropriately for assignment to Au_3. The 21200 (471 nm) band reported in an earlier study[1] without mass selection may have been contributed in part by Au_3. The counterparts of these two bands appear at 21900 (457 nm), and 19500 (513 nm) in a krypton matrix study with mass selection.[3]

In an argon matrix study with mass selection,[4] emission maxima for Au_3 were observed at 18900 (529 nm), 17300 (579 nm), and 12400 (809 nm). In a similar krypton matrix study,[3] the corresponding emission maxima were at 19600 (510 nm), 17300 (579 nm), and 12300 (816 nm).

$\tilde{a}\ ^4E'$ D_{3h}[a]

T_0=13354.15 gas MPI[2] $\tilde{a}-\tilde{X}$ 710–750 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	181.7	gas	MPI	2
e'	2	Deformation	56T	gas	MPI	2

τ_0=28(2) μs gas MPI[2]

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

[a]Distorted by Jahn–Teller interaction.

References

[1] W. Klotzbücher and G. A. Ozin, Inorg. Chem. **19**, 3767 (1980).
[2] G. A. Bishea and M. D. Morse, J. Chem. Phys. **95**, 8779 (1991).
[3] W. Harbich, S. Fedrigo, J. Buttet, and D. M. Lindsay, J. Chem. Phys. **96**, 8104 (1992).
[4] S. Fedrigo, W. Harbich, and J. Buttet, J. Chem. Phys. **99**, 5712 (1993).

Nb_3

In an argon matrix, absorption maxima have been observed[1] near 20300 (492 nm), 18800 (532 nm), and 17000 (587 nm).

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	335(3)	Ar	Ra	1
e'	2	Deformation	227(3)	Ar	Ra	1

Reference

[1] H. Wang, R. Craig, H. Haouari, Y. Liu, J. R. Lombardi, and D. M. Lindsay, J. Chem. Phys. **105**, 5355 (1996).

cyc-Fe_2N

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			811.2	Ar	IR	2
			779.0	N_2	IR	1,2
			719.0	N_2	IR	2

References

[1] L. Andrews, G. V. Chertihin, A. Citra, and M. Neurock, J. Phys. Chem. **100**, 11235 (1996).
[2] G. V. Chertihin, L. Andrews, and M. Neurock, J. Phys. Chem. **100**, 14609 (1996).

FeFeN

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	FeN stretch	771.0T	Ar	IR	1

Reference

[1] G. V. Chertihin, L. Andrews, and M. Neurock, J. Phys. Chem. **100**, 14609 (1996).

B_3

$\tilde{X}\ ^2A_1'$ D_{3h} Structure: ESR[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	2		886.2	Ar	IR	2

References

[1] Y. M. Hamrick, R. J. Van Zee, and W. Weltner, Jr., J. Chem. Phys. **96**, 1767 (1992).
[2] S. Li, R. J. Van Zee, and W. Weltner, Jr., Chem. Phys. Lett. **262**, 298 (1996).

Al_3

T_0[a]=16610 gas MPI[1] 516–602 nm

Overlapping continuum with high-frequency edge at 19378(10). This continuum may be associated with unresolved high vibrational levels of another electronic state.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1		270.6	gas	MPI	1
	2		205	gas	MPI	1

Lifetimes (possibly radiative) vary[1] from 98 to 21 μs.

$^4A_2$ C_{2v}

Ref. 3 has suggested that the gas-phase band spacing of 133, assigned by Ref. 1 to the ground state of Al_3, may instead be contributed by a fundamental of the low-lying $^4A_2$ state.

$^2B_1$ C_{2v}

T_0=1770.4(3) Ne IR[3]
1756.9(3) Ar IR[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	319(2)	Ne	IR	3
			317	Ar	IR	3

$\tilde{X}$ $^2A_1'$ D_{3h} Structure: ESR[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	2		245(2)	Ne	IR	3
			245	Ar	IR	3

[a] Possibly a 1_0^n band.

References

[1] Z. Fu, G. W. Lemire, Y. M. Hamrick, S. Taylor, J.- C. Shui, and M. D. Morse, J. Chem. Phys. **88**, 3524 (1988).
[2] Y. M. Hamrick, R. J. Van Zee, and W. Weltner, Jr., J. Chem. Phys. **96**, 1767 (1992).
[3] S. Li, R. J. Van Zee, and W. Weltner, Jr., Chem. Phys. Lett. **262**, 298 (1996).

BeOBe

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	1412.4	Ar	IR	1
			1407.5	Kr	IR	1
			1403.0	Xe	IR	1
			1408.3	N_2	IR	2

References

[1] C. A. Thompson and L. Andrews, J. Chem. Phys. **100**, 8689 (1994).
[2] L. Andrews, G. V. Chertihin, C. A. Thompson, J. Dillon, S. Byrne, and C. W. Bauschlicher, Jr., J. Phys. Chem. **100**, 10088 (1996).

TiOTi

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	736.4	Ar	IR	1

Reference

[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. **99**, 6356 (1995).

FeOFe

$\tilde{A}$

T_0=3150(240) gas PE[3]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Asym. stretch	868.6	Ar	IR	1
			878.1	N_2	IR	2
			848.6	O_2	IR	1

References

[1] G. V. Chertihin, W. Saffel, J. T. Yustein, L. Andrews, M. Neurock, A. Ricca, and C. W. Bauschlicher, Jr., J. Phys. Chem. **100**, 5261 (1996).
[2] L. Andrews, G. V. Chertihin, A. Citra, and M. Neurock, J. Phys. Chem. **100**, 11235 (1996).
[3] H. Wu, S. R. Desai, and L.-S. Wang, J. Am. Chem. Soc. **118**, 5296 (1996).

NiNiO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NiO stretch	844.6T	Ar	IR	1
			849.5T	N_2	IR	1

Reference

[1] A. Citra, G. V. Chertihin, L. Andrews, and M. Neurock, J. Phys. Chem. A **101**, 3109 (1997).

CuOCu

In an argon matrix,[1] excitation at 20725 (482 nm) yields an emission appropriate to a resonance Raman or resonance fluorescence of CuOCu.

$\tilde{D}$

T_0=14930(400) gas PE[2]

$\tilde{C}$

T_0=14120(400) gas PE[2]

$\tilde{B}$

T_0=12590(400) gas PE[2]

$\tilde{A}$

T_0=11540(400) gas PE[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	625T	Ar	LF	1
	2	Bend	200U	gas	PE	2

References

[1] D. E. Tevault, J. Chem. Phys. **76**, 2859 (1982).
[2] L.-S. Wang, H. Wu, S. R. Desai, and L. Lou, Phys. Rev. B **53**, 8028 (1996).

Al_2C

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	CAl a-stretch	802.0	Ar	IR	1

Reference

[1] G. V. Chertihin, L. Andrews, and P. R. Taylor, J. Am. Chem. Soc. **116**, 3513 (1994).

FeCC

$\tilde{A}$
T_0=8000(800) gas PE[1]

Reference

[1] J. Fan and L.-S. Wang, J. Phys. Chem. **98**, 11814 (1994).

$FeCC^-$

Threshold for electron detachment from ground-state $FeCC^-$=15400(800) gas PE[1]

Reference

[1] J. Fan and L.-S. Wang, J. Phys. Chem. **98**, 11814 (1994).

MgCN

$\tilde{X}$ $^2\Sigma^+$ $C_{\infty v}$
B_0=0.170 MW[1]

Reference

[1] M. A. Anderson, T. C. Steimle, and L. M. Ziurys, Astrophys. J. **429**, L41 (1994).

MgNC

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	86T	gas	MW	3

B_0=0.199 MW[1]

References

[1] K. Kawaguchi, E. Kagi, T. Hirano, S. Takano, and S. Saito, Astrophys. J. **406**, L39 (1993).
[2] M. A. Anderson and L. M. Ziurys, Chem. Phys. Lett. **231**, 164 (1994).
[3] E. Kagi, K. Kawaguchi, S. Takano, and T. Hirano, J. Chem. Phys. **104**, 1263 (1996).

CaNC

$\tilde{C}$ $^2\Pi$ $C_{\infty v}$
Unstructured absorption gas LF[1] $\tilde{C}-\tilde{X}$ 385–418 nm
τ=165(38) ns gas LF[1]

$\tilde{A}$ $^2\Pi$ $C_{\infty v}$
T_0=16229.54 gas LF[1,3-6,9]CL[2] $\tilde{A}-\tilde{X}$ 572–670 nm
τ (607 nm)=40.8(1.5) ns gas LF[1]
A=77.64 gas LF[6,9]
B_0=0.150 LF[6,9]

$\tilde{X}$ $^2\Sigma^+$ $C_{\infty v}$ Structure: LF[9]
B_0=0.135 gas LF[4,6,9]MW[7,8]

References

[1] L. Pasternack and P. J. Dagdigian, J. Chem. Phys. **65**, 1320 (1976).
[2] N. Furio and P. J. Dagdigian, Chem. Phys. Lett. **115**, 358 (1985).
[3] L. C. Ellingboe, A. M. R. P. Bopegedera, C. R. Brazier, and P. F. Bernath, Chem. Phys. Lett. **126**, 285 (1986).
[4] C. J. Whitham, B. Soep, J.-P. Visticot, and A. Keller, J. Chem. Phys. **93**, 991 (1990).
[5] M. Douay and P. F. Bernath, Chem. Phys. Lett. **174**, 230 (1990).
[6] T. C. Steimle, D. A. Fletcher, K. Y. Jung, and C. T. Scurlock, J. Chem. Phys. **97**, 2909 (1992); **100**, 4025 (1994).
[7] T. C. Steimle, S. Saito, and S. Takano, Astrophys. J. **410**, L49 (1993).
[8] C. T. Scurlock, T. C. Steimle, R. D. Suenram, and F. J. Lovas, J. Chem. Phys. **100**, 3497 (1994).
[9] C. T. Scurlock, D. A. Fletcher, and T. C. Steimle, J. Chem. Phys. **101**, 7255 (1994).

cyc-BCC

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CBC s-stretch	1194.6	Ar	IR	1,2

References

[1] J. M. L. Martin, P. R. Taylor, J. T. Yustein, T. R. Burkholder, and L. Andrews, J. Chem. Phys. **99**, 12 (1993).
[2] J. D. Presilla-Márquez, C. W. Larson, P. G. Carrick, and C. M. L. Rittby, J. Chem. Phys. **105**, 3398 (1996).

YCC

T_0=12889.5 gas LF[1] 725–950 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	CY s-stretch	494.5(5.0)	gas	LF	1
	3	CY a-stretch	331.6(2.2)	gas	LF	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CY s-stretch	561.1(2.8)	gas	LF	1
b_2	3	CY a-stretch	369.6(1.7)	gas	LF	1

Reference

[1] T. C. Steimle, A. J. Marr, J. Xin, A. J. Merer, K. Athanassenas, and D. Gillett, J. Chem. Phys. **106**, 2060 (1997).

cyc-BBN

In the argon-matrix study,[2] the $\nu_1+\nu_3$ combination band at 1998.3 and other combination bands between 3250 and 6150 are moderately intense, suggesting strong vibronic coupling to a low-lying excited electronic state.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	BN s-stretch	1116[a]	Ar	IR	2
b_2	3	BN a-stretch	882.3s	Ar	IR	2–4
			910.4	N_2	IR	1
			890.3	N_2	IR	1

[a] $(\nu_1+\nu_3)-\nu_3$.

References

[1] P. Hassanzadeh and L. Andrews, J. Phys. Chem. **96**, 9177 (1992).
[2] L. Andrews, P. Hassanzadeh, T. R. Burkholder, and J. M. L. Martin, J. Chem. Phys. **98**, 922 (1993).
[3] C. A. Thompson and L. Andrews, J. Am. Chem. Soc. **117**, 10125 (1995).
[4] S. Li, R. J. Van Zee, and W. Weltner, Jr., Chem. Phys. Lett. **262**, 298 (1996).

BNB

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	1736.5	Ar	IR	1,2

References

[1] L. Andrews, P. Hassanzadeh, T. R. Burkholder, and J. M. L. Martin, J. Chem. Phys. **98**, 922 (1993).
[2] C. A. Thompson and L. Andrews, J. Am. Chem. Soc. **117**, 10125 (1995).

Ga_2P

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	281.2	Ar	IR	1

Reference

[1] S. Li, R. J. Van Zee, and W. Weltner, Jr., J. Phys. Chem. **97**, 11393 (1993).

Ga_2As

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	205.4	Ar	IR	1

Reference

[1] S. Li, R. J. Van Zee, and W. Weltner, Jr., J. Phys. Chem. **97**, 11393 (1993).

Ga_2Sb

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	167.4	Ar	IR	1

Reference

[1] S. Li, R. J. Van Zee, and W. Weltner, Jr., J. Phys. Chem. **97**, 11393 (1993).

In_2P

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	249.3T	Ar	IR	1

Reference

[1] S. Li, R. J. Van Zee, and W. Weltner, Jr., J. Phys. Chem. **98**, 2275 (1994).

In_2As

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	176.9T	Ar	IR	1

Reference

[1] S. Li, R. J. Van Zee, and W. Weltner, Jr., J. Phys. Chem. **98**, 2275 (1994).

In_2Sb

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	143.9T	Ar	IR	1

Reference

[1] S. Li, R. J. Van Zee, and W. Weltner, Jr., J. Phys. Chem. **98**, 2275 (1994).

$FeOFe^-$

Threshold for electron detachment from ground-state $FeOFe^-$ = 13150(320) gas PE[1]

Reference

[1] H. Wu, S. R. Desai, and L.-S. Wang, J. Am. Chem. Soc. **118**, 5296 (1996).

$CuOCu^-$

Threshold for electron detachment from ground-state $CuOCu^-$ = 8880(240) gas PE[1]

Reference

[1] L.-S. Wang, H. Wu, S. R. Desai, and L. Lou, Phys. Rev. B **53**, 8028 (1996).

ScCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1950brT	Ar	IR	1

Reference

[1] S. B. H. Bach, C. A. Taylor, R. J. Van Zee, M. T. Vala, and W. Weltner, Jr., J. Am. Chem. Soc. **108**, 7104 (1986).

TiCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1854.4	Ar	IR	1

Reference

[1] G. V. Chertihin and L. Andrews, J. Am. Chem. Soc. **117**, 1595 (1995).

TiNN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NN stretch	1847.1	Ar	IR	1
	3	TiN stretch	766.2	Ar	IR	1

Reference

[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. **98**, 5891 (1994).

VCO

$\tilde{X}\ ^6\Sigma$ $C_{\infty v}$ Structure: ESR[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1904	Ar	IR	1
			1890	Kr	IR	1
			1868	Xe	IR	1

References

[1] L. Hanlan, H. Huber, and G. A. Ozin, Inorg. Chem. **15**, 2592 (1976).
[2] R. J. Van Zee, S. B. H. Bach, and W. Weltner, Jr., J. Phys. Chem. **90**, 583 (1986).

TaCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1831T 1819T	Ar	IR	1

Reference

[1] R. L. DeKock, Inorg. Chem. **10**, 1205 (1971).

CrCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1977	Ar	IR	1

Reference

[1] S. B. H. Bach, C. A. Taylor, R. J. Van Zee, M. T. Vala, and W. Weltner, Jr., J. Am. Chem. Soc. **108**, 7104 (1986).

NFeN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	903.4	Ar	IR	2
			903.6	N_2	IR	1,2

References

[1] L. Andrews, G. V. Chertihin, A. Citra, and M. Neurock, J. Phys. Chem. **100**, 11235 (1996).
[2] G. V. Chertihin, L. Andrews, and M. Neurock, J. Phys. Chem. **100**, 14609 (1996).

FeNN

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NN stretch	2017.8	Ar	IR	1
			2017.8	N_2	IR	1
			2012.0	N_2	IR	1

Reference

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FeCO

$\tilde{a}$ $^5\Sigma^-$ $C_{\infty v}$
T_0=1135(25) gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1990(15)	gas	PE	3
Π	2	Bend	180(60)	gas	PE	3
Σ^+	3	FeC stretch	460(15)	gas	PE	3

$\tilde{X}$ $^3\Sigma^-$ $C_{\infty v}$ Structure: MW[4,6]DL[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1946.47	gas	PE,DL	2,3,5
			1898T	Ar	IR	1
			1884T	Kr	IR	1
Π	2	Bend	330(50)	gas	PE	3
Σ^+	3	FeC stretch	530(10)	gas	PE	3

B_0=0.146 MW[4,6]DL[5]

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CoCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1956	Ar	IR	1
			1949			
			1952	Kr	IR	1
			1944			
			1947	Xe	IR	1
			1941			

Reference

[1] L. A. Hanlan, H. Huber, E. P. Kündig, B. R. McGarvey, and G. A. Ozin, J. Am. Chem. Soc. **97**, 7054 (1975).

NiCO

T_0=11050(240) gas PE[2]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1940(80)	gas	PE	2
			1996	Ar	IR	1

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PdCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	2050	Ar	IR	1,2
			2045	Kr	IR	2
			316.8T	Kr	IR	2

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[1] E. P. Kündig, M. Moskovits, and G. A. Ozin, Can. J. Chem. **50**, 3587 (1972).
[2] J. H. Darling and J. S. Ogden, J. Chem. Soc., Dalton Trans. **1973**, 1079.

PtCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	2052	Ar	IR	1

Reference

[1] E. P. Kündig, D. McIntosh, M. Moskovits, and G. A. Ozin, J. Am. Chem. Soc. **95**, 7234 (1973).

CuCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	2010.4	Ar	IR	1

Reference

[1] H. Huber, E. P. Kündig, M. Moskovits, and G. A. Ozin, J. Am. Chem. Soc. **97**, 2097 (1975).

CUO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	UC stretch	852.6	Ar	IR	1
	3	UO stretch	804.4	Ar	IR	1

Reference

[1] T. J. Tague, Jr., L. Andrews, and R. D. Hunt, J. Phys. Chem. **97**, 10920 (1993).

UCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1832T 1817T	Ar	IR	1

Reference

[1] J. L. Slater, R. K. Sheline, K. C. Lin, and W. Weltner, Jr., J. Chem. Phys. **55**, 5129 (1971).

NPuN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	1029.7	Ar	IR	1

Reference

[1] D. W. Green and G. T. Reedy, J. Chem. Phys. **69**, 552 (1978).

C_3

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

T_0=52826(30) Ar AB[15] 170–190 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1080(30)	Ar	AB	15
Π_u	2	Bend	300(30)H	Ar	AB	15
Σ_u^+	3	Asym. stretch	780(30)H[a]	Ar	AB	15

$\tilde{B}$

In 2-photon ionization studies of jet-cooled C_3, a complicated group of bands, all with rotational structure appropriate for a $\Sigma_u^+-\Sigma_g^+$ vibronic transition arising from the $\tilde{X}$ state, has been observed between 266 and 302 nm.[20] Lifetimes of these bands range from 0.4 to 2.5 μs, and the B′ value for the first intense band, at 33153(5), is 0.396(3). These same bands, as well as bands at somewhat lower energies (possibly below the ionization threshold) and some bands arising from a $\Sigma_u^+-\Pi_g$ vibronic transition, have also been studied using LF measurements on cooled beams.[23] In a neon matrix,[39] absorptions attributable to the $\tilde{B}-\tilde{X}$ transition of C_3 are observed between 281 and 302 nm, with the first intense band at 33149(20), and in an argon matrix,[30] absorptions arising from this transition of C_3 are observed between 280 and 284 nm.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			444(20)	Ne	AB	39
			390	Ar	AB	30

In an argon matrix,[30] bands attributable to C_3 have been observed between 367 and 373 nm.

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

T_0=24675.5 gas EM[1,2,6]AB[3,6,9]LF[17,23,33,35,36,42,43] $\tilde{A}-\tilde{X}$ 335–640 nm
24640 Ne AB[4,5,8]EM[5]LF[11] $\tilde{A}-\tilde{X}$ 347–488 nm
24370[b] Ar AB[4,5,7]LF[11] $\tilde{A}-\tilde{X}$ 352–411 nm
24350 Kr AB[7]
23610 Xe AB[4,7]
24635 N_2 AB[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1085.9	gas	AB,LF	6,33
			1094(6)	Ne	AB	5
			1093(6)	Ar	AB	5,7
			1090	Kr	AB	7
			1120	Xe	AB	7
			1050	N_2	AB	7
Π_u	2	Bend	307.9[c]	gas	AB	6
Σ_u^+	3	Asym. stretch	541.7[d]	gas	LF	36

τ_0=200(10) ns gas LF[12,13]

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

B_0=0.430 UV[6]

$\tilde{b}$ $^3\Pi_g$ $D_{\infty h}$ Structure: DL,EM[29]

T_0=23570(210) gas DL[29]EM[29,37] $\tilde{b}-\tilde{a}$ 1530–1640 nm
23584[e] Ne IR[32]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	345(40)[f]	gas	EM	37

A=14.77(24) EM[37]

B_0=0.424 DL[29]EM[29]

$\tilde{a}\ ^3\Pi_u$ $D_{\infty h}$ Structure: DL,EM[29]

T_0=17090(210) gas DL[29]EM[29,37]PE[31] $\tilde{b}-\tilde{a}$ 1530–1640 nm

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

IR[32] $\tilde{b}-\tilde{a}$ 1250–1538 nm

16930 Ar EM[5,34]

IR[32] $\tilde{b}-\tilde{a}$ 1253–1544 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1156.5[g]	Ne	IR	32
			1154.2[g]	Ar	IR	32
Π_u	2	Bend	505(40)[h]	gas	EM	37
Σ_u^+	3	Asym. stretch	1449.53	gas	DL	38
			1454.1	Ne	IR	32
			1455.3	Ar	IR	32

$\tau \cong 0.02$ s Ne EM[5]

A=15.16(4) EM[37]

B_0=0.417 DL[29,38]EM[29]

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

This state of C_3 is highly anharmonic. The term values of many excited vibrational energy levels have been determined in SEP[21,26,27] and LF[23] studies. Analysis of data from the SEP studies[28] using the semirigid bender model indicates that the molecule is linear in its ground state but that on excitation of ν_3 a potential barrier appears at the linear configuration.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1224.5	gas	AB,LF	9,17,23,33
			1226	Ne	EM	5
			1212(2)	Ar	IR,EM	19,34
			1215.8T	Kr	IR	41
			1234[g]	N_2	IR	19
Π_u	2	Bend	63.41[i]	gas	UV,DL	6,22,23
					SEP,TF	24,25
			70T[j]	Ne	AB	5
			82H	Ar	EM	34
Σ_u^+	3	Asym. stretch	2040.02	gas	IR,DL	16,18
					LF	23
			2042	Ne	IR	4
			2038s	Ar	IR	4,10
			2033.3	Kr	IR	41
			2036.0	H_2	IR	40
			2031	N_2	IR	19

B_0=0.431 UV[6]IR[16]DL[18]TF[25]

[a]Alternate assignment gives 1320.

[b]In the LF studies,[11] a second site was observed with T_0=24408.

[c]ω. Large Renner splitting, with ε=0.537.[6] Detailed comparisons of gas-phase with neon- and argon-matrix band positions are given in Refs. 8 and 14. Ref. 14 also gives a more detailed analysis of electronic orbital angular momentum effects in the gas-phase molecule.

[d]In the gas phase,[35] the $\tilde{A}(002)-\tilde{X}(000)$ transition appears at 26348.0, giving $2\nu_3$=1672.5, and the corresponding transition observed in a neon matrix[8] yields $2\nu_3$=1680. Ref. 36 suggests that this fundamental of C_3 $\tilde{A}\ ^1\Pi_u$ has a large quartic anharmonicity.

[e]Sum of values for $\tilde{a}-\tilde{X}$ and $\tilde{b}-\tilde{a}$ transitions.

[f]ω. Large Renner splitting, with ε=0.447.[37]

[g]$(\nu_1+\nu_3)-\nu_3$.

[h]ω. Large Renner splitting, with ε=0.566.[37]

[i]Most precise value with tunable far infrared laser spectrometer (TF).[25] $\cong$ 45 in $\tilde{X}(011)$.[22]

[j]Greatly broadened in a rare-gas matrix by interaction with lattice modes.[11]

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SiCC

$\tilde{A}\ ^1B_2$ C_{2v} Structure: PI^5AB^{11}

T_0=20065.505 gas $EM^1AB^{3,11}LF^{4,15}$ $\tilde{A}-\tilde{X}$ 402–507 nm

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CC stretch	1462	gas	EM,AB LF	1,3,4, 11,15
			1462	Ne	AB,LF	2,4
			1457	Ar	AB	9
	2	CSi s-stretch	455.04	gas	LF,EM	4,11,15
			462	Ne	AB,LF	2,4
			448	Ar	AB	9
b_2	3	CSi a-stretch	487	gas	LF	15

τ_0=370 ns gas LF^4

310 ns Ne LF^4

A_0=1.589; B_0=0.411; C_0=0.324 AB^{11}

$\tilde{X}\ ^1A_1$ C_{2v} Structure: $PI^5MW^{6,7}AB^{11}$

The triangular configuration lies 1883(200) below the linear configuration.[17]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CC stretch	1746.0(2.8)	gas	EM,LF	1,15
			1746s	Ne	IR,LF	2,4
			1741.3	Ar	IR	8,14
	2	CSi s-stretch	840.6(1.2)	gas	EM,LF	1,10,15
			836m	Ne	IR,LF	2,4
			824.3	Ar	IR	8,14
b_2	3	CSi a-stretch	196.37(4)	gas	MW,LF	13,15
			172H[a]	Ne	LF	4
			160.4	Ar	IR	14

A_0=1.729; B_0=0.436; C_0=0.348 $MW^{6,7,12,13,16}AB^{11}$

[a]In neon-matrix emission measurements, Ref. 4 identified $2\nu_3$ at 344. The gas-phase term energy for $2\nu_3$, obtained in the SEP study of Ref. 17, is 352.85.

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Si_3

$\tilde{G}\ ^1B_2$ C_{2v}

T_0=25753(13)T Ne AB^6 $\tilde{G}-\tilde{X}$ 330–390 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			350T	Ne	AB	6

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

T_0=19146(7) Ne AB^6 $\tilde{F}-\tilde{X}$ 430–540 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	360T	Ne	AB	6

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

T_0=17250(6) Ne $AB^{1,6}$ $\tilde{E}-\tilde{X}$ 530–580 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	250T	Ne	AB	6

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

T_0=13470(80) gas PE^2

12839(3) Ne AB^6 $\tilde{D}-\tilde{X}$ 700–780 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	480(40)	gas	PE	2
			470T	Ne	AB	6

$\tilde{C}$

T_0=8880(80) gas PE^2

$\tilde{B}$

T_0=7180(80) gas PE^2

$\tilde{A}$

T_0=3630(80) gas PE^2EM^3

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	480(25)	gas	PE,EM	2,3

$\tilde{a}\ ^3A_2'$ D_{3h}

T_0<350 gas TPE^4

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	501(10)	gas	TPE	4
e'	2	Deformation	337(10)	gas	EM,TPE	2–4

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	550T	Ne	IR	5
			550.6	Ar	IR	5
			546.7	Kr	IR	5
b_2	3	Asym. stretch	525.5	Ne	IR	5
			525.1	Ar	IR	5
			523.1	Kr	IR	5

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Ge_3

$^1B_1$ C_{2v}
T_0=13640(100) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			266T	gas	PE	1

$^3B_1$ C_{2v}
T_0=8070(100) gas PE[1]

$^3A_1$ C_{2v}
T_0=6540(100) gas PE[1]

$^1B_2$ C_{2v}
T_0=1690(100) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			355T	gas	PE	1

$\tilde{X},\tilde{A}\ ^3A_2',^1A_1$ D_{3h}, C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	3		150T	gas	PE	1

Reference

[1] G. R. Burton, C. Xu, C. C. Arnold, and D. M. Neumark, J. Chem. Phys. **104**, 2757 (1996).

$OBeO^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	988.6T	Ar	IR	1
			993.0T	Kr	IR	1
			993.6T	Xe	IR	1
			970.8T	N_2	IR	2

References

[1] C. A. Thompson and L. Andrews, J. Chem. Phys. **100**, 8689 (1994).
[2] L. Andrews, G. V. Chertihin, C. A. Thompson, J. Dillon, S. Byrne, and C. W. Bauschlicher, Jr., J. Phys. Chem. **100**, 10088 (1996).

$NiCO^-$

Threshold for electron detachment from ground-state $NiCO^-$=6490(100) gas PE[1]

Reference

[1] A. E. Stevens, C. S. Feigerle, and W. C. Lineberger, J. Am. Chem. Soc. **104**, 5026 (1982).

NFeO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		FeN stretch	971.1	N_2	IR	1
		FeO stretch	798.1	Ar	IR	2
			796.4	N_2	IR	1

References

[1] L. Andrews, G. V. Chertihin, A. Citra, and M. Neurock, J. Phys. Chem. **100**, 11235 (1996).
[2] G. V. Chertihin, L. Andrews, and M. Neurock, J. Phys. Chem. **100**, 14609 (1996).

FeNO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO stretch	1746.8	N_2	IR	1
			1731.0			

Reference

[1] L. Andrews, G. V. Chertihin, A. Citra, and M. Neurock, J. Phys. Chem. **100**, 11235 (1996).

$CuOO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OO stretch	1544.7T	Ar	IR	1

Reference

[1] G. V. Chertihin, L. Andrews, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **101**, 4026 (1997).

NUO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	UN stretch	983.6	Ar	IR	1,2
	3	UO stretch	818.9	Ar	IR	2

References

[1] D. W. Green and G. T. Reedy, J. Chem. Phys. **65**, 2921 (1976).
[2] G. P. Kushto, P. F. Souter, L. Andrews, and M. Neurock, J. Chem. Phys. **106**, 5894 (1997).

UNO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO stretch	1757.3 1749.2	Ar	IR	1

Reference

[1] G. P. Kushto, P. F. Souter, L. Andrews, and M. Neurock, J. Chem. Phys. **106**, 5894 (1997).

AlCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1867.7	Ar	IR	1–3
			1883.1	N_2	IR	3
			1878.3			
	3	AlC stretch	656.2wT	N_2	IR	3

References

[1] G. V. Chertikhin, I. L. Rozhanskii, L. V. Serebrennikov, and V. F. Shevel'kov, Zh. Fiz. Khim. **62**, 2256 (1988); Russ. J. Phys. Chem. **62**, 1165 (1988).
[2] C. Xu, L. Manceron, and J. P. Perchard, J. Chem. Soc. Faraday Trans. **89**, 1291 (1993).
[3] A. Feltrin, M. Guido, and S. Nunziante Cesaro, Vib. Spectrosc. **8**, 175 (1995).

GaCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1898.1	Ar	IR	1
			1886.5			
			1897.0	N_2	IR	1
			1886.0			

Reference

[1] A. Feltrin, M. Guido, and S. Nunziante Cesaro, Vib. Spectrosc. **8**, 175 (1995).

GaP_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	322	Kr	IR	1
	2	Bend	220.9	Ar	IR	1

Reference

[1] S. Li, R. J. Van Zee, and W. Weltner, Jr., J. Phys. Chem. **97**, 11393 (1993).

$GaAs_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	231.0	Ar	IR	1
	2	Bend	171.4	Ar	IR	1

Reference

[1] S. Li, R. J. Van Zee, and W. Weltner, Jr., J. Phys. Chem. **97**, 11393 (1993).

$GaSb_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	183T	Ar	IR	1
	2	Bend	158T	Ar	IR	1

Reference

[1] S. Li, R. J. Van Zee, and W. Weltner, Jr., J. Phys. Chem. **97**, 11393 (1993).

C_3^-

Threshold for electron detachment from ground-state C_3^- =15980(160) gas PE[1–3]

$\tilde{X}\ ^2\Sigma_g^+$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1075(100)	gas	PE	3
Σ_u^+	3	Asym. stretch	1721.8T	Ar	IR	4

References

[1] J. M. Oakes and G. B. Ellison, Tetrahedron **42**, 6263 (1986).
[2] S. Yang, K. J. Taylor, M. J. Craycraft, J. Conceicao, C. L. Pettiette, O. Cheshnovsky, and R. E. Smalley, Chem. Phys. Lett. **144**, 431 (1988).
[3] D. W. Arnold, S. E. Bradforth, T. N. Kitsopoulos, and D. M. Neumark, J. Chem. Phys. **95**, 8753 (1991).
[4] J. Szczepanski, S. Ekern, and M. Vala, J. Phys. Chem. A **101**, 1841 (1997).

Si_3^-

Threshold for electron detachment from ground-state Si_3^- =18565(10) gas PE[1]TPE[2]

$^2A_1$ C_{2v}

T_0=9946(2) Ne AB[3] $^2A_1$–$\tilde{X}$ 820–1040 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	495(5)	Ne	AB	3
	2	Bend	402(5)	Ne	AB	3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	565(15)T	gas	TPE	2

References

[1] T. N. Kitsopoulos, C. J. Chick, A. Weaver, and D. M. Neumark, J. Chem. Phys. **93**, 6108 (1990).
[2] C. C. Arnold and D. M. Neumark, J. Chem. Phys. **100**, 1797 (1994).
[3] J. Fulara, P. Freivogel, M. Grutter, and J. P. Maier, J. Phys. Chem. **100**, 18042 (1996).

Ge_3^-

Threshold for electron detachment from ground-state Ge_3^- =17990(80) gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			290T	gas	PE	1

Reference

[1] G. R. Burton, C. Xu, C. C. Arnold, and D. M. Neumark, J. Chem. Phys. **104**, 2757 (1996).

CCN

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

T_0=26661.80 gas AB[1]LF[14] $\tilde{C}$–$\tilde{X}$ 310–375 nm

Evidence for predissociation above 29100.[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Stretch	1859.20	gas	AB,LF	1,14
Π	2	Bend	469.9(4)	gas	AB,LF	1,14
Σ^+	3	Stretch	1257(4)[a]	gas	LF	14

B_0=0.413 AB[1]LF[14]

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

T_0=22413.25 gas AB[1] $\tilde{B}$–$\tilde{X}$ 442–446 nm

22180 Ar AB[3]

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

B_0=0.405 AB[1]

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

T_0=21259.203 gas AB[1]LF[4]EM[9] $\tilde{A}$–$\tilde{X}$ 376–471 nm

21377 Ar LF[2]AB[3] $\tilde{A}$–$\tilde{X}$ 373–550 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Stretch	1770.77	gas	AB	1
			1732(2)	Ar	LF	2
Π	2	Bend	457.1[a]	gas	AB,LF	1,6,14
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]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Stretch	1923.25	gas	LF,EM	5,8,9
					LMR	12
					DL	10,11
			1717	Ar	LF	2
Π	2	Bend	324	gas	AB,LF	1,8
			179.27[b]	gas	LF	14
Σ^+	3	Stretch	1050.76	gas	LF,EM	5,8,9
			1066	Ar	LF	2

A_0=42.328(2), $\varepsilon\omega_2$=132.8 gas LF[8]DL[10,11]LMR[12]

B_0=0.398 AB[1]LF[4,6]DL[10,11]LMR[12]MW[13]

[a] ω.
[b] $\mu^2\Sigma$ component.

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[2] V. E. Bondybey and J. H. English, J. Mol. Spectrosc. **70**, 236 (1978).
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[13] Y. Ohshima and Y. Endo, J. Mol. Spectrosc. **172**, 225 (1995).
[14] H. Kohguchi, Y. Ohshima, and Y. Endo, J. Chem. Phys. **106**, 5429 (1997).

SiNSi

$^2\Sigma_u^+$ $D_{\infty h}$ Structure: MPI[1]
T_0=34314.29 gas MPI[1] $^2\Sigma_u^+ - \tilde{X}$ 275–315 nm
B_0=0.113 MPI[1]

$\tilde{X}$ $^2\Pi_{g,1/2}$ $D_{\infty h}$ Structure: MPI[1]
B_0=0.112 MPI[1]

Reference

[1] D. J. Brugh and M. D. Morse, Chem. Phys. Lett. **267**, 370 (1997).

OBeO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	1431.4	Ne	IR	1
			1413.2	Ar	IR	1
			1408.2	Kr	IR	1
			1415.7	Xe	IR	1

Reference

[1] C. A. Thompson and L. Andrews, J. Chem. Phys. **100**, 8689 (1994).

OMgO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	767.7	Ar	IR	1
			723.6	N_2	IR	2

References

[1] L. Andrews and J. T. Yustein, J. Phys. Chem. **97**, 12700 (1993).
[2] L. Andrews, G. V. Chertihin, C. A. Thompson, J. Dillon, S. Byrne, and C. W. Bauschlicher, Jr., J. Phys. Chem. **100**, 10088 (1996).

cyc-MgO_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	MgO_2 s-stretch	621.1T	Ar	IR	1

Reference

[1] L. Andrews and J. T. Yustein, J. Phys. Chem. **97**, 12700 (1993).

OCaO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	515.7	Ar	IR	1
			497.0	N_2	IR	2

References

[1] L. Andrews, J. T. Yustein, C. A. Thompson, and R. D. Hunt, J. Phys. Chem. **98**, 6514 (1994).
[2] L. Andrews, G. V. Chertihin, C. A. Thompson, J. Dillon, S. Byrne, and C. W. Bauschlicher, Jr., J. Phys. Chem. **100**, 10088 (1996).

cyc-CaO_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	O–O stretch	736.2	Ar	IR	1
			742.1	N_2	IR	2
	2	OCaO s-stretch	555.7	N_2	IR	2
b_2	3	OCaO a-stretch	505.5	N_2	IR	2

References

[1] L. Andrews, J. T. Yustein, C. A. Thompson, and R. D. Hunt, J. Phys. Chem. **98**, 6514 (1994).
[2] L. Andrews, G. V. Chertihin, C. A. Thompson, J. Dillon, S. Byrne, and C. W. Bauschlicher, Jr., J. Phys. Chem. **100**, 10088 (1996).

OSrO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	532.4	Ar	IR	1
			496.1	N_2	IR	2

References

[1] L. Andrews, J. T. Yustein, C. A. Thompson, and R. D. Hunt, J. Phys. Chem. **98**, 6514 (1994).
[2] L. Andrews, G. V. Chertihin, C. A. Thompson, J. Dillon, S. Byrne, and C. W. Bauschlicher, Jr., J. Phys. Chem. **100**, 10088 (1996).

cyc-SrO_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	O–O stretch	729.9	Ar	IR	1
			729.8	N_2	IR	2
	2	SrO_2 s-stretch	509.2	Ar	IR	1
			473.1	N_2	IR	2

References

[1] L. Andrews, J. T. Yustein, C. A. Thompson, and R. D. Hunt, J. Phys. Chem. **98**, 6514 (1994).
[2] L. Andrews, G. V. Chertihin, C. A. Thompson, J. Dillon, S. Byrne, and C. W. Bauschlicher, Jr., J. Phys. Chem. **100**, 10088 (1996).

OBaO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	570.2	Ar	IR	1

Reference

[1] L. Andrews, J. T. Yustein, C. A. Thompson, and R. D. Hunt, J. Phys. Chem. **98**, 6514 (1994).

cyc-BaO_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	O–O stretch	754.5	Ar	IR	1
	2	BaO_2 s-stretch	468.3	Ar	IR	1

Reference

[1] L. Andrews, J. T. Yustein, C. A. Thompson, and R. D. Hunt, J. Phys. Chem. **98**, 6514 (1994).

OCrO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	895(20)	gas	PE	6
			914.4	Ar	IR	7
	2	Bend	220(20)	gas	PE	6
b_2	3	Asym. stretch	965.4	Ar	IR	1–5,7

References

[1] J. H. Darling, M. B. Garton-Sprenger, and J. S. Ogden, Sympos. Faraday Soc. **8**, 75 (1974).
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[3] M. J. Almond, A. J. Downs, and R. N. Perutz, Inorg. Chem. **24**, 275 (1985).
[4] M. J. Almond and A. J. Downs, J. Chem. Soc., Dalton Trans. 809 (1988).
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[7] G. V. Chertihin, W. D. Bare, and L. Andrews, J. Chem. Phys. **107**, 2798 (1997).

OMoO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	948.5	Ne	IR	1
			938.7	Ar	IR	1,2
b_2	3	Asym. stretch	899	Ne	IR	1
			885	Ar	IR	1,2

References

[1] W. D. Hewett, Jr., J. H. Newton, and W. Weltner, Jr., J. Phys. Chem. **79**, 3640 (1975).
[2] M. J. Almond and A. J. Downs, J. Chem. Soc., Dalton Trans. 809 (1988).

OWO

T_0=12672 Ne AB[1] 605–790 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	972	Ne	AB	1
	2	Bend	300	Ne	AB	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	992	Ne	IR	1
			974T	Ar	IR	1
			975.5	Kr	IR	2
b_2	3	Asym. stretch	928	Ne	IR	1
			921	Ar	IR	1
			937.2	Kr	IR	2

References

[1] W. Weltner, Jr. and D. McLeod, Jr., J. Mol. Spectrosc. **17**, 276 (1965).
[2] D. W. Green and K. M. Ervin, J. Mol. Spectrosc. **89**, 145 (1981).

OTiO

T_0=18880 Ne EM[1] 529–621 nm

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	965T	gas	IR	2
			962.0	Ne	IR	1
			946.9	Ar	IR	3
b_2	3	Asym. stretch	944	gas	IR	2
			934.8	Ne	IR	1
			917.1	Ar	IR	3

References

[1] N. S. McIntyre, K. R. Thompson, and W. Weltner, Jr., J. Phys. Chem. **75**, 3243 (1971).
[2] T. C. DeVore and T. N. Gallaher, High Temp. Sci. **16**, 269 (1983).
[3] G. V. Chertihin and L. Andrews, J. Phys. Chem. **99**, 6356 (1995).

OZrO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	884.3	Ar	IR	1
b_2	3	Asym. stretch	818.0	Ar	IR	1

Reference

[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. **99**, 6356 (1995).

OHfO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	883.4	Ar	IR	1
b_2	3	Asym. stretch	814.0	Ar	IR	1

Reference

[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. **99**, 6356 (1995).

OTaO

$\tilde{B}$

T_0=16232 Ne AB[1] $\tilde{B}-\tilde{X}$ 558–616 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	Bend	281	Ne	AB	1

$\tilde{A}$

T_0=11615 Ne AB[1] $\tilde{A}-\tilde{X}$ 716–861 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	937	Ne	AB	1
	2	Bend	285	Ne	AB	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	971	Ar	IR	1
b_2	3	Asym. stretch	912	Ar	IR	1

Reference

[1] W. Weltner, Jr. and D. McLeod, Jr., J. Chem. Phys. **42**, 882 (1965).

OFeO

$\tilde{A}$

T_0=7660(320) gas PE[7]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	797.1	Ar	IR	5,6
b_2	3	Asym. stretch	945.8	Ar	IR	1–6
			945.2	O_2	IR	6

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[7] H. Wu, S. R. Desai, and L.-S. Wang, J. Am. Chem. Soc. **118**, 5296 (1996).

FeOO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OO stretch	1204.5	Ar	IR	1,2
			1204.2	N_2	IR	3
			1209.8	O_2	IR	2

References

[1] L. Andrews, G. V. Chertihin, A. Ricca, and C. W. Bauschlicher, Jr., J. Am. Chem. Soc. **118**, 467 (1996).
[2] G. V. Chertihin, W. Saffel, J. T. Yustein, L. Andrews, M. Neurock, A. Ricca, and C. W. Bauschlicher, Jr., J. Phys. Chem. **100**, 5261 (1996).

[3] L. Andrews, G. V. Chertihin, A. Citra, and M. Neurock, J. Phys. Chem. **100**, 11235 (1996).

cyc-FeO_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	OO stretch	956.0	Ar	IR	1–4
			954.5	O_2	IR	4
	2	OFeO s-stretch	548.4	Ar	IR	3,4
			549.7	O_2	IR	4

References

[1] S. Chang, G. Blyholder, and J. Fernandez, Inorg. Chem. **20**, 2813 (1981).
[2] M. Fanfarillo, A. J. Downs, T. M. Greene, and M. J. Almond, Inorg. Chem. **31**, 2973 (1992).
[3] L. Andrews, G. V. Chertihin, A. Ricca, and C. W. Bauschlicher, Jr., J. Am. Chem. Soc. **118**, 467 (1996).
[4] G. V. Chertihin, W. Saffel, J. T. Yustein, L. Andrews, M. Neurock, A. Ricca, and C. W. Bauschlicher, Jr., J. Phys. Chem. **100**, 5261 (1996).

cyc-RhO_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	OO stretch	908	Ar	IR	1
			900	Xe	IR	1
	2	RhO stretch	422	Xe	IR	1

Reference

[1] A. J. L. Hanlan and G. A. Ozin, Inorg. Chem. **16**, 2848 (1977).

ONiO

$\tilde{b}$ $^1\Sigma_g^+$ $D_{\infty h}$
T_0=6210(240) gas PE[2]

$\tilde{a}$ $^1\Delta_g$ $D_{\infty h}$
T_0=3230(160) gas PE[2]

$\tilde{X}$ $^3\Sigma_g^-$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	750(30)	gas	PE	2
Σ_u^+	3	Asym. stretch	954.9	Ar	IR	1
			959.5	N_2	IR	1

References

[1] A. Citra, G. V. Chertihin, L. Andrews, and M. Neurock, J. Phys. Chem. A **101**, 3109 (1997).
[2] H. Wu and L.-S. Wang, J. Chem. Phys. **107**, 16 (1997).

cyc-NiO_2

$\tilde{A}$
T_0=8000T gas PE[3]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	OO stretch	967.1	Ar	IR	1,2
			970.1	N_2	IR	2
	2	NiO s-stretch	538.3	Ar	IR	2
b_2	3	NiO a-stretch	511.7	Ar	IR	2

References

[1] H. Huber, W. Klotzbücher, G. A. Ozin, and A. Vander Voet, Can. J. Chem. **51**, 2722 (1973).
[2] A. Citra, G. V. Chertihin, L. Andrews, and M. Neurock, J. Phys. Chem. A **101**, 3109 (1997).
[3] H. Wu and L.-S. Wang, J. Chem. Phys. **107**, 16 (1997).

NiOO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OO stretch	1221.3	Ar	IR	1

Reference

[1] A. Citra, G. V. Chertihin, L. Andrews, and M. Neurock, J. Phys. Chem. A **101**, 3109 (1997).

cyc-PdO_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	OO stretch	1023.5	Ar	IR	1
	2	PdO s-stretch	427w	Ar	IR	1

References

[1] H. Huber, W. Klotzbücher, G. A. Ozin, and A. Vander Voet, Can. J. Chem. **51**, 2722 (1973).

cyc-PtO_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	OO stretch	926.6	Ar	IR	1

Reference

[1] H. Huber, W. Klotzbücher, G. A. Ozin, and A. Vander Voet, Can. J. Chem. **51**, 2722 (1973).

OCuO

T_0=20699 Ne LF[3] 432–540 nm
20290 Ar LF[1,3]
19680 Xe UV[2] 440–586 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CuO s-stretch	610	Ne	LF	3
			615(5)	Xe	AB	2
	2	Bend	133	Ne	LF	3

$\tilde{E}$
T_0=13640(160) gas PE[5]

$\tilde{D}$
T_0=9680(160) gas PE[5]

$\tilde{C}$
T_0=6540(160) gas PE[4,5]

$\tilde{B}$
T_0=5080(160) gas PE[4,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			640(80)	gas	PE	4,5

$\tilde{A}$
T_0=2580(160) gas PE[4,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			640(80)	gas	PE	4,5

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	CuO s-stretch	658	Ne	LF	3
			668	Ar	LF	1
			670(5)	Xe	EM	2
Π_u	2	Bend	193	Ne	LF	3
Σ_u^+	3	CuO a-stretch	823.0	Ar	IR	6
			826.7	N_2	IR	6

References

[1] D. E. Tevault, J. Chem. Phys. **76**, 2859 (1982).
[2] G. A. Ozin, S. A. Mitchell, and J. García-Prieto, J. Am. Chem. Soc. **105**, 6399 (1983).
[3] V. E. Bondybey and J. H. English, J. Phys. Chem. **88**, 2247 (1984).
[4] H. Wu, S. R. Desai, and L.-S. Wang, J. Chem. Phys. **103**, 4363 (1995).
[5] H. Wu, S. R. Desai, and L.-S. Wang, J. Phys. Chem. A **101**, 2103 (1997).
[6] G. V. Chertihin, L. Andrews, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **101**, 4026 (1997).

CuOO

In a xenon matrix, an absorption maximum at 44640 (224 nm) has been attributed[1] to CuOO.

$\tilde{A}$
T_0=7400(400) gas PE[2]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OO stretch	1089.6	Ar	IR	3
	3	CuO stretch	530(50)	gas	PE	2
			550.4	Ar	IR	3
			530	Xe	IR	1

References

[1] G. A. Ozin, S. A. Mitchell, and J. García-Prieto, J. Am. Chem. Soc. **105**, 6399 (1983).
[2] H. Wu, S. R. Desai, and L.-S. Wang, J. Chem. Phys. **103**, 4363 (1995).
[3] G. V. Chertihin, L. Andrews, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **101**, 4026 (1997).

AgOO

$\tilde{X}$ C_s Structure: IR[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OO stretch	1084.4	Ar	IR	1
			1078.9			
	3	AgO stretch	445.2	Ar	IR	1

Reference

[1] D. E. Tevault, R. R. Smardzewski, M. W. Urban, and K. Nakamoto, J. Chem. Phys. **77**, 577 (1982).

cyc-AuO_2

In an argon matrix, relatively weak absorption maxima at 40980 (244 nm), 36230 (276 nm), and 31950 (313 nm) and a prominent, broad absorption maximum at 23640 (423 nm) have been attributed[1] to Au(OO).

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	OO stretch	1091.7	Ar	IR	1

Reference

[1] D. McIntosh and G. A. Ozin, Inorg. Chem. **15**, 2869 (1976).

OZnO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	748.2	Ar	IR	1
			748.1	N_2	IR	1

Reference

[1] G. V. Chertihin and L. Andrews, J. Chem. Phys. **106**, 3457 (1997).

OCdO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	626.6	Ar	IR	1

Reference

[1] G. V. Chertihin and L. Andrews, J. Chem. Phys. **106**, 3457 (1997).

OCeO

T_0=20067 Ne EM[1] 498–649 nm
19836 Ar EM[1] 504–660 nm
19259 N_2 EM[1] 519–633 nm
τ=200(50) ms Ar EM[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	777w	Ne	IR,EM	1
			757.0w	Ar	IR,EM	1,2
			714	N_2	IR,EM	1
b_2	3	Asym. stretch	759s	Ne	IR	1
			736.9s	Ar	IR	1,2
			719	N_2	IR	1

References

[1] R. L. DeKock and W. Weltner, Jr., J. Phys. Chem. **75**, 514 (1971).
[2] S. D. Gabelnick, G. T. Reedy, and M. G. Chasanov, J. Chem. Phys. **60**, 1167 (1974).

OPrO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	730.4	Ar	IR	1,2

References

[1] R. L. DeKock and W. Weltner, Jr., J. Phys. Chem. **75**, 514 (1971).
[2] S. D. Gabelnick, G. T. Reedy, and M. G. Chasanov, J. Chem. Phys. **60**, 1167 (1974).

OTbO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	758.8	Ar	IR	2
b_2	3	Asym. stretch	718.8	Ar	IR	1,2

References

[1] R. L. DeKock and W. Weltner, Jr., J. Phys. Chem. **75**, 514 (1971).
[2] S. D. Gabelnick, G. T. Reedy, and M. G. Chasanov, J. Chem. Phys. **60**, 1167 (1974).

OThO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	787.4	Ar	IR	1
b_2	3	Asym. stretch	735.4	Ar	IR	1

Reference

[1] S. D. Gabelnick, G. T. Reedy, and M. G. Chasanov, J. Chem. Phys. **60**, 1167 (1974).

OUO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	776.1	Ar	IR	1,2
			768.0	Kr	IR	1

References

[1] S. D. Gabelnick, G. T. Reedy, and M. G. Chasanov, J. Chem. Phys. **58**, 4468 (1973).
[2] R. D. Hunt and L. Andrews, J. Chem. Phys. **98**, 3690 (1993).

OPuO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	794.2	Ar	IR	1
			786.8	Kr	IR	1

Reference

[1] D. W. Green and G. T. Reedy, J. Chem. Phys. **69**, 544 (1978).

CCO

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

$\tilde{A}$ $^3\Pi$ $C_{\infty v}$ Structure: AB[3]
T_0=11651.182 gas AB[2,3,14]LF[6]DL[10-12,14] $\tilde{A}-\tilde{X}$ 500–860 nm
11860 Ar AB[5] $\tilde{A}-\tilde{X}$ 600–850 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	2045.7	gas	AB	3
Π	2	Bend	594.75[a]	gas	AB,DL	3,12
Σ^+	3	CC stretch	1283.60	gas	AB,DL	3,14

The fluorescence decay pattern[7] of CCO $\tilde{A}(101)$ 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.
$A=-35.36$; $\varepsilon=-0.172$ gas AB^3DL^{10}
$B_0=0.407$ AB^3DL^{10}

$\tilde{b}\ ^1\Sigma^+$ $C_{\infty v}$
$T_0=8190(145)$ gas PE[15]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	2010(170)	gas	PE	15

$\tilde{a}\ ^1\Delta$ $C_{\infty v}$
$T_0=5310(145)$ gas PE[15]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1950(170)	gas	PE	15

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1970.86	gas	LF,DL	6,9,16
			1969s	Ar	IR	1,4
			1978 N_2	Ar	IR	1
			1987	N_2	IR	1
Π	2	Bend	379.53	gas	AB,DL	3,11
			381m	Ar	IR	1
Σ^+	3	CC stretch	1063	gas	LF	6
			1064w	Ar	IR	1
			1074 N_2	Ar	IR	1
			1077	N_2	IR	1

$B_0=0.385$ $AB^3MW^{8,13}$

[a]ω.

References

[1] M. E. Jacox, D. E. Milligan, N. G. Moll, and W. E. Thompson, J. Chem. Phys. **43**, 3734 (1965).
[2] C. Devillers, Compt. Rend. Acad. Sci. (Paris) **262C**, 1485 (1966).
[3] C. Devillers and D. A. Ramsay, Can. J. Phys. **49**, 2839 (1971).
[4] R. L. DeKock and W. Weltner, Jr., J. Am. Chem. Soc. **93**, 7106 (1971).
[5] G. R. Smith and W. Weltner, Jr., J. Chem. Phys. **62**, 4592 (1975).
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[15] V. Zengin, B. J. Persson, K. M. Strong, and R. E. Continetti, J. Chem. Phys. **105**, 9740 (1996).
[16] N. Moazzen-Ahmadi, D. W. D. Sandilands, and R. T. Boeré, Chem. Phys. Lett. **265**, 563 (1997).

GeCO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1918.9	Ar	IR	2
			1908	Kr	IR	1
			1921.3	N_2	IR	2
			1924.0	CO	IR	2

References

[1] A. Bos, J. Chem. Soc. Chem. Commun. **1972**, 26.
[2] A. Feltrin, S. Nunziante Cesaro, and F. Ramondo, Vib. Spectrosc. **10**, 139 (1996).

SnCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1921	Kr	IR	1

Reference

[1] A. Bos, J. Chem. Soc. Chem. Commun. **1972**, 26 (1972).

NCN

$^1\Delta_u$ $D_{\infty h}$
gas AB^6 250–290 nm

$\tilde{B}\ ^3\Sigma_u^-$ $D_{\infty h}$
$T_0 \leqslant 33512$ gas AB^6 $\tilde{B}-\tilde{X}$ 258–300 nm
33100 Ar AB^2 $\tilde{B}-\tilde{X}$ 240–302 nm
33215 N_2 AB^2 $\tilde{B}-\tilde{X}$ 240–301 nm

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

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

$\tilde{b}\ ^1\Pi_u$ $D_{\infty h}$ Structure: AB^5
T_0=x+30045.76 gas AB^5 $\tilde{b}-\tilde{a}$ 330–334 nm

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

$\varepsilon\omega_2=-84.2$ gas AB^5
$B_0=0.395$ AB^5

$\tilde{A}\ ^3\Pi_u$ $D_{\infty h}$ Structure: AB^1LF^{10}
T_0=30383.967 gas $AB^1LF^{10,12}$ $\tilde{A}-\tilde{X}$ 326–329 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1254(5)	gas	LF	8
Π_u	2	Bend	534T	gas	LF	12

$A=-37.57; \varepsilon\omega_2=-91.12$ gas AB^1LF^{12}
τ_0=183(6) ns gas LF^8
B_0=0.397 $AB^1LF^{10,12}$

$\tilde{a}\ ^1\Delta_g$ $D_{\infty h}$ 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^1LF^{10}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1197[a]	Ar	IR	4
Π_u	2	Bend	437T	gas	LF	12
			423m	Ar	IR	2,4
Σ_u^+	3	Asym. stretch	1466.51	gas	IR, LMR	9,11
			1475vs	Ar	IR	2,4
			1478vs	N_2	IR	2–4

B_0=0.397 $AB^1LF^{9,10}IR^9$

[a]Frequency deduced from weak combination with ν_3 which appears at 2672.

References

[1] G. Herzberg and D. N. Travis, Can. J. Phys. **42**, 1658 (1964).
[2] D. E. Milligan, M. E. Jacox, and A. M. Bass, J. Chem. Phys. **43**, 3149 (1965).
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[4] D. E. Milligan and M. E. Jacox, J. Chem. Phys. **45**, 1387 (1966).
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[12] S. A. Beaton and J. M. Brown, J. Mol. Spectrosc. **183**, 347 (1997).

N_3^+

$\tilde{A}\ ^3\Pi_u$ $D_{\infty h}$ Structure: PF^2
T_0[a]≅35370 gas PF^2 $\tilde{A}-\tilde{X}$ 245–283 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1300T	gas	PF	2
Π_u	2	Bend	440T	gas	PF	2
Σ_u^+	3	Asym. stretch	1700T	gas	PF	2

τ>50 ps gas PF^2
A_{100}=−39.67 gas PF^2
B_{100}=0.429 gas PF^2

$\tilde{b}\ ^1\Sigma^+$
T_0=14520(160) gas PE^1

$\tilde{a}\ ^1\Delta$
T_0=9120(160) gas PE^1

$\tilde{X}\ ^3\Sigma_g^-$ $D_{\infty h}$ Structure: PE^1PF^2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1170(30)	gas	PE	1

B_0=0.424 PF^2
[a]T_{100}=36671.81 gas PF^2.

References

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[2] A. Friedmann, A. M. Soliva, S. A. Nizkorodov, E. J. Bieske, and J. P. Maier, J. Phys. Chem. **98**, 8896 (1994).

PbOPb

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	486.8	Ar	IR	1

Reference

[1] G. V. Chertihin and L. Andrews, J. Chem. Phys. **105**, 2561 (1996).

MgF_2^+

$\tilde{C}\ ^2\Sigma_g^+$ $D_{\infty h}$
T^a=12500(560) gas PE^1

$\tilde{B}\ ^2\Sigma_u^+$ $D_{\infty h}$
T^a=7500(560) gas PE^1

$\tilde{A}\ ^2\Pi_u$ $D_{\infty h}$
T^a=5240(560) gas PE^1

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

[a]From vertical ionization potential.

Reference

[1] J. M. Dyke, D. Haggerston, M. P. Hastings, and T. G. Wright, Chem. Phys. **181**, 355 (1994).

$OTiO^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	878.4	Ar	IR	1

Reference

[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. **99**, 6356 (1995).

$OZrO^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	761.4	Ar	IR	1

Reference

[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. **99**, 6356 (1995).

$OHfO^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	747.9	Ar	IR	1

Reference

[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. **99**, 6356 (1995).

$OCrO^-$

Threshold for electron detachment from ground-state $OCrO^-$ =19470(65) gas EB[1]PE[2]

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$OFeO^-$

Threshold for electron detachment from ground-state $OFeO^-$ =19040(240) gas PE[1,2]

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[1] J. Fan and L.-S. Wang, J. Chem. Phys. **102**, 8714 (1995).
[2] H. Wu, S. R. Desai, and L.-S. Wang, J. Am. Chem. Soc. **118**, 5296 (1996).

$ONiO^-$

Threshold for electron detachment from ground-state $ONiO^-$ =24610(80) gas PE[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	886.8	Ar	IR	1
			894.4	N_2	IR	1

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cyc-NiO_2^-

Threshold for electron detachment from ground-state *cyc*-NiO_2^- =6620(240) gas PE[1]

Reference

[1] H. Wu and L.-S. Wang, J. Chem. Phys. **107**, 16 (1997).

$OCuO^-$

Threshold for electron detachment from ground-state $OCuO^-$ =27920(320) gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	600(80)	gas	PE	2
Σ_u^+	3	Asym. stretch	839.6T	Ar	IR	3

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[1] H. Wu, S. R. Desai, and L.-S. Wang, J. Chem. Phys. **103**, 4363 (1995).
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$CuOO^-$

Threshold for electron detachment from ground-state $CuOO^-$ =12130(80) gas PE[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OO stretch	1009.5	Ar	IR	2

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[1] H. Wu, S. R. Desai, and L.-S. Wang, J. Chem. Phys. **103**, 4363 (1995).
[2] G. V. Chertihin, L. Andrews, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **101**, 4026 (1997).

BS_2

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

T_0=24072(5) Ne AB[2] $\tilde{B}-\tilde{X}$ 395–412 nm

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

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

$\tilde{A}\ ^2\Pi_u$ $D_{\infty h}$
T_0=13766(2) Ne AB[2] $\tilde{A}-\tilde{X}$ 514–721 nm
gas AB[1,3] $\tilde{A}-\tilde{X}$ 592–800 nm

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

A=−263(2) Ne AB[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	510	Ne	AB	2
Π_u	2	Bend	120[a]T	Ne	AB	2
Σ_u^+	3	Asym. stretch	1014.6(5)s	Ne	IR	2
			1015.7	Ar	IR	4

A=−440 gas AB[1,2]

[a]Estimated from isotope shift in origin of $\tilde{A}-\tilde{X}$ transition.

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$ClBS^+$

$\tilde{C}\ ^2\Sigma^+$ $C_{\infty v}$
T^a=50500(1000) gas PE[1]

$\tilde{B}\ ^2\Pi_{3/2}$ $C_{\infty v}$
T_0=26019 gas EF[2] $\tilde{B}-\tilde{X}$ 405–516 nm

$\tilde{A}\ ^2\Sigma^+$ $C_{\infty v}$
T_0=24961.5(4) gas EF[2] $\tilde{A}-\tilde{X}$ 392–440 nm

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

τ=240(13) ns gas EF[2]

$\tilde{X}\ ^2\Pi_{3/2}$ $C_{\infty v}$ Structure: PE[1,3]

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]
B_0=0.093 EF[2]

[a]From vertical ionization potential.

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OAlO

$D_{\infty h}$
T_0=17465 Ar LF[1] 495–620 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	790	Ar	LF	1
Π_u	2	Bend	70	Ar	LF	1
Σ_u^+	3	Asym. stretch	1015	Ar	LF	1

$\tilde{B}\ ^2\Sigma_g^+$ $D_{\infty h}$
T_0=6860(180) gas PE[3]

$\tilde{A}\ ^2\Pi_u$ $D_{\infty h}$
T_0=5240(180) gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	810(60)	gas	PE	3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	635	Ar	LF	1
Π_u	2	Bend	70	Ar	LF	1
Σ_u^+	3	Asym. stretch	1129.5	Ar	IR	2

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CCO^-

Threshold for electron detachment from ground-state CCO^- is 18470(145).[2]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1900T	gas	PE	1,2

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NCO

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

T_0=31751.1(5) gas UV[2]LF[18,30]PD[27] $\tilde{B}-\tilde{X}$ 265–320 nm
31616(25) Ne UV[3] $\tilde{B}-\tilde{X}$ 260–320 nm
31437(25) Ar UV[3] $\tilde{B}-\tilde{X}$ 232–315 nm
31339(25) N_2 UV[3] $\tilde{B}-\tilde{X}$ 256–315 nm

All vibrational states are predissociated.[27]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Stretch	2303	gas	UV	2
			2295(50)	Ne	UV	3
			2303(50)	Ar	UV	3
	3	Stretch	1047	gas	UV	2
			1033(50)	Ne	UV	3
			1053(50)	Ar	UV	3
			1025(50)	N_2	UV	3

τ_0=63(3) −152(5) ns for various rovibronic bands gas LF[13,30]
A=−76.6 gas LF[18]
B_0=0.356 LF[18]

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

T_0=22754.020(2) gas AB[1]LF[23,30]SEP[26]EM[28] $\tilde{A}-\tilde{X}$ 304–512 nm
22800(10) Ne AB[3] $\tilde{A}-\tilde{X}$ 398–440 nm
22712(2) Ar LF[8] $\tilde{A}-\tilde{X}$ 390–530 nm
22956(10) N_2 AB[3] $\tilde{A}-\tilde{X}$ 395–440 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Stretch	2338.0	gas	UV	1
			2325(20)	Ne	UV	3
			2332(4)	Ar	UV,LF	3,8
			2321(20)	N_2	UV	3
Π	2	Bend	680.8	gas	UV	1
			673(20)	Ne	UV	3
Σ^+	3	Stretch	1289.3[a]	gas	UV	1
			1270(20)	Ne	UV	3
			1291(4)	Ar	UV,LF	3,8

τ_0=435(10) ns gas LF[9,13]
350(30) ns gas LF[11,12]
170 ns Ar LF[8]
B_0=0.402 UV[1]

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$ Structure: UV[1,7,20]MW[4–6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Sym. stretch	1266.63(8)[b]	gas	LF,LMR	14,15,17
					SEP	19,23,26,29
			1275vw	Ar	IR,LF	3,8
Π	2	Bend	534.06(3)[c]	gas	UV,LF	1,7,15
					SEP	23,29
			529.5[d]	Ar	LF	8
Σ^+	3	Asym. stretch	1921.28[e]	gas	LMR	10,14,15
					LF,DL	21,23
					EM	28
					SEP	25
			1923m	Ar	IR,LF	3,8
			1935	N_2	IR	3

A_0=−95.589(3), $\varepsilon\omega_2$=−78.37(3) gas LF[23]SEP[26,29]EM[28]
B_0=0.390 UV[1]MW[16]LMR[22]EM[28]

[a]In Fermi resonance with $2\nu_2$, at 1385.3.
[b]For $\tilde{X}\ ^2\Pi_{1/2}$, 1362.87 gas LF[14,15,19,23,24]SEP[26]
[c]ω_2.
[d]Lowest frequency component ($^2\Sigma^+$) contributes a strong infrared absorption at 487.[3] Four components ($^2\Sigma^+$, $^2\Delta_{5/2}$, $^2\Delta_{3/2}$, $^2\Sigma^-$) observed at 484, 531, 626, and 672 in LF experiments.[8] Components of (0n0), n⩾2, have also been assigned in gas-phase studies.[19,23,26]
[e]For $\tilde{X}\ ^2\Pi_{1/2}$, 2017.7(5) gas LF[14,15,23,24]

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CO_2^+

$\tilde{C}\ ^2\Sigma_g^+$ $D_{\infty h}$ Structure: MP[24]

T_0=45157(3) gas TPE[21]PE[23]MP[24] $\tilde{C}-\tilde{A}$ 585–640 nm

The band origin is perturbed by another state of $^2\Sigma_g^+$ symmetry at 45188 which has a rotational constant of 0.353.[24] This state may be an excited vibrational level of the $\tilde{A}$ or $\tilde{B}$ state.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1352(4)[a]	gas	PE	23
Π_u	2	Bend	614(4)	gas	TPE, PE	21,23
Σ_u^+	3	Asym. stretch	1567(4)	gas	PE	23

B_0=0.395 MP[24]

$\tilde{B}\ ^2\Sigma_u^+$ $D_{\infty h}$ Structure: EM[9]

T_0=34591.6[b] gas EM[1,9,29,30]EF[29] $\tilde{B}-\tilde{X}$ 287–291 nm

Perturbations by the $\tilde{A}$ state are considered in Refs. 14–16 and Ref. 29.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1275(1)	gas	TPE, PE	21,23
Π_u	2	Bend	557(4)	gas	EM,PE	9,23
Σ_u^+	3	Asym. stretch	1847(10)	gas	PE,EM	17,23,30

τ_0=140(7) ns gas T-PEFCO[10]PEFCO[13]LF[16]
B_0=0.380 EM[1,29]

$\tilde{A}\ ^2\Pi_u$ $D_{\infty h}$ Structure: EM[11]

T_0=28500.35 gas EM[2,6,11,30]LF[27,30]PE[31] $\tilde{A}-\tilde{X}$ 253–490 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1126	gas	EM PE	2,5,11 23,31
Π_u	2	Bend	461	gas	EM,PE	11,23,31
Σ_u^+	3	Asym. stretch	2685.3	gas	LF,EM	30

τ_0=102(8) ns gas EF[7]T-PEFCO[10]
124(6) ns gas PEFCO[13]HFD[18]
A=−95.51 gas EM[11]LF[27]PE[31]
B_0=0.350 EM[2,11]LF[27]

$\tilde{X}\ ^2\Pi_g$ $D_{\infty h}$ 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 PE	4,5,8,12 22,31
Π_u	2	Bend	511.4(3)	gas	EM,DL PE TPE	11,19,22 28,31
			462.6[c]	Ne	IR	32
Σ_u^+	3	Asym. stretch	1423.08	gas	DL,PE	19,31
			1421.7	Ne	IR	25,32

A=−161.02(6);[d] $\varepsilon\omega_2$=−98.8(3)[d] gas EM[1,9,11]DL[20,22]TPE[28]
B_0=0.380 EM[1,3,9,11]

[a]Corrected for Fermi resonance.
[b]Measured from lowest rotational level of $\tilde{X}$ state,[29] 34672.33.
[c]$\mu\ ^2\Sigma_u^+$ level (gas-phase value[20]=467.26).
[d]Reanalysis by Ref. 26 gives A=−161.48(5) and $\varepsilon\omega_2$=−100.4.

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OCS^+

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

T_0=54640(30) gas PI[4]PE[10]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	2202(2)	gas	PE	10
Π	2	Bend	454(5)	gas	PE	10
Σ^+	3	CS stretch	926(5)	gas	PI,PE	4,10

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

T_0=39180(20) gas PI[4]PF[9]PE[10]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1850(8)	gas	PE	10
Π	2	Bend	515(3)	gas	PF,PE	9,10
Σ^+	3	CS stretch	829[a]	gas	PF	9

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

T_0=31404.099(7) gas EF[1]LF[8]PF[9,11] $\tilde{A}-\tilde{X}$ 282–432 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	2027	gas	PE,PF	10,11
Π	2	Bend	336(20)H	gas	PE	10
Σ^+	3	CS stretch	807[b]	gas	PF	9,11

τ_0=93(9) ns[c] gas PEFCO[5]
τ_0 (ω=3/2)=105(3) ns; τ_0 (ω=1/2)=77(3) ns gas HFD[6]EF[7]
A=−111.8 gas EF[1]PF[9,11]
B_0=0.186 LF[8]PF[9,11]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	2066	gas	EF,PF	1,11
Π	2	Bend	476(16)	gas	PE	10
Σ^+	3	CS stretch	697[d]	gas	PF	9,11

A=−367.2 gas EF[1]PF[9]
B_0=0.194 LF[8]PF[9,11]

[a]Ref. 10 gives value of 742(7).
[b]817 for ω=1/2.[9,11]
[c]Absence of emission from states above the $\tilde{A}\ ^2\Pi$ band origin in photoionization experiments[2] suggested that the molecule is predissociated into CO +S$^+$ ($^4S^o$), as was later confirmed.[3] PEFCO studies[5] have yielded the branching ratio for photoexcitation vs predissociation for the transition origin, permitting an estimate of 550(50) ns for the radiative lifetime.
[d]699.7 for ω=1/2.[9,11]

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CS_2^+

$\tilde{C}\ ^2\Sigma_g^+$ $D_{\infty h}$ Structure: MP[15]

T_0=49064 gas PI[5]PF[13]MP[15] $\tilde{C}-\tilde{B}$ 658–724 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	652(2)	gas	PI,PE	5,9,11
					PF,MP	13–15,19
Π_u	2	Bend	348(9)	gas	PF,PE	13,14,19
Σ_u^+	3	Asym. stretch	1024(6)T	gas	PE	14

τ_0=11(2) ps gas MP[15]
B_0=0.111 PF[13]MP[15]

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

T_0=35238.01 gas EM[1] $\tilde{B}-\tilde{X}$ 277–307 nm
35270 Ne LF[7]
35226

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	602	gas	EM,PE	3,19
Π_u	2	Bend	351(5)	gas	PE	14,19
Σ_u^+	3	Asym. stretch	1320(5)	gas	PE	14,19

τ_0=290(10) ns gas EF[2]PIFCO[4]PEFCO[8]UV[12]
There is also a long-lifetime component, with τ=1.44(22) μs.[8,12]
B_0=0.108 EM[1]

$\tilde{A}\ ^2\Pi_u$ $D_{\infty h}$ Structure: EM[3]

T_0=20975 gas EM[3] $\tilde{A}-\tilde{X}$ 426–512 nm
21017 Ne LF[6,7,17] $\tilde{A}-\tilde{X}$ 400–638 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	550[a]T	gas	EM	3
			557	Ne	LF	6,7,18
Π_u	2	Bend	305HT	gas	EM	3
			309H	Ne	LF	6,7,18
Σ_u^+	3	Asym. stretch	1644H	Ne	LF	7

τ=4.09(19) μs gas PIFCO[4]ID[10]UV[12]
2.3(1) μs Ne LF[6,7]
A=−176 gas EM[3]PE[14,19]
B_0=0.101 EM[3]

$\tilde{X}\ ^2\Pi_g$ $D_{\infty h}$ Structure: EM[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	617[a]	gas	EM,TPE	3,16,21
			618[a]	Ne	LF	6,7,17,18
Π_u	2	Bend	332[b]	gas	TPE	16,21
			349H	Ne	LF	6,7,17,18
Σ_u^+	3	Asym. stretch	1188(8)	gas	EM,PE	3,14,19
			1207.1	Ne	LF,IR	6,7,17,18
						20

A=−440.39(3) gas EM[1,2]TPE[16,21]
B_0=0.109 EM[1]

[a]Strong Fermi resonance with $2\nu_2$; assignment of Refs. 7 and 18 adopted for the $\tilde{A}$ state.
[b]Renner–Teller components are observed for $\tilde{X}\ ^2\Pi_{g,3/2}$ at 330 ($^2\Sigma^+$) and 336 ($^2\Delta_{3/2}$) in a gas-phase TPE study[21]. For $\tilde{X}\ ^2\Pi_{g,1/2}$, components at 320 ($^2\Delta_{u,3/2}$) and 341 ($^2\Sigma_u^-$) are observed in gas-phase TPE studies.[16,21]

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$BrCN^+$

$\tilde{C}\ ^2\Sigma^+$ $C_{\infty v}$
T_0=50200(200) gas PE[1,2,13]

$\tilde{B}\ ^2\Pi_{3/2}$ $C_{\infty v}$
T_0=18759.78(4) gas EF[7]LF[10,11]PE[13] $\tilde{B}-\tilde{X}$ 445–620 nm
18586(14) Ne AB[5] $\tilde{B}-\tilde{X}$ 418–538 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡N stretch	1958(2)	gas	EF,LF,PE	7,10,13
			1830(10)	Ne	AB	5
Π	2	Bend	395.7(2)H	gas	EF,LF	7,10
			377(10)	Ne	AB	5
Σ^+	3	CBr stretch	473.1(2)	gas	EF,LF,PE	7,10,13
			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=−774(20) gas PE[13]
B_0=0.127 gas LF[10,11]

$\tilde{A}\ ^2\Sigma^+$ $C_{\infty v}$
T_0=13699(1) gas EF[7]PE[13] $\tilde{A}-\tilde{X}$ 708–853 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CN stretch	1930(2)	gas	EF	7
Π	2	Bend	421(2)	gas	EF	7
Σ^+	3	CBr stretch	584(2)	gas	EF	7

τ=2750(100) ns gas T-PEFCO[8]

$\tilde{X}\ ^2\Pi_{3/2}$ $C_{\infty v}$ Structure: LF[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡N stretch	1905.94	gas	EF,LF	7,10
					DL,PE	12,13
Π	2	Bend	287.2(2)H	gas	EF,LF	7,10
Σ^+	3	CBr stretch	649.4(5)	gas	EF,LF	7,10,13
					PE	

A=−1477(2) gas EF[3]PIFCO[4]
B_0=0.141 gas LF[10,11]DL[12]

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PNP

$\tilde{A}\ ^2\Sigma_u^+$ $D_{\infty h}$
T_0=28300 Ar AB[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	560(20)	Ar	AB	1,2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	1179.3	Ar	IR	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]PF[15] $\tilde{B}-\tilde{A}$ 538–866 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Sym. stretch	900[b]T	gas	PE	1

$\tilde{A}\ ^2\Sigma^+$ $C_{\infty v}$ Structure: EM[3]PF[16]

T_0=28162.33 gas EM[3,14]PF[6,10,11,16,18] $\tilde{A}-\tilde{X}$ 317–421 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Sym. stretch	1345.52	gas	EM,PF	3,10
Π	2	Bend	614.45	gas	EM	3,14
Σ^+	3	Asym. stretch	2451.7	gas	EM	3

τ=230(10) ns gas EF[2,9]PIFCO[4]PEFCO[7]ID[8]EM[12]HFD[13]

B_0=0.433 EM[3,14]PF[10,11]

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$ Structure: EM[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Sym. stretch	1126.51	gas	EM	3
			1135.5	Ne	IR	17
Π	2	Bend	452.42	gas	EM,PF	3,11,14
Σ^+	3	Asym. stretch	1737.6	gas	EM	3
			1741.4wm	Ne	IR	17

$A=-132.434$, $\varepsilon\omega_2=-90.2$ gas EM[3,14]PF[11,16,18]

B_0=0.412 EM[3]PF[10,11,16]

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

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ArBeO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BeO stretch	1526.1	Ar	IR	1

Reference

[1] C. A. Thompson and L. Andrews, J. Am. Chem. Soc. **116**, 423 (1994).

KrBeO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BeO stretch	1521.8	Ar	IR	1
			1511.8	Kr	IR	2

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[1] C. A. Thompson and L. Andrews, J. Am. Chem. Soc. **116**, 423 (1994).
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XeBeO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BeO stretch	1516.7	Ar	IR	1
			1498.3	Xe	IR	2

References

[1] C. A. Thompson and L. Andrews, J. Am. Chem. Soc. **116**, 423 (1994).
[2] C. A. Thompson and L. Andrews, J. Chem. Phys. **100**, 8689 (1994).

FBO

$\tilde{X}$ $C_{\infty v}$ Structure: MW,DL[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	B=O stretch	2078.87	gas	DL	2
			2081	Ne	IR	1,3
			2071	Ar	IR	1
Π	2	Bend	502	Ne	IR	1,3
			493	Ar	IR	1

B_0=0.312 MW,DL[2]

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[1] A. Snelson, High Temp. Sci. **4**, 141 (1972).
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ClBO

$\tilde{X}$ $C_{\infty v}$ Structure: MW,DL[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	B=O stretch	1958s	Ar	IR	1
	2	Bend	404s	Ar	IR	1
	3	BCl stretch	676.04	gas	DL	2
			673wm	Ar	IR	1

B_0=0.174 MW,DL[2]

References

[1] A. Snelson, High Temp. Sci. **4**, 318 (1972).
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ClBS

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BS stretch	1408	gas	IR	3,4
Π	2	Bend	300(40)	gas	MW	2
Σ^+	3	BCl stretch	525	gas	IR	3,4

B_0=0.093 MW[1,2]

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[1] C. Kirby, H. W. Kroto, and N. P. C. Westwood, J. Am. Chem. Soc. **100**, 3766 (1978).
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BF_2^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	2026.1	Ne	IR	1

Reference

[1] M. E. Jacox and W. E. Thompson, J. Chem. Phys. **102**, 4747 (1995).

BCl_2^+

Emission between 280 and 350 nm which results on excitation of BCl_3 by radiation with a threshold of 74 nm has been attributed[1] to BCl_2^+. A band spacing of 650(30) observed in this emission has not been definitively assigned.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	1439.7	Ne	IR	2
			1436.3			

References

[1] H. Biehl, J. C. Creasey, D. M. Smith, R. P. Tuckett, K. R. Yoxall, H. Baumgartel, H. W. Jochims, and U. Rockland, J. Chem. Soc. Faraday Trans. **91**, 3073 (1995).
[2] M. E. Jacox, K. K. Irikura, and W. E. Thompson, J. Chem. Phys. **104**, 8871 (1996).

BBr_2^+

Emission between 250 and 300 nm, with a maximum at 290 nm (34500), which appears when BBr_3 is excited by radiation with a threshold at 78 nm (15.8 eV), has been attributed[1] to transitions of BBr_2^+.

Reference

[1] H. Biehl, D. M. Smith, R. P. Tuckett, K. R. Yoxall, H. Baumgartel, H. W. Jochims, and U. Rokland, Mol. Phys. **87**, 1199 (1996).

$OAlO^-$

Threshold for electron detachment from ground-state $OAlO^-$=34130(160) gas PE[1]

Reference

[1] S. R. Desai, H. Wu, C. M. Rohlfing, and L.-S. Wang, J. Chem. Phys. **106**, 1309 (1997).

OSiSe

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Si=O stretch	1254.2	Ar	IR	1

Reference

[1] L. Andrews, P. Hassanzadeh, D. V. Lanzisera, and G. D. Brabson, J. Phys. Chem. **100**, 16667 (1996).

$SiSe_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	SiSe a-stretch	750.8	Ar	IR	1

Reference

[1] L. Andrews, P. Hassanzadeh, D. V. Lanzisera, and G. D. Brabson, J. Phys. Chem. **100**, 16667 (1996).

OSnO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	863.1	Kr	IR	1
			877.8	N_2	IR	1

Reference

[1] A. Bos and J. S. Ogden, J. Phys. Chem. **77**, 1513 (1973).

OPbO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	658.6T^a	Ar	IR	1
Σ_u^+	3	Asym. stretch	764.8	Ar	IR	1
			775.9	N_2	IR	1

[a]From combination band.

Reference

[1]G. V. Chertihin and L. Andrews, J. Chem. Phys. **105**, 2561 (1996).

cyc-PbO_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	OO stretch	728.7	Ar	IR	1,2
			730.6	N_2	IR	2
	2	PbO stretch	437.3	Ar	IR	1,2
			449.6	N_2	IR	2

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FCP

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	C≡P stretch	1670.84	gas	IR	2
	2	Bend	375.43	gas	IR	2
	3	CF stretch	780.1(2)	gas	IR	2

B_0=0.175 MW[1]IR[2]

References

[1]H. W. Kroto, J. F. Nixon, and N. P. C. Simmons, J. Mol. Spectrosc. **82**, 185 (1980).
[2]K. Ohno, H. Matsuura, H. Murata, and H. W. Kroto, J. Mol. Spectrosc. **100**, 403 (1983).

ClCP

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	C≡P stretch	1477.34	gas	IR	3
	2	Bend	303.41	gas	IR	3
	3	CCl stretch	573.92(6)	gas	IR	3

B_0=0.101 MW[1,2]IR[3]

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[1]T. J. Dennis, S. Firth, H. W. Kroto, D. R. M. Walton, and C.-Y. Mok, J. Chem. Soc., Chem. Commun. 1430 (1990).
[2]S. Firth, S. Khalaf, and H. W. Kroto, J. Chem. Soc. Faraday Trans. **88**, 3393 (1992).
[3]D. McNaughton and D. N. Bruget, J. Mol. Spectrosc. **161**, 336 (1993).

NO_2^+

$^3B_2$ C_{2v}
T_0^a=74580(100) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1113(20)	gas	PE	1,2
	2	Bend	686(20)	gas	PE	1,2

$\tilde{d}$ $^3A_1$ C_{2v}
T^a≅67600 gas PE[2]

$\tilde{C}$ $^1B_1$ C_{2v}
T_0^a=60670(100) gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1017(20)	gas	PE	1,2

$\tilde{c}$ $^3B_1$ C_{2v}
T_0^a=60100(100) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1041(20)	gas	PE	1,2

$\tilde{B}$ $^1B_2$ C_{2v}
T_0^a=38940(100) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1025(20)	gas	PE	2
	2	Bend	573(20)	gas	PE	1,2

$\tilde{A}$ $^1A_2$ C_{2v}
T_0^a=35900(100) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	984(20)	gas	PE	1,2
	2	Bend	694(20)	gas	PE	1,2

$\tilde{b}$ $^3A_2$ C_{2v}
T_0^a=32110(100) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	662(20)	gas	PE	1,2

$\tilde{a}\ ^3B_2$ C_{2v}
T_0[a]=26170(100) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	654(20)	gas	PE	1,2

$\tilde{X}\ ^1\Sigma_g^+$ $D_{\infty h}$ Structure: TPE[4,5,7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1396	gas	TPE	5,7
			1362.4[b]	Ne	IR	6
Π	2	Bend	639	gas	TPE	5,7
Σ_u^+	3	Asym. stretch	2362	gas	TPE	5,7
			2348.2	Ne	IR	6

B_0=0.417 TPE[4,7]

[a]The band origins given here have been calculated using a first ionization potential of 9.62(1) eV for NO_2, as found in the photoionization study of Ref. 3.
[b]$(\nu_1+\nu_3)-\nu_3$.

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[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. Scr. **1**, 127 (1970).
[3] P. C. Killgoar, Jr., G. E. Leroi, W. A. Chupka, and J. Berkowitz, J. Chem. Phys. **59**, 1370 (1973).
[4] G. P. Bryant, Y. Jiang, M. Martin, and E. R. Grant, J. Phys. Chem. **96**, 6875 (1992).
[5] G. Bryant, Y. Jiang, and E. Grant, Chem. Phys. Lett. **200**, 495 (1992).
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[7] G. P. Bryant, Y. Jiang, M. Martin, and E. R. Grant, J. Chem. Phys. **101**, 7199 (1994).

SNO^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NO stretch	1975.2	Ar	IR	1

Reference

[1] L. Andrews, P. Hassanzadeh, G. D. Brabson, A. Citra, and M. Neurock, J. Phys. Chem. **100**, 8273 (1996).

SNS^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	1499.7	Ar	IR	1,2

References

[1] P. Hassanzadeh and L. Andrews, J. Am. Chem. Soc. **114**, 83 (1992).
[2] L. Andrews and P. Hassanzadeh, J. Chem. Soc., Chem. Commun. 1523 (1994).

$SeNSe^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	1250.7	Ar	IR	1,2

References

[1] L. Andrews and P. Hassanzadeh, J. Chem. Soc., Chem. Commun. 1523 (1994).
[2] L. Andrews, P. Hassanzadeh, D. V. Lanzisera, and G. D. Brabson, J. Phys. Chem. **100**, 16667 (1996).

P_2O

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	P=O stretch	1278.677	gas	DL	2
			1270.4	Ar	IR	1

References

[1] Z. Mielke, M. McCluskey, and L. Andrews, Chem. Phys. Lett. **165**, 146 (1990).
[2] H.-B. Qian, P. B. Davies, and P. A. Hamilton, J. Chem. Soc. Faraday Trans. **91**, 2993 (1995).

INC

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NC stretch	2057	Ar	IR	1,2
			2063	Kr	IR	1
			2055			
			2053	Xe	IR	1
			2058	N_2	IR	1
Π	2	Bend	200T	Ar	IR	2
Σ^+	3	IN stretch	494	Ar	IR	2

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[1] R. Fraenkel and Y. Haas, Chem. Phys. Lett. **214**, 234 (1993); **226**, 610 (1994).
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BF_2

$\tilde{C}\ ^2\Pi(3p)$ $D_{\infty h}$
T_{vert}=63100T gas MPI[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_g	2	Bend	600(50)	gas	MPI	6

$\tilde{B}\ ^2A_1$ (3s) C_{2v}
T_{vert}=59100T gas $EF^1EM^{2,3}MPI^6$ $\tilde{B}-\tilde{A},\tilde{X}$ 190–650 nm
$\tau \cong 11$ ns EF^1EM^3

$\tilde{A}\ ^2B_1$ C_{2v}
T_{vert}=35100 gas $EF^1EM^{2,3}MPI^6$ $\tilde{A}-\tilde{X}$ 220–650 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	310(20)	gas	MPI	6

$\tau \cong 49$ ns EM^3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1151.4vs	Ne	IR	5
	2	Bend	525(30)	gas	EM	3
			523.7m	Ne	IR	5
b_2	3	Asym. stretch	1393.5vs	Ne	IR	5
			1389.9	Ar	IR	4
			1384.8	N_2	IR	4

References

[1] J. E. Hesser and K. Dressler, J. Chem. Phys. **47**, 3443 (1967).
[2] M. Suto, C. Ye, and L. C. Lee, Phys. Rev. A **42**, 424 (1990).
[3] J. C. Creasey, P. A. Hatherly, H. M. Jones, I. R. Lambert, and R. P. Tuckett, Mol. Phys. **78**, 837 (1993).
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[5] M. E. Jacox and W. E. Thompson, J. Chem. Phys. **102**, 4747 (1995).
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BCl_2

Emission which is observed between 200 and 260 nm on excitation of BCl_3 by radiation of wavelength shorter than 91 nm has been attributed[5] to BCl_2.

$\tilde{B},\tilde{C}$

Emission which is observed between 200 and 500 nm on excitation of BCl_3 by radiation of wavelength between 100 and 124 nm (9.99–12.27 eV) has been attributed[8,9] to the $\tilde{B}-\tilde{X}$ and $\tilde{C}-\tilde{X}$ transitions of BCl_2. Other studies are consistent with contributions from two different emission systems, as summarized below.

Emission which is observed between 240 and 380 nm on excitation of BCl_3 by radiation of wavelength shorter than 118 nm[4,5] and on electron impact[6] has been attributed to BCl_2, as has been a similar chemiluminescence emission observed[1,2] on reaction of H atoms with BCl_3. The electron impact study[6] yielded a radiative lifetime of 1.65(20) μs and suggested that the lower state is the ground state of BCl_2.

Emission which is observed between 280 and 380 nm on excitation of BCl_3 by radiation of wavelength shorter than 124 nm[4,5] and on electron impact[6] has also been attributed to BCl_2.

$\tilde{A}$

Emission which is observed between 380 and 650 nm on excitation of BCl_3 by radiation of wavelength shorter than 138 nm[4,5,8] and on electron impact[6] has been attributed to the $\tilde{A}-\tilde{X}$ transition of BCl_2. The electron impact study indicated that the lower state is the ground state of BCl_2.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	731w	Ar	IR	3
b_2	3	Asym. stretch	977.5	Ne	IR	10
			976.4			
			965.6vs	Ar	IR	3,7

References

[1] O. Dessaux, P. Goudmand, and G. Pannetier, Compt. Rend. Acad. Sci. Paris C **265**, 480 (1967).
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BBr_2

Emission between 240 and 390 nm, with a lifetime ranging from 18(2) to 26(2) ns, which occurs when BBr_3 is excited by radiation of wavelength between 116 and 140 nm, has been attributed[4] to two or more band systems of BBr_2.

In an argon matrix, an absorption maximum at 15900 (630 nm) has been attributed[2] to BBr_2.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	551.0w	Ar	IR	2
b_2	3	Asym. stretch	833.4s	Ar	IR	1–3

References

[1] J. H. Miller and L. Andrews, J. Am. Chem. Soc. **102**, 4900 (1980).
[2] A. Moroz and R. L. Sweany, Inorg. Chem. **31**, 5236 (1992).
[3] P. Hassanzadeh and L. Andrews, J. Phys. Chem. **97**, 4910 (1993).
[4] H. Biehl, D. M. Smith, R. P. Tuckett, K. R. Yoxall, H. Baumgartel, H. W. Jochims, and U. Rokland, Mol. Phys. **87**, 1199 (1996).

AlF_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	755.3	Ar	IR	1
b_2	3	Asym. stretch	887.5	Ar	IR	1

Reference

[1] P. Hassanzadeh, A. Citra, L. Andrews, and M. Neurock, J. Phys. Chem. **100**, 7317 (1996).

$AlCl_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	461.0	Ar	IR	2,3
b_2	3	Asym. stretch	563.6	Ar	IR	1–3

References

[1] G. A. Olah, O. Farooq, S. M. F. Farnia, M. R. Bruce, F. L. Clonet, P. R. Morton, G. K. S. Prakash, R. C. Stevens, R. Bau, K. Lammertsma, S. Suzer, and L. Andrews, J. Am. Chem. Soc. **110**, 3231 (1988).
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[3] P. Hassanzadeh, A. Citra, L. Andrews, and M. Neurock, J. Phys. Chem. **100**, 7317 (1996).

$AlBr_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	348.3T	Ar	IR	1
b_2	3	Asym. stretch	458.4	Ar	IR	1

Reference

[1] P. Hassanzadeh, A. Citra, L. Andrews, and M. Neurock, J. Phys. Chem. **100**, 7317 (1996).

AlI_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	385.9	Ar	IR	1

Reference

[1] P. Hassanzadeh, A. Citra, L. Andrews, and M. Neurock, J. Phys. Chem. **100**, 7317 (1996).

GaF_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	642.0	Ar	IR	1
			638.9			
	2	Bend	158T	Ar	IR	1
b_2	3	Asym. stretch	746.6	Ar	IR	1
			744.5			

Reference

[1] S. B. Osin, E. D. Samsonova, and V. F. Shevel'kov, Zh. Fiz. Khim. **68**, 2009 (1994); Russ. J. Phys. Chem. **68**, 1823 (1994).

CO_2^-

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1253.8w	Ne	IR	2
	2	Bend	714.1w	Ne	IR	2
b_2	3	Asym. stretch	1658.3vs	Ne	IR	1,2

References

[1] M. E. Jacox and W. E. Thompson, J. Chem. Phys. **91**, 1410 (1989).
[2] W. E. Thompson and M. E. Jacox (unpublished).

FCO

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

T_0=28500(25)	gas	$AB^{2,7,8}$	$\tilde{C}-\tilde{X}$ 220–280 nm
⩽35587	Ar	AB^3	$\tilde{C}-\tilde{X}$ 234–281 nm
⩽35211	CO	$AB^{1,3}$	$\tilde{C}-\tilde{X}$ 217–284 nm

In the gas phase,[2] bands are diffuse, and the onset of predissociation is estimated[6] to lie at a wavelength longer than 294 nm. In an argon matrix,[3] the threshold for photodissociation into F + CO was observed near 280 nm.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1458(6)[a]	gas	AB	8
	2	Bend	651(5)[a]	gas	AB	2,7,8
			650T	Ar	AB	3
			650T	CO	AB	1,3

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

T_0⩽27000	gas	$CL^5AB^{7,8}$	$\tilde{B}-\tilde{X}$ 280–455 nm
⩾24000	gas	AB^8	
⩽29586	Ar	AB^3	$\tilde{B}-\tilde{X}$ 284–338 nm
⩽29516	CO	$AB^{1,3}$	$\tilde{B}-\tilde{X}$ 289–339 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1180(35)[a]	gas	AB	8
	2	Bend	770(30)[a]	gas	AB	8
			700T	Ar	AB	3
			700T	CO	AB	1,3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CO stretch	1861.64	gas	DL	4
			1857vs	Ar	IR	3
			1855vs	CO	IR	1
	2	Bend	627.5m	Ar	IR	3
			626m	CO	IR	1
	3	CF stretch	1026.13	gas	DL	4
			1023vs	Ar	IR	3
			1018s	CO	IR	1

A_0=6.38; B_0=0.382; C_0=0.360 DL[4]

[a] ω.

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[1] D. E. Milligan, M. E. Jacox, A. M. Bass, J. J. Comeford, and D. E. Mann, J. Chem. Phys. **42**, 3187 (1965).
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[8] M. M. Maricq, J. J. Szente, Y. Su, and J. S. Francisco, J. Chem. Phys. **100**, 8673 (1994).

CS_2^-

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	1159.4	Ne	IR	1

Reference

[1] T. M. Halasinski, J. T. Godbout, J. Allison, and G. E. Leroi, J. Phys. Chem. **100**, 14865 (1996).

SiO_2^-

Threshold for electron detachment from ground-state $SiO_2^- \leqslant 16940(800)$ gas PE[1]

Reference

[1] L.-S. Wang, H. Wu, S. R. Desai, J. Fan, and S. D. Colson, J. Phys. Chem. **100**, 8697 (1996).

GeO_2^-

Threshold for electron detachment from ground-state $GeO_2^- = 20170(800)$ gas PE[1]

Reference

[1] L.-S. Wang, H. Wu, S. R. Desai, J. Fan, and S. D. Colson, J. Phys. Chem. **100**, 8697 (1996).

FCS

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CF stretch	1297.4	Ar	IR	1
	2	Bend	457T	Ar	IR	1
	3	C=S stretch	917.9	Ar	IR	1

Reference

[1] N. Caspary, B. E. Wurfel, A. Thoma, G. Schallmoser, and V. E. Bondybey, Chem. Phys. Lett. **212**, 329 (1993).

PO_2

$^2B_1$? C_{2v}

T_0=30378(3) gas AB^1LF^3 $^2B_1-\tilde{X}$ 268–600 nm

Ar AB^6 $^2B_1-\tilde{X}$ 292–301 nm

In LF studies,[3] there was an apparently continuous background signal, with a maximum between 400 and 500 nm. The similarity of the behavior of this band system to that of the visible bands of NO_2 suggests that the quasicontinuum may be contributed by high vibrational levels of the ground state.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	933	gas	AB	1
			942	Ar	AB	6
	2	Bend	396	gas	AB	1

$\tau \cong 500$ ns gas LF^3

$\tau_{cont} \cong 4.5\ \mu s$ gas LF^3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PO s-stretch	1117(20)	gas	MW LMR LF	2,3
	2	Bend	387(20)	gas	MW,LF LMR	2,3
			386.4	Ar	IR	7
b_2	3	PO a-stretch	1327.53	gas	DL	8,9
			1319.1	Ar	IR	4,5,7

A_0=3.486; B_0=0.287; C_0=0.264 MW,LMR^2

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[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).
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[4] L. Andrews and R. Withnall, J. Am. Chem. Soc. **110**, 5605 (1988).
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[6] R. Withnall, M. McCluskey, and L. Andrews, J. Phys. Chem. **92**, 126 (1989).
[7] Z. Mielke, M. McCluskey, and L. Andrews, Chem. Phys. Lett. **165**, 146 (1990).
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[9] H.-B. Qian, P. B. Davies, and P. A. Hamilton, J. Chem. Soc. Faraday Trans. **91**, 2993 (1995).

SNO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO stretch	1522.8s[a]	Ar	IR	1–3
	3	NS stretch	790.2m	Ar	IR	1–3

[a] In Fermi resonance with $2\nu_3$.

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SeNO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO stretch	1570.0	Ar	IR	1

Reference

[1] L. Andrews, P. Hassanzadeh, D. V. Lanzisera, and G. D. Brabson, J. Phys. Chem. **100**, 16667 (1996).

NS_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NS_2 s-stretch	660T	Ar	IR	1
b_2	3	NS_2 a-stretch	1225.2	Ar	IR	1,2

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NSe_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	436T	Ar	IR	1
b_2	3	Asym. stretch	1019.0	Ar	IR	1

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[1] L. Andrews and P. Hassanzadeh, J. Chem. Soc., Chem. Commun. 1523 (1994).
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SeSeN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SeN stretch	614.7	Ar	IR	1

Reference

[1] L. Andrews, P. Hassanzadeh, D. V. Lanzisera, and G. D. Brabson, J. Phys. Chem. **100**, 16667 (1996).

SO_2^+

$\tilde{F}\ ^2A_1$ C_{2v}
T_0=62200(500) gas PE[2]

$\tilde{E}\ ^2B_1$ C_{2v}
T_0=33090(20) gas PE[2,6,7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	960(10)	gas	PE	7
	2	Bend	444(10)	gas	PE	7

$\tilde{D}\ ^2A_1$ C_{2v}
T_0=32190(50) gas PE[1,2,6,7]PF[5] $\tilde{D}-\tilde{X}$ 300–317 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	912(1)	gas	PE,PF	1,2,5–7
	2	Bend	411(60)	gas	PF	5

$\tilde{C}\ ^2B_2$ C_{2v}
T_0=28670(50) gas PE[1,2,6,7]PF[5] $\tilde{C}-\tilde{B}$ 511–437 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	800(4)	gas	PE	6,7
	2	Bend	371(10)	gas	PF,PE	4–7

$\tilde{B}\ ^2B_2$ C_{2v}
T_0=7034(80) gas PE[1,6,7]PF[4,5] $\tilde{C}-\tilde{B}$ 437–511 nm[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	465(9)	gas	PE,PF	1,4–7
b_2	3	Asym. stretch	1320(8)HT	gas	PE	7

$\tau \cong 25\ \mu s$ gas PF[5]

$\tilde{A}\ ^2A_2$ C_{2v}
T_0=5156(65) gas PE[1,6,7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	981(60)	gas	PE	6,7
	2	Bend	353(7)	gas	PE	6,7
b_2	3	Asym. stretch	202(13)	gas	PE	6,7

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	404.2(5)	gas	PE	1,6,7

Barrier to linearity ca. 3200 PE[6,7]

[a] Attributed by Ref. 5 to the $\tilde{C}-\tilde{A}$ transition.

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CF_2

$\tilde{B}$ [a]

$T_0 \cong 72740$ gas AB[10] $\tilde{B}-\tilde{X}$ 131–138 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	Bend	625	gas	AB	10

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

T_0=37226 gas EM[1]AB[2,3,5,10]LF[20,42] $\tilde{A}-\tilde{X}$ 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	1	Sym. stretch	1011(2)	gas	LF	42
	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
b_2	3	Asym. stretch	1180(2)	gas	LF	42

τ_0=50(5) ns gas LF[20,21,28,30,33]EM[35,39]EF[37]
31 ns Ne LF[17]
27 ns Ar LF[17]
23 ns Kr LF[17]
A_0=4.577; B_0=0.334; C_0=0.311 AB[10]

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

T_0=19828 gas CL[18,19,22,24,29]PE[34] $\tilde{a}-\tilde{X}$ 430–800 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	517	gas	CL	18,22, 24,29

$\tau \cong 1$ s gas CL[19]

$\tilde{X}\ ^1A_1$ C_{2v} Structure: MW[8]AB[9,10]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1225.08	gas	DL,IR PE	23,31,32 34,36
			1221.9	Ne	IR,LF	12,17,40
			1222vs	Ar	IR,LF	6,11,17
	2	Bend	666.25	gas	UV,PE DL	1,10,34 41
			668vw	Ar	IR,LF	6,11,17
b_2	3	Asym. stretch	1114.44	gas	IR,DL	7,13,27 32,38
			1105.8	Ne	IR	12,40
			1102vs	Ar	IR	6,11

A_0=2.947; B_0=0.417; C_0=0.365 MW[8,15,26]AB[9,10]

[a] Tentative assignment. This band system was associated with the $\tilde{C}-\tilde{X}$ transition in Ref. 10. Subsequent studies[14,25] have dictated the reassignment to CF_3 of almost all of the bands between 136 and 160 nm which had tentatively been attributed[10] to CF_2.

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SiF_2

$\tilde{B}\ ^1B_2$ C_{2v}
T_0=62280 gas UV[11]MPI[15,16,19] $\tilde{B}-\tilde{X}$ 158–165 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	790T	gas	AB MPI	11,19
	2	Bend	320T	gas	AB	11

$\tilde{A}\ ^1B_1$ C_{2v} Structure: AB[9]
T_0=44113.9 gas EM[1,2]AB[5,9]LF[14,17] $\tilde{A}-\tilde{X}$ 213–276 nm
≅43964 Ne AB[7] $\tilde{A}-\tilde{X}$ 216–225 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	250.1(3) 253T	gas Ne	AB,LF AB	5,9,17,18 7

$\tau \leqslant 20$ ns gas LF[17]
A_0=1.446; B_0=0.241; C_0=0.206 AB[9]

$\tilde{a}\ ^3B_1$ C_{2v} Structure: LF[18]
T_0=26319.478(6) gas EM[10]MPI[16,19]LF[18] $\tilde{a}-\tilde{X}$ 364–420 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	278.2	gas	EM,MPI,LF	10,16,18

A_0=1.367; B_0=0.253; C_0=0.213 LF[18]

$\tilde{X}\ ^1A_1$ C_{2v} Structure: MW[3,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	855.01	gas	IR,LF	6,13,17
			851s	Ne	IR	8
			843s	Ar	IR	7,8
	2	Bend	345	gas	MW,UV, LF,MPI	4,5 17,19
			343	Ar	IR	7
b_2	3	Asym. stretch	870.40	gas	IR	6,13
			864.6s	Ne	IR	8
			855vs	Ar	IR	7,8

A_0=1.021; B_0=0.294; C_0=0.228 MW[3,4]

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$SiCl_2$

$\tilde{A}\ ^1B_1$ C_{2v} Structure: LF[10]
T_0=30013.5(2) gas AB[4]EM[5-7,15]LF[8,10,13] $\tilde{A}-\tilde{X}$ 295–430 nm
In an argon matrix, unstructured absorption attributable to $SiCl_2$ has been observed[1] between 310 and 320 nm, with a maximum at approximately 315 nm.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	428.9	gas	LF	8,13
	2	Bend	149.8	gas	UV,LF	3,7,8,13

τ_{070}=77(3) ns gas LF[8,15]
A_{060}=0.909; B_{060}=0.076; C_{060}=0.069 LF[10]

$\tilde{a}\ ^3B_1$ C_{2v}
T_0=18943T gas EM[11,12,15] $\tilde{a}-\tilde{X}$ 500–650 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	159(2)	gas	EM	11,12

τ=11(2) ms gas EM[12]

$\tilde{X}\ ^1A_1$ C_{2v} Structure: ED[4]MW[9,14]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	521.6	gas	LF	13
			518.7	Ne	IR	2
			512.5s	Ar	IR	1,2
	2	Bend	200.6	gas	EM,LF	7,8,11–13
			202.2	Ar	IR	2
b_2	3	Asym. stretch	509.4	Ne	IR	2
			502vs	Ar	IR	1,2

A_0=0.493; B_0=0.094; C_0=0.079 MW[9]LF[10]

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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=43860.9 gas AB[1]LF[10] $\tilde{A}-\tilde{X}$ 222–243 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	623.8(6)	gas	LF	10
	2	Bend	159.6	gas	AB,LF	1,10

$\tilde{a}\ ^3B_1$ C_{2v}
T_0=30582.1 gas EM[6,8,9]LF[10] $\tilde{a}-\tilde{X}$ 305–370 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	673.1(5)	gas	LF	10
	2	Bend	192.2	gas	EM,LF	6,8,10

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	663	gas	IR	2
			655	Ne	IR	2
			648	Ar	IR,Ra	2,7
			653	N_2	Ra	7
	2	Bend	263(2)	gas	AB,EM	1,6,8
b_2	3	Asym. stretch	692	gas	IR	2
			685	Ne	IR	2
			676	Ar	IR	2

A_0=0.513; B_0=0.262; C_0=0.173 MW[3,4]

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$GeCl_2$

$\tilde{A}\ ^1B_1$ C_{2v}
T_0=30622(2) gas AB[2]LF[11] $\tilde{A}-\tilde{X}$ 300–330 nm

Structured absorption[2] is superposed on a continuum with maximum near 32280, presumably due to predissociation of $GeCl_2$ into GeCl + Cl. In the LF excitation spectrum,[11] there is a marked increase in the line density beyond approximately 31630.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	354	gas	LF	11
	2	Bend	104	gas	AB,LF	2,11

τ=89.7(6.8) ns gas EM[10]

$\tilde{a}\ ^3B_1$ C_{2v}
T_0=22315(2) gas CL[1]LF[11] $\tilde{a}-\tilde{X}$ 400–490 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	393	gas	LF	11
	2	Bend	118	gas	CL,LF	1,11

τ=17.4(6) μs gas EM[10]

$\tilde{X}\ ^1A_1$ C_{2v} Structure: ED[8]MW[12]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	399	gas	CL,Ra	1,4
			398.6	Ar	IR	3,5,7,9
			390	N_2	Ra	6
	2	Bend	160(4)	gas	CL,AB	1,2
					Ra	4
			163	N_2	Ra	6
b_2	3	Asym. stretch	373.5	Ar	IR	3,5,7,9
			362	N_2	Ra	6

A_0=0.241; B_0=0.087; C_0=0.064 MW[12]

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NF_2^+

$\tilde{A}\ ^1B_1$? C_{2v}
$T_0 \cong 38400^a$ gas PE[1,2]

$\tilde{a}\ ^3B_1$ C_{2v}
T_0=19610(320) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			520(20)	gas	PE	1,2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1250(20)	gas	PE	1,2
b_2	3	Asym. stretch	1233.5T	Ne	IR	3

[a]From vertical ionization potential.

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PO_2^-

Threshold for electron detachment from ground-state PO_2^- =27600(80) gas PE[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	520T	gas	PE	2
b_2	3	PO a-stretch	1198.8	Ar	IR	1

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SOO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1006.1	Ar	IR	1
			739.9	Ar	IR	1

Reference

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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 $\tilde{C}-\tilde{X}$ band system of SO_2 has been proposed.[15]

$\tilde{C}\ ^1A'$ C_s Structure: AB[11]
T_0=29687.72 gas AB[1,7,11]LF[12,13,16,17] $\tilde{C}-\tilde{X}$ 250–395 nm
29285(20) Xe AB[4] $\tilde{C}-\tilde{X}$ 280–342 nm
Predissociation limit between 31172 and 31307. AB[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SO stretch	1032	gas	AB,LF	11,13,16
	2	Bend	253	gas	AB,LF	11,13,16
	3	SS stretch	410.6	gas	AB,LF	7,11,13, 16,17
			415(20)	Xe	AB	4

τ=66(4) ns gas LF[17]
A_0=1.016; B_0=0.149; C_0=0.130 AB[11]LF[17]

$\tilde{a}\ ^3A'$ C_s
T_0=13943 gas AB[10,15]LF[13] $\tilde{a}-\tilde{X}$ 430–670 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SO stretch	1089	gas	AB	10,15
	2	Bend	332	gas	AB	10,15
	3	SS stretch	505	gas	AB	10,15

$\tilde{X}\ ^1A'$ C_s Structure: MW[2,6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SO stretch	1166.45	gas	IR,DL	1,3,14
			1156.2	Ar	IR,Ra	8,9
	2	Bend	380	gas	LF	16
			382	Ar	IR,Ra	8,9
	3	SS stretch	679.1	gas	IR,LF	1,3,13
			672.2	Ar	IR,Ra	8,9

A_0=1.398; B_0=0.169; C_0=0.150 MW[2,5,6]DL[14]

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S_3

T_0=23465(15) gas AB[1,2,5,7] 350–510 nm
23210 Ar AB[4,6,8] 355–435 nm
Kr AB[1,2] 310–420 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	420	gas	AB	2
			450T	Ar	AB	4,8
			420	Kr	AB	2
	2	Bend	340T	Ar	AB	8

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	590	gas	AB	2
			581	gas	Ra	9
			583	Ar	Ra,IR	3,6
	2	Bend	281	gas	Ra	9
b_2	3	Asym. stretch	680.0	Ar	IR	6,8
			676.2			
			674.5			

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SeO_2

$^1B_2$ C_{2v} Structure: AB[10]
T_0=31957.4 gas AB[1,9,10]EM[4] $^1B_2$–$\tilde{X}$ 225–345 nm
31065(20) Xe AB[6] $^1B_2$–$\tilde{X}$ 242–322 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	648.8	gas	AB	1,9
			620T	Xe	AB	6
	2	Bend	258	gas	AB	9

$^3B_2$ C_{2v} Structure: AB[11]
T_0=23840 gas AB[2,11]EM[4] $^3B_2$–$\tilde{X}$ 370–500 nm
Kr EM[6] $^3B_2$–$\tilde{X}$ 475–600 nm
Xe EM[6] $^3B_2$–$\tilde{X}$ 475–615 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	780	gas	AB	11
	2	Bend	199	gas	AB,EM	2,4,11
b_2	3	Asym. stretch	863	gas	AB	11

τ<200(100) μs Xe EM[6]

$\tilde{X}\ ^1A_1$ C_{2v} Structure: MW[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	922.6	gas	AB,PE	9,11,12
			923.4	Ne	IR	5
			922.0w	Ar	IR	5,8,13
	2	Bend	372	gas	AB	9,11
			366.0s	Ar	IR	8,13
			365T	Kr,Xe	EM	6
b_2	3	Asym. stretch	963	gas	IR,AB	3,11
			971.2	Ne	IR	5
			970.2			
			965.3s	Ar	IR	5,8,13

A_0=0.962; B_0=0.289; C_0=0.222 MW[7]

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SeOO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OO stretch	1061.0T	Ar	IR	1

Reference

[1] G. D. Brabson, L. Andrews, and C. J. Marsden, J. Phys. Chem. **100**, 16487 (1996).

SeSeO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SeO stretch	883.2	Ar	IR	1

Reference

[1] G. D. Brabson, L. Andrews, and C. J. Marsden, J. Phys. Chem. **100**, 16487 (1996).

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
			1071.6	Ne	IR	15
			1069m	Ar	IR	7,9
			1070	N_2	IR	2,3
	2	Bend	573w	N_2	IR	3
b_2	3	Asym. stretch	942.48	gas	IR,DL LMR	2,10, 13,14
			936.0	Ne	IR	15
			932vs	Ar	IR	7,9
			931	N_2	IR	2,3

A_0=2.351; B_0=0.396; C_0=0.338 MW[8]DL[12]

[a]Average value.

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NFCl

$\tilde{A}$ C_s
gas EM[1] $\tilde{A}-\tilde{X}$ 380–500 nm
Ar AB[3]EM[4] $\tilde{A}-\tilde{X}$ 300–525 nm

In the gas phase, an emission maximum is observed[1] near 23500 (425 nm). In an argon matrix, an absorption maximum is observed[3] at 27800 (360 nm), and an emission maximum appears[4] near 21200 (472 nm). Ref. 4 discusses reasons for the disparity between the gas-phase and the argon-matrix observations.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	340(20)	Ar	AB	3

τ<20 ns gas EM[1]
=610(40) ns Ar EM[4]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NF stretch	917[a]	Ar	IR	2
	2	Bend	390(40)	gas	EM	1
			390T	Ar	EM	4
	3	NCl stretch	720[a]	Ar	IR	2

[a]Similar values, not explicitly given, were obtained in krypton and xenon matrix experiments.

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PF_2

$\tilde{M}$ C_{2v}
T_0=68505(5) gas MPI[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	972(7)[a]	gas	MPI	4
	2	Bend	345(3)[a]	gas	MPI	4

$\tilde{L}$ C_{2v}
T_0=67922(5) gas MPI[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	956(2)	gas	MPI	4
	2	Bend	358(3)	gas	MPI	4

$\tilde{K}$ C_{2v}
T_0=66763(5) gas MPI[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	956(2)	gas	MPI	4
	2	Bend	364(1)	gas	MPI	4

$\tilde{J}$ C_{2v}
T_0=66118(5) gas MPI[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	981(4)[a]	gas	MPI	4
	2	Bend	366(1)[a]	gas	MPI	4

$\tilde{I}$ C_{2v}
T_0=65958(5) gas MPI[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	980(4)[a]	gas	MPI	4
	2	Bend	365(3)[a]	gas	MPI	4

$\tilde{H}$ C_{2v}
T_0=60962(5) gas MPI[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1004(2)	gas	MPI	4

$\tilde{G}$ C_{2v}
T_0=58184(5) gas MPI[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	998(2)	gas	MPI	4

$\tilde{F}$ $^2A_1$ C_{2v}
T_0=55126(5) gas MPI[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1008(2)	gas	MPI	4

$\tilde{E}$ $^2B_1$ C_{2v}
T_0=51932(5) gas MPI[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1016(2)[a]	gas	MPI	4
	2	Bend	408(2)[a]	gas	MPI	4

$\tilde{a}$ $^4A_2$ C_{2v}
T_0=23998(6) gas EM[3] $\tilde{a}-\tilde{X}$ 400–520 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	505(2)	gas	EM	3
	2	Bend	219	gas	EM	3

$\tau \geqslant 1.9$ ms gas EM[3]

$\tilde{X}$ $^2B_1$ C_{2v} Structure: MW[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	841(4)	gas	EM	3
			852.1ms	Ar	IR	1
	2	Bend	366	gas	MW,EM	2,3
b_2	3	Asym. stretch	848(24)	gas	MW	2
			831.4s	Ar	IR	1

A_0=0.933; B_0=0.310; C_0=0.232 MW[2]

[a]ω.

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PCl_2

$\tilde{E}(4p)$ C_{2v}
T_0=51320(10) gas MPI[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	600(15)	gas	MPI	3
	2	Bend	240(15)	gas	MPI	3

$\tilde{D}\ ^2A_1(4s)$ C_{2v}
T_0=42760(15) gas MPI[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	620(20)	gas	MPI	3
	2	Bend	230(20)	gas	MPI	3

$\tilde{A}\ ^2A_1$ C_{2v}
In the gas phase, unstructured emission at wavelengths longer than 370 nm, with a maximum at approximately 460 nm, has been attributed[2] to PCl_2.
τ=29(6) μs gas EM[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	525(10)	gas	MPI	3
			525	Ar	IR	1
b_2	3	Asym. stretch	452	Ar	IR	1

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PBr_2

$\tilde{A}\ ^2A_1$ C_{2v}
In the gas phase, unstructured emission at wavelengths longer than 510 nm, with a maximum at 527 nm, has been attributed[2] to PBr_2.
τ=21(9) μs gas EM[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	369	Ar	IR	1
	2	Bend	140T	gas	EM	3
b_2	3	Asym. stretch	410	Ar	IR	1

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AsF_2

$\tilde{H}$ C_{2v}
T_0=57480(15) gas MPI[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	810(10)	gas	MPI	3
	2	Bend	310(20)	gas	MPI	3

$\tilde{F}$ C_{2v}
T_0=54355(15) gas MPI[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	813(6)	gas	MPI	3
	2	Bend	308(5)	gas	MPI	3

When gas-phase AsF_3 is subjected to 124 nm radiation, an emission band system, tentatively assigned to AsF_2, is observed between 330 and 610 nm, with a maximum near 450 nm.[1] The radiative lifetime of the species which contributes this band system is 25.5(1.8) μs.[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	705(10)	gas	MPI	3
	2	Bend	285(10)	gas	MPI	3

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O_3^-

$\tilde{C}\ ^2A_1$ C_{2v}
T_0=21420(40) gas PF[10]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	760(20)	gas	PF	10
	2	Bend	190(20)	gas	PF	10

Threshold for electron detachment from ground-state O_3^-=16970(20) gas PE[9]PD[11]

$\tilde{A}\ ^2A_2$ C_{2v}
T_0=16508(16) gas PF[8,10]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	815(10)	gas	PF	8,10
	2	Bend	275(10)	gas	PF	8,10

$\tilde{X}\ ^2B_1$ C_{2v} Structure: $PD^{11}PE^{13}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	975(50)	gas	PD,PF PE	8–10,13
			1016 Cs	Ar	Ra	3,5
			1011 Na	Ar	Ra	3,5
	2	Bend	550(50)	gas	PD,PF PE	9,10,13
			600w Cs	Ar	IR	4
b_2	3	Asym. stretch	880(50)	gas	PE	13
			796.3	Ne	IR	12,14
			804.3	Ar	IR	6,7
			789s Cs	Ar	IR	2,4
			802s Cs			
			802s Na	Ar	IR	1,2,4

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ClOO

An unstructured absorption between 225 and 270 nm, with a maximum near 246 nm in the gas phase[3–6] and near 250 nm in a neon[8] or an argon[7] matrix, has been assigned to ClOO, which photodecomposes in that spectral region.

$\tilde{X}$ C_s Structure: IR[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OO stretch	1443[a]	gas	IR	4
			1438.6	Ne	IR	8
			1442.8vs[b]	Ar	IR	2,7
			1438	N_2	IR	1
			1428			
			1436	O_2	IR	7
	2	Bend	413.7	Ne	IR	8
			408.3vw[b]	Ar	IR	2,7
	3	ClO stretch	201.4	Ne	IR	8
			192.4w	Ar	IR	7
			203	O_2	IR	7

[a]Absorption maximum; spectral slit width 13 cm^{-1}.
[b]Peaks at 1415, 435, and 227 cm^{-1} may be contributed by ClOO trapped in a metastable site in the argon lattice.[7,8]

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[1] M. M. Rochkind and G. C. Pimentel, J. Chem. Phys. **46**, 4481 (1967).
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BrOO

In an argon matrix, a prominent absorption between 240 and 300 nm, with maximum at 38200 (262 nm), has been assigned[3] to BrOO. Irradiation at 280 nm leads to photoisomerization to OBrO.[4]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	1485.1	Ar	IR	1–4

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IOO

In an argon matrix, an absorption maximum at 39370 (254 nm) has been attributed[1] to IOO. Irradiation of the sample in the spectral region of this absorption results in photoisomerization to OIO.

Reference

[1] G. Maier and A. Bothur, Chem. Ber. **130**, 179 (1997).

SeO_2^-

Threshold for electron detachment from ground-state $SeO_2^- = 14710(400)$ gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	810(80)	gas	PE	1

Reference

[1] J. T. Snodgrass, J. V. Coe, K. M. McHugh, C. B. Freidhoff, and K. H. Bowen, J. Phys. Chem. **93**, 1249 (1989).

SSF

$\tilde{A}\ ^2A'$ C_s Structure: LF[1,2]
T_0=14922 gas LF[1,2] $\tilde{A}-\tilde{X}$ 485–700 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SF stretch	768	gas	LF	1
	2	Bend	217	gas	LF	1
	3	SS stretch	495	gas	LF	1

A_{005}=0.662; B_{005}=0.157; C_{005}=0.126 LF[1,2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SF stretch	705	gas	LF	1
	2	Bend	293	gas	LF	1
	3	SS stretch	684	gas	LF	1

A_0=0.886; B_0=0.162; C_0=0.137 LF[1]MW[3]

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SSCl

T_0=21650T gas[a] AB[1,2,5] 378–481 nm
⩽21925 Ar AB[3] 389–456 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	Stretch	480	gas	AB	5
			491(20)	Ar	AB	3
	3	Stretch	407	gas	AB	5

$\tilde{A}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SS stretch	630	gas	LF	7,8
	2	Bend	249	gas	LF	7,8
	3	SCl stretch	554	gas	LF	7,8

$\tilde{X}\ ^2A''$ C_s Structure: MW[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SS stretch	662(3)	gas	AB,Ra,LF	5,7,8
			665	Ar	IR	4
	2	Bend	196	gas	Ra,LF	7,8
	3	SCl stretch	450	gas	Ra,LF	7,8
			404	Ar	IR	4

A_0=0.611; B_0=0.094; C_0=0.082 MW[6]

[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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OClO

$\tilde{E}$
T_0=63774 gas AB[12,19,45] $\tilde{E}-\tilde{X}$ 148–157 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	1000T	gas	AB	12
	2	Bend	508	gas	AB	12,19

$\tilde{D}$
T_0=61430(20) gas AB[12,19,42,45] $\tilde{D}-\tilde{X}$ 155–163 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	1051(20)	gas	AB	12,19,42
	2	Bend	521(20)	gas	AB	12,19,42

$\tilde{C}\ ^2A_1$ C_{2v}
T_0=54689(20) gas AB[12,19,42,45] $\tilde{C}-\tilde{X}$ 176–183 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1020(20)	gas	AB	12,19,42

$^2A_1, ^2B_2$ C_{2v}
These two as yet undetected states are expected to lie close to the $\tilde{A}$ state and to interact strongly with it. One or both of them may contribute to the much-studied predissociation of the $\tilde{A}$ state.[21,24,29,35,40,46,47]

$\tilde{A}\ ^2A_2$ C_{2v}[a] Structure: AB[25]
T_0=21017.2 gas AB[1,2,5,14,25,31,32,34,35,45]LF[15,16]MPI[33,36]PF[41,43,47] $\tilde{A}-\tilde{X}$ 260–780 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	711.5	gas	AB	5,14,34
	2	Bend	292.5	gas	AB	5,14,34
b_2	3	Asym. stretch	441.2	gas	AB	25,34

τ_1[b]=56(20) ps gas AB[21,24]LF[29]
τ_2[c]=336(27) ps gas LF[29]
A_0=1.057; B_0=0.311; C_0=0.240 AB[25]

$\tilde{X}\ ^2B_1$ C_{2v} Structure: MW[6,30]IR[26]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	945.59s	gas	IR,AB	3–5,14–16
					LF	20,23,26
					LMR	
					DL,LS	28,37,39
			944.8m	Ne	IR	44
			947.6m	Ar	IR,Ra	13,17,18
						44
			942	Kr	Ra	18
			940(2)	Xe	Ra	18
			950(2)	N_2	Ra	18
	2	Bend	447.70s	gas	IR,AB	4,5,14–16
					LF	22,25,38
						39
			448.7m	Ne	IR	44
			451s	Ar	IR,LF	13,17,18
			447s			44
			447	Kr	LF	18
b_2	3	Asym. stretch	1110.11vs	gas	IR	3,14,26
						38,39
			1107.6vs	Ne	IR	44
			1106.5vs	Ar	IR	13,17,44
			1100.8vs			

A_0=1.737; B_0=0.332; C_0=0.278 MW[6-10,27]IR[37,38]

[a]Double minimum in potential for antisymmetric stretch,[11,25] with barrier height of 1153.[34]
[b]For $F_1(J=N+\frac{1}{2})$ spin states.
[c]For $F_2(J=N-\frac{1}{2})$ spin states.

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OBrO

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

$T_0 \leq 16509$ gas AB[2] $\tilde{A}-\tilde{X}$ 420–605 nm

16785(20) Ar AB[3,5] $\tilde{A}-\tilde{X}$ 400–650 nm

Irradiation of the argon-matrix deposit in this spectral region leads to photoisomerization to BrOO.[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	615T	gas	AB	2
			631T	Ar	AB	5
	2	Bend	200T	gas	AB	2
			221T	Ar	AB	5
b_2	3	Asym. stretch	365HT	gas	AB	2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	795.7	Ar	IR	3,5
	2	Bend	317.0	Ar	IR	5
b_2	3	Asym. stretch	848.6	gas	IR	4
			845.2	Ar	IR	1,3,5

A_0=0.935; B_0=0.275; C_0=0.212 MW[4]

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OIO

$\tilde{A}$ C_{2v}
T_0=14553(7)T gas AB[2] $\tilde{A}-\tilde{X}$ 480–662 nm

In an argon matrix, structured absorption between 467 and 634 nm, with maximum at 18180 (550 nm), has been assigned[3] to OIO.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	631(3)	gas	AB	2
	2	Bend	177(2)	gas	AB	2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	765(25)	gas	PE	1
			768.0wm	Ar	IR	3
			769.5	O_2	IR	3
	2	Bend	192(35)	gas	PE	1
b_2	3	Asym. stretch	800.3vs	Ar	IR	3
			801.3	O_2	IR	3

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NF_2^-

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	994.7m	Ne	IR	1
	2	Bend	431H	Ne	IR	1
b_2	3	Asym. stretch	862.4s	Ne	IR	1

Reference

[1] M. E. Jacox and W. E. Thompson, J. Chem. Phys. **102**, 6 (1995).

BrOCl

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ClO stretch	675.9	Ar	IR	1
	3	BrO stretch	559.5	Ar	IR	1

Reference

[1] M. Bahou, L. Schriver-Mazzuoli, A. Schriver, and P. Chaquin, Chem. Phys. **216**, 105 (1997).

BrOBr

In the gas phase, a prominent absorption maximum near 50000 (200 nm) and a less prominent absorption maximum near 31800 (314 nm), with a broad shoulder which has its onset near 22700 (440 nm) and on which structure with separations of ~500 is partially resolved, have been assigned[4] to BrOBr.

In a nitrogen matrix, a strong absorption maximum at approximately 47000, a weaker shoulder near 31200, and a much weaker shoulder near 22100 have been attributed[3] to electronic transitions of BrOBr.

$\tilde{X}$ C_{2v} Structure: EXAFS[3] MW[5,6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	526.1s	Ar	IR	1,2
			528	N_2	IR	3
b_2	3	Asym. stretch	623.4w	Ar	IR	2
			626	N_2	IR	3

A_0=1.108; B_0=0.046; C_0=0.044 MW[5,6]

References

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SF_2

$\tilde{E}$ **4*p* Rydberg state** C_{2v}
T_0=62015(30) gas MPI[10]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	931(59)	gas	MPI	10
	2	Bend	383(42)	gas	MPI	10

$\tilde{C}$
gas MPI[10] $\tilde{C}-\tilde{X}$ 165–175 nm

$\tilde{B}$ $^1B_1(4s)$ C_{2v}
T_0=54433(30) gas MPI[10]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	991(12)	gas	MPI	10
	2	Bend	361(24)	gas	MPI	10

$\tilde{A}$

T_0=18100(1000) gas CL[7,8,11] $\tilde{A}-\tilde{X}$ 550–850 nm

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	Bend	243(6)	gas	CL	11

$\tilde{X}$ C_{2v} Structure: MW[1,2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	838.53	gas	IR,CL	5,7–9,11
			834	Ne	IR	3
			832vs	Ar	IR	3,12
			825	N_2	IR	3
	2	Bend	355(2)	gas	MW,CL	2,7–9,11
			358	Ne	IR	3
			358m	Ar	IR	3
			358	N_2	IR	3
b_2	3	Asym. stretch	813.04	gas	IR,CL	5,11
			807.5	Ne	IR	3
			804vs	Ar	IR	3,12
			795	N_2	IR	6

A_0=0.898; B_0=0.307; C_0=0.228 MW[1,2,13]

References

[1] D. R. Johnson and F. X. Powell, Science **164**, 950 (1969).
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FSCl

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SF stretch	781vs	Ne	IR	1
			778vs	Ar	IR	1
	2	Bend	277vw	Ne	IR	1
			274vw	Ar	IR	1
	3	SCl stretch	552s[a]	Ne	IR	1
			543s[a]	Ar	IR	1

A_0=0.738; B_0=0.157; C_0=0.130 MW[2]

[a]In Fermi resonance with $2\nu_2$.

References

[1] H. Willner, Z. Naturforsch. **39B**, 314 (1984).
[2] J. Preusser and M. C. L. Gerry, J. Chem. Phys. **106**, 10037 (1997).

FSBr

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SF stretch	765	Ar	IR	1
	3	SBr stretch	434	Ar	IR	1

Reference

[1] C. O. Della Védova and H.-G. Mack, Inorg. Chem. **32**, 948 (1993).

SeF_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	699	Ar	IR	1
b_2	3	Asym. stretch	672	Ar	IR	1

Reference

[1] A. Haas and H. Willner, Z. Anorg. Allg. Chem. **454**, 17 (1979).

ClClO

In an argon matrix, an absorption maximum at 38500 (260 nm) has been attributed[5,6] to ClClO.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ClO stretch	961.6s	Ar	IR,Ra	3–6
			963	N_2	IR	1,2
	2	Bend	240.2wm	Ar	IR,Ra	3,5,6
	3	ClCl stretch	374.2ms	Ar	IR,Ra	3,5,6
			377	N_2	IR	1,2

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BrClO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ClO stretch	940.5	Ar	IR	1,2

°References

[1] L. Schriver-Mazzuoli, O. Abdelaoui, C. Lugez, and A. Schriver, Chem. Phys. Lett. **214**, 519 (1993).
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ClBrO

In an argon matrix, irradiation at 633 nm results in isomerization to BrClO, and irradiation at 870 nm to BrOCl.[2]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	BrO stretch	819.6	Ar	IR	1,2

References

[1] L. Schriver-Mazzuoli, O. Abdelaoui, C. Lugez, and A. Schriver, Chem. Phys. Lett. **214**, 519 (1993).
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BrBrO

In an argon matrix, irradiation at 870 nm results in photoisomerization to BrOBr.[3]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	BrO stretch	805.4	Ar	IR	1–3
	3	BrBr stretch	236	Ar	IR	1

References

[1] D. E. Tevault, N. Walker, R. R. Smardzewski, and W. B. Fox, J. Phys. Chem. **82**, 2733 (1978).
[2] L. Schriver-Mazzuoli, O. Abdelaoui, C. Lugez, and A. Schriver, Chem. Phys. Lett. **214**, 519 (1993).
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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[3,7]

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	235.05	gas	IR	2,6
			236m	Ar	IR	1
Σ_u^+	3	Asym. stretch	592.52	gas	IR	2,3,7
			580s	Ar	IR	1

B_0=0.125 IR[3,6,7]

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XeF_2

$6p\ ^1\Sigma_g$ $D_{\infty h}$
T_0=87400 gas AB[11] $6p\ ^1\Sigma_g-\tilde{X}$ 114 nm
A higher member of this Rydberg series has also been reported.[11]

$5d\ ^1\Pi_{u,1/2}$ $D_{\infty h}$
T_0=86000 gas AB[3,4,11] $5d\,^1\Pi_{u,1/2}-\tilde{X}$ 116 nm
Higher members of this Rydberg series have also been reported.[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	484(24)	gas	AB	11
Π_u	2	Bend	200T	gas	AB	11

$5d\ ^1\Pi_{u,3/2}$ $D_{\infty h}$
T_0=80800 gas AB[3,4,11] $5d\,^1\Pi_{u,3/2}-\tilde{X}$ 124 nm
Higher members of this Rydberg series have also been reported.[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	524(8)	gas	AB	11
Π_u	2	Bend	200T	gas	AB	11

$6s\ ^1\Pi_{u,1/2}$ $D_{\infty h}$
T_0=73870 gas AB[3,4,8,11] $6s\,^1\Pi_{u,1/2}-\tilde{X}$ 135 nm
Higher members of this Rydberg series have also been reported.[3,4,11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	500(16)	gas	AB	11

6s $^1\Pi_{u,3/2}$ $D_{\infty h}$
T_0=69300 gas AB[3,4,8,11] $6s\,^1\Pi_{u,3/2}-\tilde{X}$ 144 nm
Higher members of this Rydberg series have also been reported.[3,4,11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	532(8)	gas	AB	11
Π_u	2	Bend	73(8)	gas	AB	11

$\tilde{B}$ $^1\Sigma_u$ $D_{\infty h}$
T^a=63300 gas AB[3,4,11] $\tilde{B}-\tilde{X}$ 158 nm

$\tilde{A}$ $^1\Pi_g$ $D_{\infty h}$
T^a=43500 gas AB[3,4,6,11] $\tilde{A}-\tilde{X}$ 230 nm

$\tilde{X}$ $^1\Sigma_g$ $D_{\infty h}$ Structure: IR[7,14,16]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	516.5(5)	gas	Ra	9,13
			512	Ar	Ra	10
			512	Xe	Ra	10
Π_u	2	Bend	213.08s	gas	IR	5,14,15
			215	Ar	IR	12
Σ_u^+	3	Asym. stretch	561.94s	gas	IR	1,5,7,14
			547	Ar	IR	2

B_0=0.113 IR[7,14,15]

[a]Absorption maximum.

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[16] H. Bürger, R. Kuna, S. Ma, J. Breidung, and W. Thiel, J. Chem. Phys. **101**, 1 (1994).

Ar_2F

4 $^2\Gamma$ C_{2v}
Unstructured gas-phase emission[1–3] between 250 and 340 nm, with maximum near 34250 (292 nm). Predissociated at 248 nm to ArF + Ar.[5] In a neon matrix, the emission maximum is shifted to 33240 (301 nm),[7] and in an argon matrix to 28170 (355 nm).[6]
τ=185(46) ns gas EM[4]
180(10) ns Ar EM[6]

References

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[2] N. G. Basov, V. A. Danilychev, V. A. Dolgikh, O. M. Kerimov, V. S. Lebedev, and A. G. Molchanov, Pis'ma Zh. Éksp. Teor. Fiz. **26**, 20 (1977); J. Exp. Theor. Phys. Lett. **26**, 16 (1977).
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ArKrF

Unstructured gas-phase emission[1,2] between 240 and 370 nm, with maximum near 32790 (305 nm). In solid argon, the emission maximum appears near 29150 (343 nm) and has a radiative lifetime of 60(5) ns.[3]

References

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Kr_2F

9 $^2\Gamma$ C_{2v}
gas AB[6,8,9,12] $9^2\Gamma-4^2\Gamma$ 280–360 nm
Broad absorption, with maximum near 31750 (315 nm). Predissociated into KrF (D) + Kr.[12]

6 $^2\Gamma$ C_{2v}
gas AB[12] $6^2\Gamma-4^2\Gamma$ 590–840 nm
Broad absorption, with maximum near 14080 (710 nm). Predissociated into KrF (C) + Kr.[12]

4 $^2\Gamma$ C_{2v}
Unstructured gas-phase emission[1–4] between 340 and 480 nm, with maximum near 24390 (410 nm). In solid neon, the emission maximum is shifted to 23240 (430 nm).[11] In solid argon, the emission maximum appears near 22780 (439 nm), and in solid krypton the excitation maximum appears near 36360 (275 nm) and the emission maximum near 22080 (453 nm).[10]
τ=200(28) ns gas LF[5]EF[7]
140(10) ns Kr LF[10]

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[2] N. G. Basov, V. A. Danilychev, V. A. Dolgikh, O. M. Kerimov, V. S. Lebedev, and A. G. Molchanov, Pis'ma Zh. Éksp. Teor. Fiz. **26**, 20 (1977); J. Exp. Theor. Phys. Lett. **26**, 16 (1977).
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KrXeF

Unstructured gas-phase emission between 340 and 460 nm, with maximum near 400 nm, has been attributed[1–3] to KrXeF.

References

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Xe_2F

4 $^2\Gamma$ C_{2v}
gas EM[1–3] $4^2\Gamma-1,2^2\Gamma$
Unstructured emission maximum at 16300 (614(5) nm), with bandwidth (FWHM) of 125(5) nm.

Ne LF[5] $4^2\Gamma-1,2^2\Gamma$
Excitation maximum near 28600 (350 nm), and emission maximum at 14000 (714 nm).

Xe EM[4] $4^2\Gamma-1,2^2\Gamma$
Unstructured emission maximum at 12900 (775 nm), with bandwidth (FWHM) of 2300 cm^{-1}.
τ=152(+19,−10) ns gas EM[2]
250 ns Ne LF[5]
190(10) ns Xe EM[4]

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8.4. Four-Atomic Trihydrides

TiH_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		TiH stretch	1580.6	Ar	IR	1

TiD_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		TiD stretch	1147.2	Ar	IR	1

Reference

[1] G. V. Chertihin and L. Andrews, J. Am. Chem. Soc. **116**, 8322 (1994).

ZrH_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ZrH stretch	1545.3	Ar	IR	1

ZrD_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ZrD stretch	1110.3	Ar	IR	1

Reference

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HfH_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		HfH stretch	1646	Ar	IR	1

HfD_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		HfD stretch	1180.2	Ar	IR	1

Reference

[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. **99**, 15004 (1995).

FeH_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		FeH_3 stretch	1646.1	Ar	IR	1

FeD_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		FeD_3 stretch	1193.2	Ar	IR	1

Reference

[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. **99**, 12131 (1995).

ThH_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	ThH_3 stretch	1435.4 1434.1	Ar	IR	1

ThD_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	ThD_3 stretch	1025.9 1024.8	Ar	IR	1

Reference

[1] P. F. Souter, G. P. Kushto, L. Andrews, and M. Neurock, J. Phys. Chem. A **101**, 1287 (1997).

UH_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	UH_3 stretch	1346.8	Ar	IR	1

UD_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	UD_3 stretch	962.5	Ar	IR	1

Reference

[1] P. F. Souter, G. P. Kushto, L. Andrews, and M. Neurock, J. Am. Chem. Soc. **119**, 1682 (1997).

BH_3

$\tilde{X}\ ^1A_1'$ D_{3h} Structure: IR[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	1147.50 1129.2	gas Ar	DL,IR IR	2,5 1,4
e'	3	BH_3 stretch	2601.57 2587.3	gas Ar	IR IR	3 4
	4	Deformation	1196.7	gas	IR	5

$B_0 = 7.874$; $C_0 \cong 3.879$ IR[3]

BD_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	878.5	Ar	IR	4
e'	3	BD_3 stretch	1953.4	Ar	IR	4

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AlH_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	697.8m	Ar	IR	1–3
e'	3	AlH_3 stretch	1882.8vs	Ar	IR	1–3
	4	Deformation	783.4m	Ar	IR	1–3

AlD_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	512.5s	Ar	IR	1–3
e'	3	AlD_3 stretch	1377.9vs	Ar	IR	1–3
	4	Deformation	568.5m	Ar	IR	1–3

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[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. **97**, 10295 (1993).
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GaH_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	717.4ms	Ar	IR	1
e'	3	GaH_3 stretch	1923.2vs	Ar	IR	1
	4	Deformation	758.7s	Ar	IR	1

GaD_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	517.5s	Ar	IR	1
e'	3	GaD_3 stretch	1387.7vs	Ar	IR	1
	4	Deformation	544.0m	Ar	IR	1

Reference

[1] P. Pullumbi, Y. Bouteiller, L. Manceron, and C. Mijoule, Chem. Phys. **185**, 25 (1994).

InH_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	613.2m	Ar	IR	1
e'	3	InH_3 stretch	1754.5vs	Ar	IR	1
	4	Deformation	607.8s	Ar	IR	1

InD_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	439.7	Ar	IR	1
e'	3	InD_3 stretch	1261.2	Ar	IR	1
	4	Deformation	433.3	Ar	IR	1

Reference

[1] P. Pullumbi, Y. Bouteiller, L. Manceron, and C. Mijoule, Chem. Phys. **185**, 25 (1994).

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	3–5

B_0=9.362 LD[3-5]

CD_3^+

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	1070(30)	gas	PE	2

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SiH_3^+

$\tilde{X}$ D_{3h} Structure: DL[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	838.067	gas	DL	1,2
e'	4	SiH stretch	938.397	gas	DL	2

B_0=5.214; C_0=2.585 DL[1,2]

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CH_3

4f $^2E'$ [a] D_{3h}
T_0 = 72508 gas MPI[12]
Higher member of Rydberg series observed at 74961. MPI[12]

4p $^2A_2''$ D_{3h}
T_0 = 69853.44(13) gas MPI[15]
B_0 = 9.90 gas MPI[15]

3d $^2A_1'$ D_{3h} Structure: AB[2]
T_0 = 66805 gas AB[1,2] $3d^2A_1'-\tilde{X}$ 147–150 nm
Ar AB[3] $3d^2A_1'-\tilde{X}$ ~150.3 nm
First member of Rydberg series converging to 79392(5). Higher members observed at 72326, 74851, 76256, 77090, and 77643. AB[2]
B_0 = 10.72(8) AB[2]

3d $^2E''$ D_{3h} Structure: AB[2]
T_0=66536 gas AB[1,2]MPI[10] $3d^2E''-\tilde{X}$ 144-150 nm
Ar AB[3] $3d^2E''-\tilde{X}$ ~150.3 nm
Diffuse. First member of Rydberg series converging to 79392(5). Higher members observed at 72165, 74851, 76256, 77090, and 77643. AB[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	1372H	gas	AB,MPI	2,10

3p $^2A_2''$ D_{3h} Structure: MPI[12]
T_0=59972 gas MPI[12,28]
Higher member of Rydberg series observed at 69837. MPI[12]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	CH stretch	2914	gas	MPI	12
a_2''	2	OPLA	1334	gas	MPI	12

B_0=9.51(7); C_0=4.62(3) MPI[28]

3s $^2A_1'$ D_{3h} Structure: AB[2]
T_0=46205 gas AB[1,2,7]Ra[24] $3s^2A_1'-\tilde{X}$ 216 nm
Diffuse. First member of Rydberg series converging to 79392(5). Next member observed at 71042. AB[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	CH stretch	2040T	gas	Ra	24

$\tilde{X}$ $^2A_2''$ D_{3h} Structure: AB[2]IR[9,18]CAR[23,26]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	CH stretch	3004.43(2)	gas	CAR	13,16,23
					Ra	26
a_2''	2	OPLA	606.453	gas	IR,DL	5,9,21
			617vs	Ne	IR	4
			603[b]	Ar	IR	3,8
			611	N_2	IR	3
e'	3	CH stretch	3160.821	gas	LD	11,25,27
					CC	30
			3162wm	Ne	IR	4
			3150	Ar	IR	6
			3171.4	H_2	IR	29
			3170.6			
	4	Deformation	1396w	Ne	IR	4
			1398[c]	Ar	IR	8
			1402.7	H_2	IR	29
			1401.6			

B_0=9.578 AB[2]DL[9]; C_0=4.742 DL[9]

CD_3

4f $^2E'$ [a] D_{3h}
T_0=72431 gas MPI[12]
Higher member of Rydberg series observed at 74885. MPI[12]

4p $^2A_2''$ D_{3h}
T_0=69777.40(4) gas MPI[15]
B_0=4.846(2) gas MPI[15]

3d $^2A_1'$ D_{3h} Structure: AB[2]
T_0=66715 gas AB[1,2] $3d^2A_1'-\tilde{X}$ 145–150 nm
Ar AB[3] $3d^2A_1'-\tilde{X}$ ~150.3 nm
First member of Rydberg series converging to 79315(5). Higher members observed at 72296, 74781, 76181, 77023, 77562, and 77933. AB[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	1040H	gas	AB	2

B_0=5.14 AB[2]

3d $^2E''$ D_{3h} Structure: AB[2]
T_0=66465 gas AB[1,2]MPI[10] $3d^2E''-\tilde{X}$ 146–150 nm
Ar AB[3] $3d^2E''-\tilde{X}$ ~150.3 nm
Diffuse. First member of Rydberg series converging to 79315(5). Higher members observed at 72180, 74753, 76166, 77023, 77562, and 77933. AB[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	1031H	gas	AB,MPI	2,10

3p $^2A_2''$ D_{3h} Structure: MPI[1]
T_0=59886 gas MPI[12,17]
Higher members of Rydberg series observed at 69789, 73645, and 75557. MPI[12]

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

B_0=4.76(2); C_0=2.38 MPI[12,17]

3s $^2A_1'$ D_{3h} Structure: AB^2

T_0=46629 gas $AB^{1,2,7}Ra^{24}$ $3s^2A_1'-\tilde{X}$ 204–225 nm

First member of Rydberg series converging to 79315(5). Higher members observed at 70910, 74246, 75869, and 76830. AB^2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	CD stretch	1684[d]	gas	AB	7
a_2''	2	OPLA	1094	gas	AB,Ra	7,24

B_0=4.42 AB^2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	CD stretch	2157.5(2)	gas	Ra, CAR	19,20
a_2''	2	OPLA	457.81	gas	DL	14,18
			463s	Ne	IR	4
			453[b]	Ar	IR	3,8
			463	N_2	IR	3
e'	3	CD stretch	2381.09	gas	IR,DL	22,31
			2381w	Ne	IR	4
			2369	Ar	IR	6
	4	Deformation	1026vw	Ne	IR	4
			1029	Ar	IR	6

B_0=4.802 AB^2DL[14]

[a]Tentative assignment.
[b]Band center. Rotational structure assigned.[8]
[c] $^RR(0_0)$ transition.
[d]Approximate value; perturbed by Fermi resonance.

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SiH_3

$\tilde{M}$ $^2A_2''$ (6p) D_{3h}

T_0=60341 gas MPI[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	800(30)	gas	MPI	7

$\tilde{L}$ (5d) D_{3h}

T_0=59615(30)[c] gas MPI[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	839(26)	gas	MPI	8

$\tilde{J}'$ (4d) D_{3h}

T_0=57726(30) gas MPI[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	835(26)	gas	MPI	8

$\tilde{J}$ $^2A_2''$ (5p) D_{3h}

T_0=56929 gas MPI[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	821(4)	gas	MPI	7

$\tilde{I}'$ (4d) D_{3h}

T_0=56253(30) gas MPI[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	814(25)	gas	MPI	8

$\tilde{D}\ ^2A_1'$ (3*d*) D_{3h}
T_0=49787(30) gas MPI[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	810(31)	gas	MPI	8

$\tilde{E}\ ^2A_2''$ (4*p*) D_{3h}
T_0=48438 gas MPI[5,7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	796(7)	gas	MPI	5,7
e'	4	Deformation	870(5)H	gas	MPI	7

$\tilde{A}\ ^2A_1$ C_{3v}
gas AB[9] $\tilde{A}-\tilde{X}$ 205–250 nm

$\tilde{X}\ ^2A_1$ C_{3v} Structure: ESR[1,2]DL[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Umbrella	727.94[a]	gas	DL,MPI	3,6,7
			721.05[b]	gas	DL,MPI	3,6,7
e	3	SiH_3 stretch	2185.2	gas	DL	10

Barrier to inversion=1935 gas PE[4]MPI[7]
B_0=4.763 DL[3]

SiD_3

$\tilde{P}\ ^2A_2''$ (7*p*) D_{3h}
T_0=62002 gas MPI[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	615(3)	gas	MPI	7

$\tilde{N}\ ^2E'$ (5*f*) D_{3h}
T_0=61005 gas MPI[7,8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	619(7)	gas	MPI	7

$\tilde{M}\ ^2A_2''$ (6*p*) D_{3h}
T_0=60267 gas MPI[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	615(4)	gas	MPI	7

$\tilde{K}\ ^2E'$ (4*f*) D_{3h}
T_0=58417 gas MPI[7,8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	602(10)	gas	MPI	8

$\tilde{J}'$ (4*d*) D_{3h}
T_0=57840(30)[c] gas MPI[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	603(20)	gas	MPI	8

$\tilde{J}\ ^2A_2''$ (5*p*) D_{3h}
T_0=56874 gas MPI[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	608(3)	gas	MPI	7

$\tilde{I}'$ (4*d*) D_{3h}
T_0=56205(30) gas MPI[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	600(17)	gas	MPI	8

$\tilde{H}\ ^2E'$ (4*p*) D_{3h}
$T_0 \cong 50000$ gas MPI[7,8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	602(5)	gas	MPI	7

$\tilde{D}\ ^2A_1'$ (3*d*) D_{3h}
T_0=49685(30)[c] gas MPI[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	600(28)	gas	MPI	8

$\tilde{E}\ ^2A_2''$ (4*p*) D_{3h}
T_0=48391 gas MPI[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	SiD_3 stretch	1576(3)	gas	MPI	7
a_2''	2	OPLA	589(3)	gas	MPI	7
e'	4	Deformation	635(6)H	gas	MPI	7

$\tilde{X}\ ^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Umbrella	545[a]	gas	MPI	7
			542[b]	gas	MPI	7

Barrier to inversion = 1925 gas MPI[7]

[a] $1^- - 0^+$ transition.
[b] $1^+ - 0^-$ transition.
[c] Extrapolated value.

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[2] G. S. Jackel and W. Gordy, Phys. Rev. **176**, 443 (1968).

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NH_3^+

$\tilde{A}\ ^2E$ D_{3h}

T_0 = 36590(100) gas PE[3,4]

Broad, partially resolved vibrational structure has been discussed[3] in terms of the expected Jahn–Teller distortion. Continuous background absorption may be associated with the formation of NH_2^+, for which the threshold is ~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	3150(100)	gas	PE	5,10
a_2''	2	OPLA	903.39	gas	PE,DL	3,7
			916.8	Ne	IR	11
e'	3	NH stretch	3388.65	gas	LD	6
			3404.6	Ne	IR	11
	4	Bend	1507.1	gas	PE,TPE	8–10
			1516.8	Ne	IR	11

B_0 = 10.644; C_0 = 5.247 LD[6]DL[7]

ND_3^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	ND stretch	2453(56)	gas	PE	10
a_2''	2	OPLA	725(25)	gas	PE	2
			683.3	Ne	IR	11
e'	3	ND stretch	2551.8	Ne	IR	11
	4	Bend	1138(56)	gas	PE	10
			1114.6	Ne	IR	11

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H_3S^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SH stretch	2521.05	gas	LD	3
	2	Umbrella	1033.31	gas	DL	2
e	3	SH stretch	2525.74	gas	LD	1,3

B_0=4.895; C_0=4.228 LD[1,3]DL[2]MW[4]

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[3] T. Nakanaga and T. Amano, J. Mol. Spectrosc. **133**, 201 (1989).
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8.5. Four-Atomic Dihydrides

HBeBeH

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	BeH a-stretch	1900.6	Ar	IR	1

DBeBeD

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	BeD a-stretch	1533.0	Ar	IR	1

Reference

[1] T. J. Tague, Jr. and L. Andrews, J. Am. Chem. Soc. **115**, 12111 (1993).

HMgMgH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		MgH stretch	1491.8	Ar	IR	1

DMgMgD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		MgD stretch	1084.3	Ar	IR	1

Reference

[1] T. J. Tague, Jr. and L. Andrews, J. Phys. Chem. **98**, 8611 (1994).

br-$(MgH)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1022.8	Ar	IR	1
			605.4	Ar	IR	1

br-$(MgD)_2$

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

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

Reference

[1] T. J. Tague, Jr. and L. Andrews, J. Phys. Chem. **98**, 8611 (1994).

HZnZnH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ZnH stretch	1740.3	Ar	IR	1

DZnZnD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ZnD stretch	1254.9	Ar	IR	1

Reference

[1] T. M. Greene, W. Brown, L. Andrews, A. J. Downs, G. V. Chertihin, N. Runeberg, and P. Pyykkö, J. Phys. Chem. **99**, 7925 (1995).

HHgHgH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		HgH stretch	1792.0T	N_2	IR	1

DHgHgD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		HgD stretch	1286.6T	N_2	IR	1

Reference

[1] N. Legay-Sommaire and F. Legay, J. Phys. Chem. **99**, 16945 (1995).

cyc-U_2H_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}		UH stretch	1182.4	Ar	IR	1

cyc-U_2D_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}		UD stretch	845.6	Ar	IR	1

Reference

[1] P. F. Souter, G. P. Kushto, L. Andrews, and M. Neurock, J. Am. Chem. Soc. **119**, 1682 (1997).

$CrCH_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s-stretch	2907.4	Ar	IR	1
	3	CrC stretch	567.0	Ar	IR	1
b_1	4	OPLA	687.7	Ar	IR	1
b_2	5	CH_2 a-stretch	2966.7	Ar	IR	1
	6	CH_2 rock	450.3	Ar	IR	1

$CrCD_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CrC stretch	525.7	Ar	IR	1
b_1	4	OPLA	538.8	Ar	IR	1
b_2	6	CD_2 rock	346.2	Ar	IR	1

Reference

[1] W. E. Billups, S.-C. Chang, R. H. Hauge, and J. L. Margrave, Inorg. Chem. **32**, 1529 (1993).

$CoCH_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s-stretch	2918.0	Ar	IR	1,2
	2	CH_2 scissors	1327.0	Ar	IR	1,2
	3	CoC stretch	655.4	Ar	IR	1,2
b_1	4	OPLA	757.4	Ar	IR	1,2
b_2	5	CH_2 a-stretch	2979.7	Ar	IR	1,2
	6	CH_2 rock	587.5	Ar	IR	1,2

$CoCD_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_2 scissors	993.2	Ar	IR	1,2
	3	CoC stretch	608.2	Ar	IR	1,2
b_1	4	OPLA	599.5	Ar	IR	1,2
b_2	6	CD_2 rock	455.4	Ar	IR	1,2

References

[1] W. E. Billups, S.-C. Chang, R. H. Hauge, and J. L. Margrave, J. Am. Chem. Soc. **115**, 2039 (1993).
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$NiCH_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s-stretch	2917.1	Ar	IR	1
	2	CH_2 scissors	1328.5	Ar	IR	1
	3	NiC stretch	696.2	Ar	IR	1
b_1	4	OPLA	791.9	Ar	IR	1
b_2	5	CH_2 a-stretch	2973.2	Ar	IR	1
	6	CH_2 rock	586.7	Ar	IR	1

$NiCD_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_2 scissors	993.6	Ar	IR	1
	3	NiC stretch	641.7	Ar	IR	1
b_1	4	OPLA	627.0	Ar	IR	1
b_2	6	CD_2 rock	455.1	Ar	IR	1

Reference

[1] S.-C. Chang, R. H. Hauge, Z. H. Kafafi, J. L. Margrave, and W. E. Billups, Inorg. Chem. **29**, 4373 (1990).

HBBH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BH stretch	2679.9	Ar	IR	1

Reference

[1] T. J. Tague, Jr. and L. Andrews, J. Am. Chem. Soc. **116**, 4970 (1994).

cyc-Al_2H_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{1u}			1160.9	Ar	IR	1,2
b_{2u}			844	Ar	IR	1,2

cyc-Al_2D_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{1u}			852.8	Ar	IR	1
b_{2u}			617.2	Ar	IR	1

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[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. **97**, 10295 (1993).
[2] J. C. Stephens, E. E. Bolton, H. F. Schaefer III, and L. Andrews, J. Chem. Phys. **107**, 119 (1997).

H(*cyc*-AlHAl)

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1668.7	Ar	IR	1,2
			1127	Ar	IR	1,2
			890	Ar	IR	1,2

D(*cyc*-AlDAl)

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1210	Ar	IR	1,2
			811	Ar	IR	1,2

References

[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. **97**, 10295 (1993).
[2] J. C. Stephens, E. E. Bolton, H. F. Schaefer III, and L. Andrews, J. Chem. Phys. **107**, 119 (1997).

HAlAlH

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1646.9T	Ar	IR	1

DAlAlD

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1194.3T	Ar	IR	1

Reference

[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. **97**, 10295 (1993).

cyc-Ga_2H_2

In an argon or a krypton matrix, irradiation at 400–520 nm results in rearrangement to HGaGaH.[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		GaH stretch	1002.1	Ar	IR	1
			1022.3	Kr	IR	1

cyc-Ga_2D_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		GaD stretch	728.2	Ar	IR	1
			732.0	Kr	IR	1

Reference

[1] Z. L. Xiao, R. H. Hauge, and J. L. Margrave, Inorg. Chem. **32**, 642 (1993).

HGaGaH

In an argon or a krypton matrix, irradiation at 320–380 nm results in rearrangement to *cyc*-Ga_2H_2.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		GaH stretch	1686.2	Ar	IR	1

DGaGaD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		GaD stretch	1206.5	Ar	IR	1
			1218.2	Kr	IR	1

Reference

[1] Z. L. Xiao, R. H. Hauge, and J. L. Margrave, Inorg. Chem. **32**, 642 (1993).

$CaNH_2$

$\tilde{C}$ $^2A_1$ C_{2v} Structure: LF[2,7]

T_0=17375.167 gas $CL^1LF^{2,7}$ $\tilde{C}-\tilde{X}$ 575 nm

A=12.95; $\frac{1}{2}$(B+C)=0.302; $\frac{1}{4}$(B−C)=0.0018 $LF^{2,7}$

$\tilde{B}$ $^2B_1$ C_{2v} Structure: LF[7]

T_0=15885.28 gas $CL^1LF^{3-5,7}$ $\tilde{B}-\tilde{X}$ 620–650 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CaN stretch	545.8(5)	gas	LF	4

A=14.37; $\frac{1}{2}$(B+C)=0.302; $\frac{1}{4}$(B−C)=0.005 $LF^{5,7}$

$\tilde{A}$ $^2B_2$ C_{2v} Structure: LF[7]

T_0=15464.367 gas CL^1LF^{3-6} $\tilde{A}-\tilde{X}$ 620–650 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CaN stretch	549.5(1.0)	gas	LF	3,4

A_0=11.449; B_0=0.307; C_0=0.299 $LF^{5,6}$

$\tilde{X}$ $^2A_1$ C_{2v} Structure: LF[2,6,7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CaN stretch	524(10)	gas	LF	3

A=13.057; B_0=0.300; C_0=0.293 $LF^{2,5,6}$

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[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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[7] Z. Morbi, C. Zhao, and P. F. Bernath, J. Chem. Phys. **106**, 4860 (1997); J. Chem. Phys. **107**, 1297 (1997).

HBCH

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3248.8	Ar	IR	1
	2	BH stretch	2724.6	Ar	IR	1
	3	B=C stretch	1475.3	Ar	IR	1

DBCD

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2464.3	Ar	IR	1
	2	BD stretch	2097.8	Ar	IR	1

Reference

[1] P. Hassanzadeh, Y. Hannachi, and L. Andrews, J. Phys. Chem. **97**, 6418 (1993).

$HCCH^+$

$\tilde{C}$ $^2\Sigma^+$ $D_{\infty h}$
T_0=92460(80) gas PE[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	2	CC stretch	1370T	gas	PE	6

$\tilde{B}$ $^2\Sigma_u^+$ $D_{\infty h}$
T_0=56380(80) gas PE[1,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	CH s-stretch	2500(20)	gas	PE	1,3
	2	CC stretch	1815(20)	gas	PE	1,3

τ<14 fs gas PE[3]

$\tilde{A}$ ^2A_g[a] C_{2h} Structure: MPD[11]
T_0=39109.7(1.0) gas PE[3]MPD[11] $\tilde{A}-\tilde{X}$ 240–255 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	CH s-stretch	2530(20)	gas	PE	3
	2	CC stretch	1730(20)	gas	PE	3
	3	Bend	793[b]	gas	MPD	11
a_u	4	Torsion	282H[b]	gas	MPD	11
b_u	6	Bend	436H[b]	gas	MPD	11

τ_0=150 ps gas MPD[11]
A_0=12.15; B_0=0.94(5) MPD[11]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	2	CC stretch	1829(3)	gas	PE	1,3
Σ_u^+	3	CH a-stretch	3135.98	gas	LD	5,9
			3137.6	Ne	IR	8
			3105.5	Ar	IR	4,8
Π_g	4	Deform.	694[c]	gas	PE,TPE	7,10
Π_u	5	Deform.	837(12)[c]	gas	PE	3

A=−30.91(2) gas LD[5,9]
B_0=1.105 LD[5,9]

$DCCD^+$

$\tilde{B}$ $^2\Sigma_u^+$ $D_{\infty h}$
T_0=56655(80) gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	CC stretch	2275(20)	gas	PE	1,3
	2	CD s-stretch	1475(20)	gas	PE	1,3

$\tilde{A}$ ^2A_g C_{2h}
T_0=39906(80) gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	CD s-stretch	2280(20)	gas	PE	3
	2	CC stretch	1450(20)	gas	PE	3
	3	Bend	339(12)	gas	PE	3
b_u	6	Bend	516(12)	gas	PE	3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	CD s-stretch	2572(16)	gas	PE	3
	2	CC stretch	1651(4)	gas	PE	1,3
Σ_u^+	3	CD a-stretch	2329.1	Ne	IR	8
			2311T	Ar	IR	4,8
Π_u	5	Bend	702(12)[c]	gas	PE	3

[a] Threshold for formation of $HCC^+ \leqslant 48000\ cm^{-1}$.[2,3]
[b] All three bending fundamentals have exceptionally large anharmonicities.
[c] ω_4. ϵ_4=0.30.[10] The identification[7,10] of the Renner components of ν_4 (Π_g) of $HCCH^+$ in the photoelectron spectrum of HCCH ($\tilde{A}$ ^1A_u) necessitates the reassignment to ν_5 (Π_u) of the peaks previously assigned[3] to ν_4 of $HCCH^+$ and $DCCD^+$.

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HBeOH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3841.8	Ar	IR	1
	2	BeH stretch	2117.7	Ar	IR	1
	3	BeO stretch	1206.9	Ar	IR	1
		Deformation	552.0	Ar	IR	1

DBeOD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2834.2	Ar	IR	1
	2	BeD stretch	1663.6	Ar	IR	1
	3	BeO stretch	1098.3	Ar	IR	1

Reference

[1] C. A. Thompson and L. Andrews, J. Phys. Chem. **100**, 12214 (1996).

HZnOH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		HZn stretch	1955.0	Ar	IR	1
		ZnO stretch	660.0	Ar	IR	1
			481.4	Ar	IR	1

DZnOD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		DZn stretch	1410.0	Ar	IR	1

Reference

[1] T. M. Greene, W. Brown, L. Andrews, A. J. Downs, G. V. Chertihin, N. Runeberg, and P. Pyykkö, J. Phys. Chem. **99**, 7925 (1995).

HCdOH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		HCd stretch	1836.9	Ar	IR	1

DCdOD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		DCd stretch	1319.8	Ar	IR	1

Reference

[1] T. M. Greene, W. Brown, L. Andrews, A. J. Downs, G. V. Chertihin, N. Runeberg, and P. Pyykkö, J. Phys. Chem. **99**, 7925 (1995).

HBNH

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NH stretch	3710.5m	Ar	IR	3,5,6
			3700.5m			
	2	BH stretch	2775.3	Ar	IR	6
	3	BN stretch	1786.19	gas	DL	4
			1788.7m	Ar	IR	3,5,6
			1782.8m			
Π	4	BH deform.	676.9	Ar	IR	6
			671.6			
	5	NH deform.	463.3m	Ar	IR	3,5,6
			461.0m			

B_0=1.099 DL[4]

DBND

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	ND stretch	2836	Ar	IR	3
	2	BD stretch	2730	Ar	IR	3
	3	BN stretch	1734	Ar	IR	3
Π	4	Bend	360	Ar	IR	3

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H_2NB

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		NH_2 scissors	1533.2	Ar	IR	1
b_1	4	OPLA	596.0	Ar	IR	1

Reference

[1] C. A. Thompson, L. Andrews, J. M. L. Martin, and J. El-Yazal, J. Phys. Chem. **99**, 13839 (1995).

H_2CSi

$^1B_2$ C_{2v}
T_0=29312.883(4) gas AB[1] $^1B_2-\tilde{X}$ 310–340 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_2 scissors	1101.96	gas	AB	1
	3	CSi stretch	702.00	gas	AB	1

A_0=8.537; B_0 = 0.509; C_0=0.479 AB[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_2 rock	331T	gas	MW	2

A_0=10.167(18); B_0=0.553; C_0=0.521 AB[1]MW[2]

D_2CSi

$^1B_2$ C_{2v}
T_0=29272 gas AB[1] $^1B_2-\tilde{X}$ 310–340 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_2 scissors	829	gas	AB	1
	3	CSi stretch	691	gas	AB	1

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br-Si_2H_2

$\tilde{X}$ C_{2v} Structure: MW[1,2]
A_0=5.244; B_0=0.243; C_0=0.240 MW[1,2]

br-Si_2D_2

$\tilde{X}$ C_{2v}
A_0=2.688; B_0=0.240; C_0=0.234 MW[2]

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HGaOH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3675	Ar	IR	1
		HGa stretch	1669.8	Ar	IR	1,2
		HGaO bend	784.9	Ar	IR	1,2
		GaO stretch	646.4	Ar	IR	1,2
		GaOH bend	520.5	Ar	IR	1

DGaOD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OD stretch	2708	Ar	IR	1
		DGa stretch	1213.8	Ar	IR	1
		GaO stretch	644.6	Ar	IR	1
		DGaO bend	582.9	Ar	IR	1

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H_2CO^+

$\tilde{C}$ $^2B_2$ C_{2v}
T_0=43172(11) gas PE[1,4,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1895T	gas	PE	4,5
			1412T	gas	PE	1,4,5

$\tilde{B}$ $^2A_1$ C_{2v}
T_0=39928(6) gas PE[1,4,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CO stretch	1304(4)	gas	PE	1,4,5

$\tilde{A}$ $^2B_1$ C_{2v}
T_0=25929(5) gas PE[1,4,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1488(4)	gas	PE	4,5
			1250(4)	gas	PE	1,4,5
b_1	4	OPLA	263(4)	gas	PE	4,5

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	2580(4)	gas	PE	1,4,5
	2	CO stretch	1675(4)	gas	PE	4,5
	3	CH_2 scissors	1210(4)	gas	PE	1,4,5
b_1	4	OPLA	777(4)	gas	PE	4,5

$A_0=8.875(3)$; $B_0=1.31(1)$; $C_0=1.14(1)$ TPE[6]

D_2CO^+

$\tilde{C}\ ^2B_2$ C_{2v}
$T_0=44600(160)$ gas PE[4,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1604T	gas	PE	4,5
			943T	gas	PE	1,4,5
			819T	gas	PE	4,5

$\tilde{B}\ ^2A_1$ C_{2v}
$T_0=39816(5)$ gas PE[1,4,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CO stretch	1311(4)	gas	PE	1,4,5
	3	CD_2 scissors	957(4)	gas	PE	1,4,5

$\tilde{A}\ ^2B_1$ C_{2v}
$T_0=25756(7)$ gas PE[1,4,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		1282(4)	gas	PE	1,4,5
	3		1064(4)	gas	PE	4,5
b_1	4	OPLA	777(4)	gas	PE	5

$\tau_0=64(22)\mu s$ gas PEPICO[3]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD stretch	1948(4)	gas	PE	1,4,5
	2	CO stretch	1657(4)	gas	PE	4,5
	3	CD_2 scissors	920(4)	gas	PE	1,4,5
b_1	4	OPLA	648(4)	gas	PE	4,5

H_2CS

$\tilde{E}\ 3p_z\ ^1B_2$ C_{2v}
$T_0=55096$ gas AB[8,19] $\tilde{E}-\tilde{X}$ 181.5 nm

$\tilde{D}\ 3p_y\ 1A_1$ C_{2v}
$T_0=53134$ gas AB[8,19] $\tilde{D}-\tilde{X}$ 188.2 nm

$\tilde{C}\ 3s\ ^1B_2$ C_{2v} Structure: AB[19]
$T_0=47110.821(9)$ gas AB[1,8,15,19] $\tilde{C}-\tilde{X}$ 212.1 nm
$A_0=8.557$; $B_0=0.603$; $C_0=0.562$ AB[19]

$\tilde{B}\ ^1A_1$[a] C_{2v}
$T_0=45197$ gas AB[8,18] $\tilde{B}-\tilde{X}$ 185–215 nm
All but the first absorption band show evidence for predissociation.[18]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CS stretch	476	gas	AB	18
b_1	4	OPLA	363H	gas	AB	18

$\tilde{A}\ ^1A_2$ C_{2v} Structure: AB[10,21]LF[28]
$T_0=16394.628(4)$ gas AB[7,9,10]LF[24,28,32,33] $\tilde{A}-\tilde{X}$ 440–610 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	3033.4[b]	gas	AB,LF	9,28
	2	CH_2 scissors	1334.5[b]	gas	LF	28
	3	CS stretch	819.7	gas	AB,LF	7,9,28
b_1	4	OPLA	370.3	gas	AB,LF	9,28,32
b_2	5	CH stretch	3054.9[b]	gas	LF	28
	6	CH_2 rock	785.2	gas	LF	28

$\tau_0=140(3)\ \mu s$ gas LF[22,25]
$A_0=9.434$; $B_0=0.538$; $C_0=0.509$ AB[10]LF[24,28]

$\tilde{a}\ ^3A_2$ C_{2v} Structure: AB[11,21]LF[29]
$T_0=14507.38$ gas AB[7,11]LF[20,24,29]CL[26,30] $\tilde{a}-\tilde{X}$ 610–800 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_2 scissors	1318.6	gas	AB,LF	11,29
	3	CS stretch	861.6	gas	AB,LF	11,23
b_1	4	OPLA	326	gas	LF,CL	20,21,26 30,32
b_2	6	CH_2 rock	762.3	gas	LF	23

$\tau>1.5$ ms gas LF[22,25]
$A_0=9.383$; $B_0=0.552$; $C_0=0.521$ AB[11]LF[24]

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$\tilde{X}\ ^1A_1$ C_{2v} Structure: MW[2,4,5]IR[3,14]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	2971.03	gas	IR	3,14
			2970w	Ar	IR	6,17
			2973w	N_2	IR	6
	2	CH_2 scissors	1455.50	gas	LF,IR	13,31
			1447	Ar	IR	17
	3	CS stretch	1059.20	gas	LS,IR	12,14
			1063w	Ar	IR	6,17
			1062w	N_2	IR	6
b_1	4	OPLA	990.19	gas	LS,IR	12,14
			993s	Ar	IR	6,17
			995s	N_2	IR	6
b_2	5	CH stretch	3024.61	gas	IR	3,14
	6	CH_2 rock	991.01	gas	LS,IR	12,14
			988m	Ar	IR	6,17

$A_0=9.729$; $B_0=0.590$; $C_0=0.555$ MW[2,4,5]AB[10]IR[31]

D_2CS

$\tilde{C}\ 3s\ ^1B_2$ C_{2v}
$T_0=47325.563(4)$ gas AB[8,19] $\tilde{C}-\tilde{X}$ 211.2 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD stretch	1783	gas	AB	8,19
	2	CD_2 scissors	746	gas	AB	19

$A_0=4.350$; $B_0=0.510$; $C_0=0.456$ AB[19]

$\tilde{B}\ ^1A_1$[a] C_{2v}
$T_0\cong 45200$ gas AB[18] $\tilde{B}-\tilde{X}$ 185–215 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CS stretch	467	gas	AB	18
b_1	4	OPLA	263H	gas	AB	18

$\tilde{A}\ ^1A_2$ C_{2v}
$T_0=16483.502(8)$ gas AB[7,9,10] $\tilde{A}-\tilde{X}$ 440–610 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD stretch	2139(2)	gas	AB	9
	2	CD_2 scissors	1013(2)	gas	AB	9
	3	CS stretch	771.3(5)	gas	AB	7,9
b_1	4	OPLA	275.33	gas	AB	9
b_2	5	CD stretch	2324.85	gas	AB	9
	6	CD_2 rock	599(2)	gas	AB	9

τ_0 = 182 μs gas LF[25]
$A_0=4.736$; $B_0=0.458$; $C_0=0.417$ AB[10]

$\tilde{a}\ ^3A_2$ C_{2v} Structure: AB[21]
$T_0=14613.54$ gas AB[7,11]CL[26,30] $\tilde{a}-\tilde{X}$ 610–815 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_2 scissors	1012	gas	AB,CL	11,30
	3	CS stretch	798	gas	AB,CL	7,11,30
b_1	4	OPLA	219.4(5.0)	gas	AB,CL	21,26,30
b_2	6	CD_2 rock	572.6(5.0)	gas	CL	30

$A_0=4.716$; $B_0=0.469$; $C_0=0.426$ AB[11]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD stretch	2158.5	gas	IR	14
			2155m	Ar	IR	17
	2	CD_2 scissors	1171.8	gas	IR	14
			1167m	N_2	IR	17
	3	CS stretch	936.13	gas	IR,LS	14,16
			941vw	Ar	IR	6,17
			939wm	N_2	IR	6
b_1	4	OPLA	781.2	gas	IR	14
			783m	Ar	IR	6,17
			784s	N_2	IR	6
b_2	6	CD_2 rock	757.4	gas	IR	14

$A_0=4.883$; $B_0=0.497$; $C_0=0.450$ MW[2]AB[10]LF[27]

[a]Barrier to inversion ≅ 50.[18]
[b]From fit to combination bands.

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H_2CSe

$\tilde{A}\ ^1A_2$ C_{2v} Structure: LF[7]
$T_0 \cong 13555$ gas LF[5,6]CL[8] $\tilde{A}-\tilde{X}$ 685–833 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	C=Se stretch	662	gas	LF	6
b_1	4	OPLA	355T	gas	LF	6

$A^a=9.015$; $B^a=0.377$; $C^a=0.360$ LF[7]

$\tilde{a}\ ^3A_2$ C_{2v} Structure: LF[9]
$T_0=12162.514$ gas AB[1]CL[3,8]LF[5,6,9] $\tilde{a}-\tilde{X}$ 658–865 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_2 scissors	1312	gas	LF	5,6
	3	C=Se stretch	704	gas	AB,CL LF	1,3,5,6,8
b_1	4	OPLA	297[b]	gas	AB,LF	1,5,6
b_2	6	HCSe bend	812H	gas	LF	5,6

$A_0=9.320$; $B_0=0.391$; $C_0=0.375$ LF[9]

$\tilde{X}\ ^1A_1$ C_{2v} Structure: MW[2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_2 scissors	1460(30)	gas	CL	8
	3	C=Se stretch	860(10)	gas	CL	8
b_1	4	OPLA	906(10)	gas	CL	8
b_2	6	HCSe bend	914(20)	gas	CL	8

$A_0=9.690$; $B_0=0.414$; $C_0=0.396$ MW[2,4]LF[7]

D_2CSe

$\tilde{A}\ ^1A_2$ C_s
$T_0=13631.4$ gas LF[6] $\tilde{A}-\tilde{X}$ 671–734 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	C=Se stretch	619	gas	LF	6

$A_0=4.711$; $B_0=0.316$; $C_0=0.296$ LF[7]

$\tilde{a}\ ^3A_2$ C_{2v}
$T_0=12258.060$ gas LF[6,9] $\tilde{a}-\tilde{X}$ 661–815 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_2 scissors	996	gas	LF	6
	3	C=Se stretch	667	gas	LF	6
b_1	4	OPLA	208[b]	gas	LF	6
b_2	6	DCSe bend	563H	gas	LF	6

$A_0=4.688$; $B_0=0.327$; $C_0=0.306$ LF[9]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	C=Se stretch	789T	gas	LF	6

$A_0=4.865$; $B_0=0.344$; $C_0=0.321$ MW[4]LF[7,9]

[a] $v_4 = 1$.
[b] From fit to double minimum potential. Barrier to inversion 13.1 for H_2CSe, 16.2 for D_2CSe.[6]

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H_2SiO

$\tilde{X}$ C_{2v} Structure: MW[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Si=O stretch	1202	Ar	IR	1,2
		SiH_2 deform.	697	Ar	IR	2

$A_0=5.559$; $B_0=0.623$; $C_0=0.558$ MW[3]

D_2SiO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Si=O stretch	1189	Ar	IR	1,2
		SiD_2 deform.	533	Ar	IR	2

$A_0=2.789$; $B_0=0.555$; $C_0=0.461$ MW[4]

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t-N_2H_2

$\tilde{C}\ ^1B_u$[a] C_{2h}
T_0=67894 gas AB[9] $\tilde{C}-\tilde{X}$ 135–147 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2	Bend	1180	gas	AB	9
	3	NN stretch	1849	gas	AB	9

$\tilde{B}\ ^1B_u$ C_{2h} Structure: AB[9]
T_0=57926.5 gas AB[2,9] $\tilde{B}-\tilde{X}$ 150–175 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	NH stretch	3092	gas	AB	9
	2	Bend	1180	gas	AB	2,9
	3	NN stretch	1875	gas	AB	2,9

A_0=15.63; B_0=1.32; C_0=1.22 AB[9]

$\tilde{A}\ ^1B_g$ C_{2h}
T[c]=23896 gas AB[4,5,8] $\tilde{A}-\tilde{X}$ 300–440 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2	Bend	1215(15)	gas	AB	5
	3	NN stretch	1550(20)	gas	AB	5

$\tilde{X}\ ^1A_g$ C_{2h} Structure: IR[2,6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	NH stretch	3128	N_2	Ra	3
	2	NH bend	1583	N_2	Ra	3
	3	N=N stretch	1529	N_2	Ra	3
a_u	4	Torsion	1288.65	gas	IR	10,11
			1283	Ar	IR	7
			1286	N_2	IR,Ra	1,3,7
b_u	5	NH stretch	3120.29	gas	IR	2,6,10,11
			3118	Ar	IR	7
			3137	N_2	IR	7
	6	NH bend	1316.41	gas	IR	10,11
			1313	Ar	IR	7
			1321	N_2	IR	3,7

A_0=10.001; B_0=1.304; C_0=1.150 IR[6,10,11]

t-N_2D_2

$\tilde{B}\ ^1B_u$ C_{2h}
T_0≅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	948.30	gas	IR	12
			946	N_2	IR	1,3,7
b_u	5	ND stretch	2315.05	gas	IR	6,12
			2308	N_2	IR	7
	6	ND bend	968.70	gas	IR	12
			972	N_2	IR	7

A_0=6.025; B_0=1.089; C_0=0.920 IR[6,12]

[a] 4pπ Rydberg transition.
[b] 3pπ Rydberg transition.
[c] 5_0^1 vibronic band origin.[8]
[d] 1-0 subband origin.

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H_2CCl

$\tilde{X}$ C_{2v} Structure: ESR[3]MW[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_2 scissors	1391wm	Ar	IR	2
	3	CCl stretch	827s	Ar	IR	1,2
b_1	4	OPLA	402s	Ar	IR	1,2

$A_0=9.152(3)$; $B_0=0.532$; $C_0=0.502$ MW[4]LMR[5]

D_2CCl

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_2 scissors	1045m	Ar	IR	1,2
	3	CCl stretch	788m	Ar	IR	1,2
b_1	4	OPLA	291m	Ar	IR	1,2

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H_2CBr

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_2 scissors	1355.7s	Ar	IR	1,2
		CH_2 rock	953w	Ar	IR	1
		CBr stretch	693.4s	Ar	IR	1,2
		Umbrella	368vs	Ar	IR	1,2

B+C=0.744(8) LMR[3]

D_2CBr

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD_2 scissors	1016.4s	Ar	IR	1,2
		CD_2 rock	708w	Ar	IR	1
		CBr stretch	656.6m	Ar	IR	1,2
		Umbrella	263vs	Ar	IR	1,2

B+C=0.621(15) LMR[3]

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H_2PO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		PH stretch	2275.7	Ar	IR	1
			2273.8			
		P=O stretch	1153.1	Ar	IR	1
			1151.7			
			1147.7			
		PH_2 rock	833.2	Ar	IR	1
		PH_2 wag	791.6	Ar	IR	1

$A_0=5.208$; $B_0=0.634$; $C_0=0.594$ MW[2]

D_2PO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		PD stretch	1648.2	Ar	IR	1
		P=O stretch	1147.3	Ar	IR	1
			1141.7			
			1137.7			
		PD_2 rock	628.4	Ar	IR	1
		PD_2 wag	602.9	Ar	IR	1

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HPSH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		PH stretch	2187.0T	Ar	IR	1
			461.2T	Ar	IR	1

Reference

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H_2PF

$\tilde{X}$ C_s Structure: MW[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	PH_2 s-stretch	2283.12	gas	IR	2–4
			2304	Ar	IR	1
	2	PH_2 deform.	1109.24	gas	IR	2,3
			1090	Ar	IR	1
	3	PH_2 deform.	976.50	gas	IR	3
			934	Ar	IR	1
	4	PF stretch	807.36	gas	IR	2,3
			795vs	Ar	IR	1
a''	5	PH_2 a-stretch	2286.97	gas	IR	2–4
			2310	Ar	IR	1

$A_0=4.364$; $B_0=0.505$; $C_0=0.499$ IR[3,4]MW[5]

D_2PF

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	PD_2 s-stretch	1660	gas	IR	2
			1673	Ar	IR	1
	3	PF stretch	808	gas	IR	2
			798	Ar	IR	1
	4	PD_2 s-deform.	701	Ar	IR	1
a''	5	PD_2 a-stretch	1667	gas	IR	2
			1680	Ar	IR	1

$A_0=2.272$; $B_0=0.465$; $C_0=0.453$ MW[5]

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H_2PCl

$\tilde{X}$ C_s Structure: MW[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	PH_2 s-stretch	2303.44	gas	IR	1–3
	2	PH_2 deform.	1095.74	gas	IR	1,2
	3	PH_2 deform.	861.05	gas	IR	1,2
	4	PCl stretch	511.23	gas	IR	1,2
a''	5	PH_2 a-stretch	2309.68	gas	IR	1–3

$A_0=4.353$; $B_0=0.225$; $C_0=0.224$ IR[2]MW[4]

D_2PCl

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	PD_2 s-stretch	1665T	gas	IR	1
	3	PD_2 deform.	633	gas	IR	1
	4	PCl stretch	510	gas	IR	1
a''	5	PD_2 a-stretch	1670T	gas	IR	1

$A_0=2.256$; $B_0=0.212$; $C_0=0.209$ MW[4]

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H_2PBr

$\tilde{X}$ C_s

$A_0=4.335(4)$; $B_0=0.142$; $C_0=0.141$ MW[1]

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H_2PI

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	PH_2 deform.	752.52	gas	IR	1
	4	PI stretch	337.60	gas	IR	1
a''	6	PH_2 deform.	742.68	gas	IR	1

$A_0=4.350(45)$; $B_0=0.105$; $C_0=0.105$ IR,MW[1]

Reference

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HOOH

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

$\tilde{X}$ C_2 Structure: IR[4,19,21]MW[8,21]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	OH s-stretch	3617.95[a]	gas	IR,Ra	3,4,10,
			3609.8			17
			3593	Ar	Ra	11
	2	OH s-bend	1393.5	gas	Ra	10
			1385	Ar	Ra	11
	3	OO stretch	877.93[a]	gas	IR	20
			865.94	gas	Ra,IR	10,20
			869	Ar	Ra	11
	4	Torsion	370.89[a]	gas	IR	6,17,18,
			254.55			19
			372br	Ar	IR	9
			264			
			378vs,br	N_2	IR	5,9
b	5	OH a-stretch	3618.84[a]	gas	IR	3,4,17
			3610.66			
			3597.0[b]	Ar	IR	9,23
			3587.8[b]			
			3583.6[b]	Kr	IR	23
			3574.0[b]			
			3568.0[b]	Xe	IR	23
			3560.0[b]			
			3587s	N_2	IR	5,9
			3582s			
	6	OH a-bend	1273.68[a]	gas	IR,DL	3,16
			1264.58			
			1277.0ms[b]	Ar	IR	9,23
			1270.9vs[b]			
			1273.7[b]	Kr	IR	23
			1268.7[b]			
			1270.3[b]	Xe	IR	23
			1265.7[b]			
			1294vs	N_2	IR	5,9

$A_0=10.069$; $B_0=0.874$; $C_0=0.838$ IR[4,17,20]MW[8,13-15,22]

DOOD

$\tilde{X}$ C_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	OD s-stretch	2668	gas	Ra	10
			2653.5	Ar	Ra	11
	2	OD s-bend	1029	gas	Ra	10
			1021.5	Ar	Ra	11
	3	OO stretch	867	gas	Ra	10
			871	Ar	Ra	11
	4	Torsion	251	Ar	IR	9
			286br	N_2	IR	9
b	5	OD a-stretch	2661m	gas	IR	3
			2655.7	Ar	IR	9,23
			2651.3			
			2645.3			
			2645.2	Kr	IR	23
			2639	Xe	IR	23
			2633.2			
			2628.4			
			2646	N_2	IR	9
	6	OD a-bend	947s	gas	IR	3
			951.3vs	Ar	IR	9,23
			949.9	Kr	IR	23
			947.8	Xe	IR	23
			966vs	N_2	IR	9

[a]Transitions to two lowest torsional levels associated with this fundamental are given.
[b]Ref. 23 attributes the doubling in the matrix absorptions to excitation from the two lowest torsional levels.

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HSSH

$\tilde{X}$ C_2 Structure: MW,IR[13,14]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	SH s-stretch	2555.78	gas	IR	3,5
	2	Deformation	883	gas	IR	3
	3	SS stretch	515.92	gas	IR,MW	3,15
	4	Torsion	417.48	gas	IR	2,3,11,15
b	5	SH a-stretch	2558.63	gas	IR	1,3,5,16
	6	Deformation	882.0	gas	IR	1,3

$A_0=4.899$; $B_0=0.233$; $C_0=0.232$ MW[4,8,9,12]IR[10,12]

DSSD

$\tilde{X}$ C_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	4	Torsion	306	gas	IR	3
b	5	SD a-stretch	1863	gas	IR	3
	6	Deformation	646.4	gas	IR	3

$A_0=2.550$; $B_0=0.218$; $C_0=0.218$ MW[4,6,7,13]IR[13]

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8.6. Four-Atomic Monohydrides

BeCCH

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	CC stretch	2018.9	Ar	IR	1
	3	BeC stretch	855.0	Ar	IR	1
Π	4	HCC bend	675.7	Ar	IR	1

BeCCD

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	CC stretch	1873.4	Ar	IR	1
	3	BeC stretch	848.9	Ar	IR	1
Π	4	DCC bend	553.8	Ar	IR	1

Reference

[1] C. A. Thompson and L. Andrews, J. Am. Chem. Soc. **118**, 10242 (1996).

MgCCH

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

T_0=22807 gas LF[2] $\tilde{A}-\tilde{X}$ 415–440 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		MgC stretch	552	gas	LF	2

A=36.4 gas LF[2]
B_0=0.175 gas LF[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	CC stretch	1984.2	Ar	IR	3
	3	MgC stretch	491.8	Ar	IR	3
Π	4	HCC bend	660.8	Ar	IR	3

B_0=0.167 MW[1]

MgCCD

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	CC stretch	1856.4	Ar	IR	3
	3	MgC stretch	485.1	Ar	IR	3

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CaCCH

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

T_0=16600T gas LF[5]

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

T_0=15525.393 gas LF[1-3,5,6] $\tilde{A}-\tilde{X}$ 640–665 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	5	CaCC bend	101.39	gas	LF	6

A=70.821 gas LF[1-3,5]
$\epsilon_5\omega_5$=3.528(14) gas LF[6]
B_0=0.115 LF[2,3,5]

$\tilde{X}$ $^2\Sigma^+$ $C_{\infty v}$ Structure: LF[2,5]

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	102.94	gas	LF	6

B_0=0.113 LF[2,3,5]MW[4]

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SrCCH

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

T_0=14176(10) gas LF[1] $\tilde{A}-\tilde{X}$ 685–725 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	SrC stretch	354(10)	gas	LF	1

A=275(10) gas LF[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	SrC stretch	343(10)	gas	LF	1
Π	5	SrCC bend	70(5)H	gas	LF	1

B_0=0.083 MW[2]

References

[1] A. M. R. P. Bopegedera, C. R. Brazier, and P. F. Bernath, Chem. Phys. Lett. **136**, 97 (1987).
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FeCCD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		FeC stretch	500(100)	gas	PE	1

Reference

[1] J. Fan and L.-S. Wang, J. Phys. Chem. **98**, 11814 (1994).

$FeCCH^-$

Threshold for electron detachment from ground-state $FeCCH^-$ = 11400(400) gas PE[1]

Reference

[1] J. Fan and L.-S. Wang, J. Phys. Chem. **98**, 11814 (1994).

HBNB

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BH stretch	2805.6	Ar	IR	1,2
	2	BNB a-stretch	1846.3	Ar	IR	1,2
	3	BNB s-stretch	1089.3	Ar	IR	1,2
Π	4	HBN deform.	746.2	Ar	IR	1,2

DBNB

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BD stretch	2218.7	Ar	IR	1,2
	2	BNB a-stretch	1717.6	Ar	IR	1,2
	3	BNB s-stretch	1062.4	Ar	IR	1,2
Π	4	DBN deform.	596.4	Ar	IR	1

References

[1] C. A. Thompson and L. Andrews, J. Am. Chem. Soc. **117**, 10125 (1995).
[2] C. A. Thompson, L. Andrews, J. M. L. Martin, and J. El-Yazal, J. Phys. Chem. **99**, 13839 (1995).

HBCC

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C≡C stretch	1995.2	Ar	IR	1

DBCC

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BD stretch	2173.3	Ar	IR	1
		C≡C stretch	1907.7	Ar	IR	1

Reference

[1] L. Andrews, P. Hassanzadeh, J. M. L. Martin, and P. R. Taylor, J. Phys. Chem. **97**, 5839 (1993).

HCCB

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C≡C stretch	2039.3	Ar	IR	1

DCCB

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C≡C stretch	1918.8	Ar	IR	1

Reference

[1] L. Andrews, P. Hassanzadeh, J. M. L. Martin, and P. R. Taylor, J. Phys. Chem. **97**, 5839 (1993).

cyc-HBC_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	BC_2 s-stretch	1122.7	Ar	IR	1,2

cyc-DBC_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	BC_2 s-stretch	1075.7	Ar	IR	1,2

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HCCAl

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CC stretch	1976.4	Ar	IR	1,2
		HCC deform.	683.5	Ar	IR	1,2
		AlC stretch	512.8	Ar	IR	1,2

DCCAl

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CC stretch	1860.8	Ar	IR	1
		DCC deform.	505.2	Ar	IR	1
		AlC stretch	456.0	Ar	IR	1

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cyc-HC_3

$\tilde{X}\ ^2B_2$ C_{2v} Structure: MW[2,4]

$A_0=1.486$; $B_0=1.135$; $C_0=0.640$ MW[1,3,4]

cyc-DC_3

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

$A_0=1.485$; $B_0=0.931$; $C_0=0.570$ MW[2,3]

References

[1] S. Yamamoto, S. Saito, M. Ohishi, H. Suzuki, S.-I. Ishikawa, N. Kaifu, and A. Murakami, Astrophys. J. **322**, L55 (1987).
[2] S. Yamamoto and S. Saito, Astrophys. J. **363**, L13 (1990).
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[4] S. Yamamoto and S. Saito, J. Chem. Phys. **101**, 5484 (1994).

HC_3

$\tilde{X}\ ^2\Pi_{1/2}$ $C_{\infty v}$ Structure: MW[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3238.0w	Ar	IR	5,6
	2	C_3 a-stretch	1832.6m 1824.7s	Ar	IR	1,5,6
	3	C_3 s-stretch	1167br 1159.8w	Ar	IR	5,6
Π	4	HCC bend	28[a]	gas	MW	4

$A=14.44$ gas MW[2–4]
$B_0=0.373$ MW[2-4]

DC_3

$\tilde{X}\ ^2\Pi_{1/2}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2424.0wmT	Ar	IR	5,6
	2	C_3 a-stretch	1778.8sh 1771.5m	Ar	IR	1,5,6
	3	C_3 s-stretch	1148br 1140.4w	Ar	IR	5,6

$A=12.53$ gas MW[4]
$B_0=0.337$ MW[4]

[a] $^2\Sigma^\mu$ component.

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HCCSi

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	CC stretch	1989.8	Ar	IR	1
	3	SiC stretch	636.0T	Ar	IR	1

DCCSi

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	CC stretch	1874.9	Ar	IR	1
	3	SiC stretch	622.4T	Ar	IR	1

Reference

[1] D. Han, C. M. L. Rittby, and W. R. M. Graham, J. Chem. Phys. **106**, 6222 (1997).

HCCN

$^3\Sigma^-$?

In the gas phase, a prominent absorption band system beginning at 340 nm has been attributed[2,3] to HCCN, but has not been analyzed. An absorption band system assigned to HCCN was observed in an argon matrix between 240 and 340 nm, with band separations of approximately 1050.[4]

$\tilde{X}$ $^3\Sigma^-$ $C_{\infty v}$ [a] Structure: ESR[1]MW[5–7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3246.66	gas	CC	8
			3229s	Ar	IR	4
	2	CCN a-stretch	1735s	Ar	IR	4
	3	CCN s-stretch	1178m	Ar	IR	4
Π	4	H deform.	383(20)	gas	CC,MW	8,9
			369.5[b]	Ar	IR	4
	5	Skel. deform.	187(20)	gas	CC	8

B_0=0.366 MW[5,7,9]

DCCN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2424ms	Ar	IR	4
	2	CCN a-stretch	1730s	Ar	IR	4
	3	CCN s-stretch	1127w	Ar	IR	4
Π	4	CCN bend	367(15)	gas	MW	9
			405wmT	Ar	IR	4
	5	D deform.	90(15)	gas	MW	9

B_0=0.330 MW[6,9]

[a]Quasi-linear,[6,7] with barrier to linearity[9] of ~235.
[b]Assignment proposed by Ref. 9. A prominent argon-matrix absorption of HCCN at 458 and of DCCN at 317.5, with counterparts at 435(20) and 311(20), respectively, in the millimeter-wave spectra, may result from $l=0$ transitions associated with overtones or combination bands.

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HCCO

$\tilde{B}$ $^2\Pi$ $C_{\infty v}$
T_0=33423.92(2) gas PF[6,7]LF[8] $\tilde{B}-\tilde{X}$ 263–300 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	CCO s-stretch	1037	gas	PF,LF	7,8
Π	4	Deformation	416T	gas	PF	7
	5	Deformation	365T	gas	PF	7

B_0=0.324 PF[7]LF[8]

Analysis of the submillimeter-wave spectrum[1] indicates that HCCO possesses a low-lying excited electronic state which, together with the ground state, is derived from a Π state by Renner-Teller interaction.

$\tilde{X}$ $^2A''$ C_s Structure: MW[1,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CCO a-stretch	2022.64	gas	DL	3
			2023.7	Ne	IR	5
			2019.5	Ar	IR	2
a''	6	CCH bend	494	gas	LF	8

A_0=41.5(1.5); B_0=0.363; C_0=0.359 MW[1,4]

DCCO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CCO a-stretch	1995.2	Ne	IR	5
			1989.9	Ar	IR	2

A_0=21.75(12); B_0=0.331; C_0=0.325 MW[1]

References

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HCCS

A $^2\Pi$ $C_{\infty v}$
T_0=24299.690(6) gas AB[1,2]EM[3]LF[4,6] $\tilde{A}-\tilde{X}$ 377–452 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	CC stretch	1843T	gas	AB	2
	3	CS stretch	740	gas	AB	1,2
Π	5	CCS bend	328H	gas	AB,EM	2,3

B_0=0.174 AB[2]

$\tilde{X}$ $^2\Pi$ $C_{\infty v}$ Structure: MW^5

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	CC stretch	2189T	gas	EM	3
	3	CS stretch	782	gas	EM	3
Π	5	CCS bend	411H[a]	gas	EM	3

$A \cong -185$[a] gas MW^5
$B_0=0.196$ AB^2MW^5

DCCS

$\tilde{A}$ $^2\Pi$ $C_{\infty v}$
$T_0=24359$ gas AB^2LF^4 $\tilde{A}-\tilde{X}$ 376–420 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	CC stretch	1718T	gas	AB	2
	3	CS stretch	725	gas	AB	2

[a]Ref. 7 estimated that $A=-270$, $\omega_4=565$, and $\omega_5=380$ by considering the relative intensities of microwave lines arising from vibrationally excited HCCS.

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HNCN

$\tilde{B}$ $^2A'$ C_s Structure: AB^1
$T_0=28994.1$ gas AB^1LF^2 $\tilde{B}-\tilde{X}$ 344–365 nm
$\tau_0=20(5)$ ns gas LF^2
$A_0=22.30$; $B_0=0.376$; $C_0=0.369$ AB^1LF^2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH stretch	3297.5m	Ar	IR	4
	2	NCN a-stretch	1843s	Ar	IR	4
	3		1146vs	Ar	IR	4
a''	6	NCN deform.	440T	gas	LF	2

$A_0=21.18(11)$; $B_0=0.370$; $C_0=0.363$ $AB^1LF^2MW^3$

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HCNN

$\tilde{A}$
$T_0=30500$ gas $AB^{1,2,4,5}$ $\tilde{A}-\tilde{X}$ 289–328 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1048	gas	AB	4

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3233.7wm	Ar	IR	3,6
			3229m	N_2	IR	3
		CNN a-stretch	1786.6s	Ar	IR	3,6
			1784s	Kr	IR	3
			1800s	N_2	IR	3
		H deform.	862.2vs	Ar	IR	3,6
			860vs	Kr	IR	3
			871m	N_2	IR	3
			863m			

DCNN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CNN a-stretch	1771vs	Ar	IR	3
		D deform.	725vs	Ar	IR	3

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HNCO

Between 132.5 and 120 nm, continuous absorption, with some diffuse bands.[5]

Relatively sharp absorption bands at 72940, 73910, and 74680 (137.1, 135.3, and 133.9 nm), which may be contributed by a Rydberg transition.[5]

Between 147 and 163 nm, diffuse bands are superposed on a continuum, with maximum near 157 nm.[5]

Continuous absorption between 163 and 185 nm, with a maximum near 166 nm.[5]

Continuous absorption has its onset near 41000 (244 nm), and extends beyond 200 nm.[4]

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

gas AB[4] $\tilde{A}-\tilde{X}$ 228–282 nm

Complicated group of progressions, possibly resulting from the occurrence of *cis*- and *trans*- rotamers in the excited state.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		NCO bend	555T	gas	AB	4

$A \cong 4.37$; $B \cong 0.388$; $C \cong 0.357$ AB[4]

$\tilde{X}\ ^1A'$ C_s Structure: MW[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH stretch	3538.25s	gas	IR,Ra	1,2,12 14,15
			3516.8wm	Ar	IR	12
			3505.7wm			
	2	NCO a-stretch	2268.89vs	gas	IR	1,2,9,10
			2259.0vs	Ar	IR	12,13
	3	NCO s-stretch	1327vw	gas	IR	1,2
	4	HNC, NCO bend	776.62wm	gas	IR	6
			769.8wm	Ar	IR	12,13
	5	HNC, NCO bend	577.35w	gas	IR	1,2,6
			573.7wm	Ar	IR	12,13
a''	6	Torsion	656.29	gas	IR	6,11

$A_0 = 30.638$; $B_0 = 0.369$; $C_0 = 0.364$ MW[7]IR[14]

DNCO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ND stretch	2637.20	gas	IR	8
			2606.9m	Ar	IR	12
	2	NCO a-stretch	2235vs	gas	IR	3
			2231.0vs	Ar	IR	12
	3	NCO s-stretch	1310	gas	IR	3
	4	DNC, NCO bend	578.6w	Ar	IR	12
	5	DNC, NCO bend	475.4w	Ar	IR	12
a''	6	Torsion	602.9	gas	IR	3

$A_0 = 17.09$; $B_0 = 0.344$; $C_0 = 0.336$ MW[7]

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$HOCS^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OH stretch	3435.16	gas	LD	1

$A_0 = 26.11$; $B_0 = 0.192$; $C_0 = 0.190$ LD[1]MW[2]

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t-HOCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3635.70	gas	LD	7
			3631.7wm	Ne	IR	9
			3628.1wm			
			3602.9	Ar	IR	2
			3456	CO	IR	1
	2	C=O stretch	1852.57	gas	DL	4
			1848.0s	Ne	IR	9
			1843.6	Ar	IR	2
			1833	CO	IR	1
	3	HOC bend	1210.4m	Ne	IR	9
			1211.2	Ar	IR	2
			1261	CO	IR	1
	4	C-O stretch	1050.4wm	Ne	IR	9
			1064.6	Ar	IR	2
			1077	CO	IR	1
	5	OCO bend	615	CO	IR	1
a''	6	Torsion	508.1wm	Ne	IR	9
			515	Ar	IR	2

$A_0 = 5.596$; $B_0 = 0.381$; $C_0 = 0.356$ MW[3]LMR[5]

t-DOCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2684.10	gas	LD	6
			2680.7wm	Ne	IR	9
			2678.1wm			
			2558	CO	IR	1
	2	C=O stretch	1851.65	gas	DL	4
			1848.0m	Ne	IR	9
			1846.2s			
			1841.7	Ar	IR	2
			1825	CO	IR	1
	3	Mixed	1082.5m	Ne	IR	9
			1092.6	Ar	IR	2
			1117	CO	IR	1
	5	OCO bend	610m	CO	IR	1
a''	6	Torsion	472wm	CO	IR	1

$A_0=5.160$; $B_0=0.356$; $C_0=0.333$ $MW^3LD^6LMR^8$

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HCO_2

$\tilde{B}$ $^2A_2$ C_{2v}
$T_0=4320$ gas PE[1] Structure: PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CO_2 bend	700(50)	gas	PE	1

$\tilde{A}$ $^2B_2$[a] C_{2v}
$T_0=220$ gas PE[1] Structure: PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CO_2 bend	550T	gas	PE	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CO_2 bend	570T[b]	gas	PE	1

DCO_2

$\tilde{B}$ $^2A_2$ C_{2v}
$T_0=4110$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CO_2 bend	700(50)	gas	PE	1

$\tilde{A}$ $^2A_1$[a] C_{2v}
$T_0=65T$ gas PE[1]

$\tilde{X}$ $^2B_2$[a] C_{2v}

[a]Strong vibronic interaction between the $\tilde{X}$ and $\tilde{A}$ states. Differences in the zero-point vibrational energies result in a reversal of the symmetries of these two states for DCO_2.
[b]Large anharmonicity.

Reference

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$HFCS^+$

$\tilde{B}$ C_s
$T_0=28720(120)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1210(80)	gas	PE	1
			980(80)	gas	PE	1

$\tilde{A}$ $^2A''$ C_s
$T_0=10810(180)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1450(80)	gas	PE	1
			750(80)	gas	PE	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1360(60)	gas	PE	1

Reference

[1] J. Baker, V. A. Butcher, J. M. Dyke, and E. P. F. Lee, J. Phys. Chem. **99**, 10147 (1995).

HBF_2

$\tilde{X}$ C_{2v} Structure: IR[2,3]MW[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	BH stretch	2620.8(5)	gas	IR	1–4
			2644	N_2	IR	6
	2	BF_2 s-stretch	1164.2(5)	gas	IR	1–4
			1156	N_2	IR	6
	3	BF_2 scissors	541.5(5)	gas	IR	1–4
			542	N_2	IR	6
b_1	4	OPLA	923.5(5)	gas	IR	1–4
			918	N_2	IR	6
b_2	5	BF_2 a-stretch	1402vs	gas	IR	1,2,4
			1385.1	N_2	IR	6

$A_0=2.485$; $B_0=0.350$; $C_0=0.306$ MW[5,7]

DBF_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	BD stretch	1960.0(5)	gas	IR	2–4
			1980	N_2	IR	6
	2	BF_2 s-stretch	1126.4(5)	gas	IR	2–4
			1121.3	N_2	IR	6
	3	BF_2 scissors	540	gas	IR	2,4
b_1	4	OPLA	785	gas	IR	2,4
			772.7	N_2	IR	6
b_2	5	BF_2 a-stretch	1392	gas	IR	2,4
			1374.5	N_2	IR	6

$A_0=1.764$; $B_0=0.350$; $C_0=0.292$ MW[5]

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$HBCl_2$

$\tilde{X}$ C_{2v} Structure: IR[4]MW[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	BH stretch	2616.9w	gas	IR	1–4
			2625	Ar	IR	6
	2	BCl_2 s-stretch	740T	gas	IR	5
b_1	4	OPLA	784T	gas	IR	5
			788	Ar	IR	6
b_2	5	HBCl bend	1089s	gas	IR	1–3,5
			1082.5	Ar	IR	6,7
	6	BCl_2 a-stretch	892s	gas	IR	1–3,5
			886.3	Ar	IR	6,7

$A_0=1.565$; $B_0=0.106$; $C_0=0.099$ IR[4]MW[8]

$DBCl_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	BD stretch	1969	gas	IR	4
b_1	4	OPLA	645T	gas	IR	5
b_2	5	BCl_2 a-stretch	1005T	gas	IR	5
			970	Ar	IR	6

$A_0=1.173$; $B_0=0.106$; $C_0=0.097$ IR[4]MW[8]

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$HBBr_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	BH stretch	2622.4	gas	IR	1–3
	2	BBr_2 s-stretch	595	gas	IR	2
b_1	4	OPLA	731	gas	IR	2
b_2	5	BBr_2 a-stretch	1036	gas	IR	2,3
			1032	Ar	IR	4
	6	HBBr deform.	772	gas	IR	2,3
			768	Ar	IR	4

$A_0=1.256$; $B_0=0.041$; $C_0\cong0.039$ gas IR[1]

$DBBr_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	BD stretch	1960.1	gas	IR	1–3
	2	BBr_2 s-stretch	585	gas	IR	2
b_1	4	OPLA	625vw	gas	IR	2
b_2	5	BBr_2 a-stretch	870	gas	IR	2,3
	6	DBBr deform.	656	gas	IR	2,3

$A_0=0.822$; $B_0=0.041$; $C_0\cong0.039$ gas IR[1]

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HCO_2^-

Threshold for electron detachment from ground-state HCO_2^- = 28220(120) gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CO_2 bend	730	gas	PE	1

DCO_2^-

Threshold for electron detachment from ground-state DCO_2^- =28320(120) gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CO_2 bend	730	gas	PE	1

Reference

[1] E. H. Kim, S. E. Bradforth, D. W. Arnold, R. B. Metz, and D. M. Neumark, J. Chem. Phys. **103**, 7801 (1995).

HCOCl

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

T_0=32754.7 gas AB[5,6] $\tilde{A}-\tilde{X}$ 230–314 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CO stretch	1153.8	gas	AB	5
	4	CCl stretch	633.6	gas	AB	5
	5	ClCO deform.	306.3	gas	AB	5
a''	6	Umbrella (OPLA)	779.5	gas	AB	5

Barrier to planarity=1608.8 gas AB[5]

$\tilde{X}$ $^1A'$ C_s Structure: MW[2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	2929.18w	gas	IR	1,3,6
	2	CO stretch	1784.14vs	gas	IR	1,3,6,8
	3	CH bend	1307.21m	gas	IR	1,3,6,7
	4	CCl stretch	738.80vs	gas	IR	1,3,6,9
	5	CCl bend	457.02vw	gas	IR	1,6,9
a''	6	OPLA	932.15vw	gas	IR	1,3,6,11

A_0=2.601; B_0=0.205; C_0=0.190 MW[2,4]IR[7]

DCOCl

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

T_0=32775.3 gas AB[5] $\tilde{A}-\tilde{X}$ 283–313 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CO stretch	1092.0	gas	AB	5
	4	CCl stretch	633.4	gas	AB	5
	5	ClCO deform.	303.1	gas	AB	5
a''	6	Umbrella (OPLA)	566.5	gas	AB	5

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CD stretch	2204.3	gas	IR	4,10
	2	CO stretch	1749.1	gas	IR	4,10
	3	CD bend	986.11	gas	IR	4,10
	4	CCl stretch	700.77	gas	IR	4,10,11
	5	CCl bend	455.78	gas	IR	10
a''	6	OPLA	781.50	gas	IR	10,11

A_0=1.904; B_0=0.203; C_0=0.184 MW[2,4]DL[10]

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HCOBr

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	2911.9	gas	IR	1
	2	CO stretch	1797.9[a]	gas	IR	1
			1799.5	Ar	IR	2
	3	H deform.	1270.9[b]	gas	IR	1
	4	CBr stretch	646.3	gas	IR	1
a''	6	OPLA	893.4	gas	IR	1

DCOBr

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CD stretch	2205.4	gas	IR	1
	2	CO stretch	1748.3	gas	IR	1
			1746.2	Ar	IR	2
	3	D deform.	975.5[c]	gas	IR	1
	4	CBr stretch	605.2	gas	IR	1
	5	CBr deform.	358T	gas	IR	1
a''	6	OPLA	746.8	gas	IR	1

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

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HCOI

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	2930Tw	gas	IR	1
	2	CO stretch	1776.3vs	gas	IR	1
	3	HCO deform.	1247.9wm	gas	IR	1
	4	CI stretch	561m	gas	IR	1

Reference

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c-HNSO[a]

gas AB^3 238–269 nm

Diffuse absorption merges into continuum with maximum near 217 nm.[3]

Photolysis in an argon matrix by 254 nm radiation leads to rapid formation of *c*-HOSN.[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	5	NSO bend	285T	gas	AB	3

$\tilde{a}\ ^3A'$ [b] C_s

Weak, unstructured absorption 325–350 nm.[3]

In an argon matrix, converted to *t*-HNSO by irradiation at wavelengths longer than 300 nm.[6]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH stretch	3308.5	gas	IR	7,9
			3308wm	Ar	IR	3,4
			3303	N_2	IR	4
	2	SO stretch	1257.58s	gas	IR	1,9,10
			1249vs	Ar	IR	3,4
			1252	N_2	IR	4
	3	NS stretch	1086.83w	gas	IR	1,9,11
			1083s	Ar	IR	3,4
			1094	N_2	IR	4
	4	HNS bend	906.3m	gas	IR	1,9
			900s	Ar	IR	3,4
			923	N_2	IR	4
	5	NSO bend	447.85m	gas	IR	1,9,11
			447s	Ar	IR	3,4
			455	N_2	IR	4
a''	6	Torsion	757.0s	gas	IR	1,9
			755vs	Ar	IR	3,4
			774	N_2	IR	4

$A_0=1.645$; $B_0=0.329$; $C_0=0.274$ MW^2

c-DNSO

gas AB^3 242–264 nm

Diffuse, merges into continuum.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	5	NSO bend	285T	gas	AB	3

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ND stretch	2454.8	gas	IR	8,9
			2453	Ar	IR	3,4
	2	SO stretch	1254.4s	gas	IR	1,9
			1245	Ar	IR	3,4
	3	NS stretch	1052.3w	gas	IR	1,9
			1048	Ar	IR	3,4
	4	DNS bend	755.0m	gas	IR	1,9
			752	Ar	IR	3,4
	5	NSO bend	400.2m	gas	IR	1,9
			400	Ar	IR	3,4
a''	6	Torsion	595.7s	gas	IR	1,9
			594	Ar	IR	3,4

$A_0=1.644(3)$; $B_0=0.318$; $C_0=0.259$ MW^2

[a]Stable rotamer.
[b]Tentative assignment.

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[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).
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[10] D.-L. Joo and D. J. Clouthier, J. Chem. Phys. **104**, 8852 (1996).
[11] D.-L. Joo, H. H. Harjanto, and D. J. Clouthier, J. Mol. Spectrosc. **178**, 78 (1996).

HPSS

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		PH stretch	2172.6	Ar	IR	1
		P=S stretch	690.6	Ar	IR	1
		S=S stretch	682.4	Ar	IR	1

DPSS

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		P=S stretch	690.3	Ar	IR	1
		S=S stretch	682.3	Ar	IR	1
		DPS deform.	588.1	Ar	IR	1

Reference

[1] Z. Mielke and L. Andrews, J. Phys. Chem. **97**, 4313 (1993).

HOClO

In an argon matrix, a dissociative excited state has its maximum near 400 nm (25000).[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OH stretch	3527.1vs	Ar	IR	1
	2	HOCl deform.	1176.9wm	Ar	IR	1
	3	ClO stretch	973.9s	Ar	IR	1
	4	OCl stretch	591.5wm	Ar	IR	1

DOClO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OD stretch	2605.4vs	Ar	IR	1
	2	ClO stretch	974.7vs	Ar	IR	1
	3	DOCl deform.	864.5wm	Ar	IR	1
	4	OCl stretch	594.5wm	Ar	IR	1

Reference

[1] K. Johnsson, A. Engdahl, and B. Nelander, J. Phys. Chem. **100**, 3923 (1996).

$HClO_2$

In an argon matrix, the onset of photodecomposition is near 290 nm (34500).[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	HCl stretch	2116wm	Ar	IR	1
	2	ClO_2 a-stretch	1132.0vs	Ar	IR	1
	5	ClO_2 s-stretch	969.4m	Ar	IR	1

$DClO_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	DCl stretch	1550.4wm	Ar	IR	1
	2	ClO_2 a-stretch	1115.9vs	Ar	IR	1
	3	ClO_2 s-stretch	969.3m	Ar	IR	1

Reference

[1] K. Johnsson, A. Engdahl, and B. Nelander, J. Phys. Chem. **100**, 3923 (1996).

8.7. Four-Atomic Nonhydrides

Ta_4

In an argon matrix,[1] there is a broad absorption maximum centered at 18800 (532 nm).

In an argon matrix,[1] a broad absorption maximum at 13020 (768 nm) has partially resolved high frequency shoulders separated by intervals of ~240.

$\tilde{X}$ T_d

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			270.2	Ar	Ra	1
			185.1	Ar	Ra	1
			130.6(2)	Ar	Ra	1

Reference

[1] H. Wang, R. Craig, H. Haouari, J.-G. Dong, Z. Hu, A. Vivoni, J. R. Lombardi, and D. M. Lindsay, J. Chem Phys. **103**, 3289 (1995).

BeBeCO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1943.6	Ar	IR	1
			483.3	Ar	IR	1

Reference

[1] L. Andrews, T. J. Tague, Jr., G. P. Kushto, and R. D. Davy, Inorg. Chem. **34**, 2952 (1995).

BeBeNN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NN stretch	1876.1	Ar	IR	1

Reference

[1] C. A. Thompson, L. Andrews, and R. D. Davy, J. Phys. Chem. **99**, 7913 (1995).

BeNNBe

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BeN stretch	1111.7	Ar	IR	1

Reference

[1] C. A. Thompson, L. Andrews, and R. D. Davy, J. Phys. Chem. **99**, 7913 (1995).

$(BeN)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BeN stretch	787.7	Ar	IR	1

Reference

[1] C. A. Thompson, L. Andrews, and R. D. Davy, J. Phys. Chem. **99**, 7913 (1995).

FeCCC

$\tilde{A}$ $C_{\infty v}$
T_0=4500(700) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Fe=C stretch	700(150)	gas	PE	1

Reference

[1] J. Fan, L. Lou, and L.-S. Wang, J. Chem. Phys. **102**, 2701 (1995).

AlCCAl

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	AlC a-stretch	605.1	Ar	IR	1

Reference

[1] G. V. Chertihin, L. Andrews, and P. R. Taylor, J. Am. Chem. Soc. **116**, 3513 (1994).

$FeCCC^-$

Threshold for electron detachment from ground-state $FeCCC^-$ =13600(600) gas PE[1]

Reference

[1] J. Fan, L. Lou, and L.-S. Wang, J. Chem. Phys. **102**, 2701 (1995).

cyc-$(BeO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1131.2	Ar	IR	1
			1120.8	Kr	IR	1
			1104.4	Xe	IR	1
			1118.0	N_2	IR	2
			866.3	Ar	IR	1
			857.2	Kr	IR	1
			845.4	Xe	IR	1
			892.4	N_2	IR	2
			522.4	Ar	IR	1
			516.9	Kr	IR	1
			514.4	Xe	IR	1
			539.1	N_2	IR	2

References

[1] C. A. Thompson and L. Andrews, J. Chem. Phys. **100**, 8689 (1994).
[2] L. Andrews, G. V. Chertihin, C. A. Thompson, J. Dillon, S. Byrne, and C. W. Bauschlicher, Jr., J. Phys. Chem. **100**, 10088 (1996).

BeOBeO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1572.9T	Ar	IR	1,2
			1552Tbr	N_2	IR	2

References

[1] C. A. Thompson and L. Andrews, J. Chem. Phys. **100**, 8689 (1994).
[2] L. Andrews, G. V. Chertihin, C. A. Thompson, J. Dillon, S. Byrne, and C. W. Bauschlicher, Jr., J. Phys. Chem. **100**, 10088 (1996).

MgOMgO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			971.7A[a]	Ar	IR	1
			943.1B	Ar	IR	1
			591.7A	Ar	IR	1
			567.2B	Ar	IR	1

[a]It is uncertain whether the absorptions labelled A and B are contributed by two different MgOMgO structures (A and B) or whether they correspond to the same molecule trapped in two different matrix sites.

Reference

[1]L. Andrews and J. T. Yustein, J. Phys. Chem. **97**, 12700 (1993).

cyc-$(CaO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}	5		584.6	Ar	IR	1
			559.5	N_2	IR	2
b_{3u}	6		516.3	Ar	IR	1
			497.0	N_2	IR	2

References

[1]L. Andrews, J. T. Yustein, C. A. Thompson, and R. D. Hunt, J. Phys. Chem. **98**, 6514 (1994).
[2]L. Andrews, G. V. Chertihin, C. A. Thompson, J. Dillon, S. Byrne, and C. W. Bauschlicher, Jr., J. Phys. Chem. **100**, 10088 (1996).

CaOCaO

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

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

Reference

[1]L. Andrews, J. T. Yustein, C. A. Thompson, and R. D. Hunt, J. Phys. Chem. **98**, 6514 (1994).

cyc-$(SrO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}	5		530.1	Ar	IR	1
			502.7	N_2	IR	2
b_{3u}	6		441.3	Ar	IR	1
			423T	N_2	IR	2

References

[1]L. Andrews, J. T. Yustein, C. A. Thompson, and R. D. Hunt, J. Phys. Chem. **98**, 6514 (1994).
[2]L. Andrews, G. V. Chertihin, C. A. Thompson, J. Dillon, S. Byrne, and C. W. Bauschlicher, Jr., J. Phys. Chem. **100**, 10088 (1996).

cyc-$(BaO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}	5		501.2	Ar	IR	1,2
b_{3u}	6		401.4	Ar	IR	1,2

References

[1]D. M. Thomas and L. Andrews, J. Mol. Spectrosc. **50**, 220 (1974).
[2]L. Andrews, J. T. Yustein, C. A. Thompson, and R. D. Hunt, J. Phys. Chem. **98**, 6514 (1994).

BaOBaO

$\tilde{X}$

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

References

[1]D. M. Thomas and L. Andrews, J. Mol. Spectrosc. **50**, 220 (1974).
[2]L. Andrews, J. T. Yustein, C. A. Thompson, and R. D. Hunt, J. Phys. Chem. **98**, 6514 (1994).

cyc-$(TiO)_2$

$\tilde{X}$

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

Reference

[1]G. V. Chertihin and L. Andrews, J. Phys. Chem. **99**, 6356 (1995).

cyc-$(ZrO)_2$

$\tilde{X}$

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

Reference

[1]G. V. Chertihin and L. Andrews, J. Phys. Chem. **99**, 6356 (1995).

cyc-$(HfO)_2$

$\tilde{X}$

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

Reference

[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. **99**, 6356 (1995).

$(FeO)_2$

$\tilde{A}$

T_0=3550(400) gas PE[6]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			670(70)	gas	PE	6
	5		517.4	Ar	IR	1–4
			535.5	N_2	IR	5

References

[1] S. Abramowitz, N. Acquista, and I. W. Levin, Chem. Phys. Lett. **50**, 423 (1977).
[2] S. Chang, G. Blyholder, and J. Fernandez, Inorg. Chem. **20**, 2813 (1981).
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[4] G. V. Chertihin, W. Saffel, J. T. Yustein, L. Andrews, M. Neurock, A. Ricca, and C. W. Bauschlicher, Jr., J. Phys. Chem. **100**, 5261 (1996).
[5] L. Andrews, G. V. Chertihin, A. Citra, and M. Neurock, J. Phys. Chem. **100**, 11235 (1996).
[6] H. Wu, S. R. Desai, and L.-S. Wang, J. Am. Chem. Soc. **118**, 5296 (1996).

cyc-$(NiO)_2$

$\tilde{X}$

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

Reference

[1] A. Citra, G. V. Chertihin, L. Andrews, and M. Neurock, J. Phys. Chem. A **101**, 3109 (1997).

NiONiO

$\tilde{X}$

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

Reference

[1] A. Citra, G. V. Chertihin, L. Andrews, and M. Neurock, J. Phys. Chem. A **101**, 3109 (1997).

Cu_2O_2

$\tilde{C}$

T_0=6780(400) gas PE[1]

$\tilde{B}$

T_0=5320(400) gas PE[1]

$\tilde{A}$

T_0=3630(400) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			650(30)	gas	PE	1

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			630(30)	gas	PE	1

Reference

[1] L.-S. Wang, H. Wu, S. R. Desai, and L. Lou, Phys. Rev. B **53**, 8028 (1996).

ZnOZnO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			882br	Ar	IR	1
			877br			
			877br	N_2	IR	1
			848.5	Ar	IR	1

Reference

[1] G. V. Chertihin and L. Andrews, J. Chem. Phys. **106**, 3457 (1997).

CdOCdO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			682.0	Ar	IR	1
			675.5			

Reference

[1] G. V. Chertihin and L. Andrews, J. Chem. Phys. **106**, 3457 (1997).

C_4

$^3\Sigma_u^-$ $D_{\infty h}$
T_0=26323(15) Ne AB[11] $^3\Sigma_u^- - \tilde{X}$ 325–380 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1822(20)	Ne	AB	11
	2	C–C stretch	903(20)	Ne	AB	11
Π_g	4	Bend	370(20)H	Ne	AB	11
Π_u	5	Bend	175(20)H	Ne	AB	11

$^1\Delta_g$ $D_{\infty h}$
T_0=2640(50) gas PE[6]

$\tilde{X}$ $^3\Sigma_g^-$ $D_{\infty h}$ [a] Structure: ESR[2,5]DL[3,7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	2032(50)	gas	PE	6
Σ_u^+	3	Asym. stretch	1548.61	gas	DL	3
			1547.0	Ne	IR	8,10
			1543.4	Ar	IR	1
			1539.5	Kr	IR	12
Π_g	4	Bend	352(15)	gas	PE,DL	6,9
Π_u	5	Bend	160(4)[b]	gas	DL	7
			172.4	Ar	IR	4
			170.4			

B_0=0.166 DL[4,8]

[a]ESR measurements[2,5] suggest that C_4 may deviate by a few degrees from the linear structure.
[b]Estimated from *l*-doubling parameter for ν_5.

References

[1] L. N. Shen and W. R. M. Graham, J. Chem. Phys. **91**, 5115 (1989).
[2] H. M. Cheung and W. R. M. Graham, J. Chem. Phys. **91**, 6664 (1989).
[3] J. R. Heath and R. J. Saykally, J. Chem. Phys. **94**, 3271 (1991).
[4] P. A. Withey, L. N. Shen, and W. R. M. Graham, J. Chem. Phys. **95**, 820 (1991).
[5] Q. Jiang and W. R. M. Graham, J. Chem. Phys. **95**, 3129 (1991).
[6] D. W. Arnold, S. E. Bradforth, T. N. Kitsopoulos, and D. M. Neumark, J. Chem. Phys. **95**, 8753 (1991).
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[11] P. Freivogel, M. Grutter, D. Forney, and J. P. Maier, Chem. Phys. Lett. **249**, 191 (1996).
[12] J. Szczepanski, S. Ekern, C. Chapo, and M. Vala, Chem. Phys. **211**, 359 (1996).

Si_2C_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{1u}	3		982.9vs	Ar	IR	1
b_{2u}	4		382.2wm	Ar	IR	1

Reference

[1] J. D. Presilla-Márquez, S. C. Gay, C. M. L. Rittby, and W. R. M. Graham, J. Chem. Phys. **102**, 6354 (1995).

Si_4

$^1B_{1u}$ D_{2h}
T_0=23635T[a] gas EM[3] $^1B_{1u}-\tilde{X}$ 418–448 nm
21432(9) Ne AB[1,7] $^1B_{1u}-\tilde{X}$ 410–470 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1		431(14)	Ne	AB	7
	2		310(25)	gas	EM	3
			317(14)	Ne	AB	1,7

$^3B_{1u}$ D_{2h}
T_0=16220(160) gas PE[2]TPE[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1		450(65)	gas	PE,TPE	2,4

$^1B_{3u}$ D_{2h}
T_0=11050(80) gas PE[2]TPE[4]
10807(2) Ne AB[7] $^1B_{3u}-\tilde{X}$ 790–930 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g			300(8)	gas	TPE	4
			300(6)	Ne	AB	7

$^3B_{3u}$ D_{2h}
T_0=6580(80) gas PE[2]TPE[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2		312	gas	PE,TPE	2,4

$\tilde{X}$ ^1A_g D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1		470	N_2	Ra	5
	2		360(25)	gas	PE	2
			345	N_2	Ra	5
b_{1u}	4		501.9	Ne	IR	6
			500.9	Ar	IR	6
			498.5	Kr	IR	6

[a]Attributed by Refs. 1 and 3 to Si_3.

References

[1] W. Weltner, Jr. and D. McLeod, Jr., J. Chem. Phys. **41**, 235 (1964).
[2] T. N. Kitsopoulos, C. J. Chick, A. Weaver, and D. M. Neumark, J. Chem. Phys. **93**, 6108 (1990).
[3] C. B. Winstead, K. X. He, D. Grantier, T. Hammond, and J. L. Gole, Chem. Phys. Lett. **181**, 222 (1991).
[4] C. C. Arnold and D. M. Neumark, J. Chem. Phys. **99**, 3353 (1993).
[5] E. C. Honea, A. Ogura, C. A. Murray, K. Raghavachari, W. O. Sprenger, M. F. Jarrold, and W. L. Brown, Nature **366**, 42 (1993).
[6] S. Li, R. J. Van Zee, W. Weltner, Jr., and K. Raghavachari, Chem. Phys. Lett. **243**, 275 (1995).
[7] J. Fulara, P. Freivogel, M. Grutter, and J. P. Maier, J. Phys. Chem. **100**, 18042 (1996).

Ge_4

$\tilde{a}\ ^3B_{3u}$ D_{2h}
T_0=6000T gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		Breathing	173T	gas	TPE	1

Reference

[1] G. R. Burton, C. Xu, C. C. Arnold, and D. M. Neumark, J. Chem. Phys. **104**, 2757 (1996).

$Fe_2O_2^-$

Threshold for electron detachment from ground-state $Fe_2O_2^-$ =19040(400) gas PE[1]

Reference

[1] H. Wu, S. R. Desai, and L.-S. Wang, J. Am. Chem. Soc. **118**, 5296 (1996).

$Cu_2O_2^-$

Threshold for electron detachment from ground-state $Cu_2O_2^-$ =19850(240) gas PE[1]

Reference

[1] L.-S. Wang, H. Wu, S. R. Desai, and L. Lou, Phys. Rev. B **53**, 8028 (1996).

C_4^-

Threshold for electron detachment from ground-state C_4^- =31320(80) gas PE[1,2]

(3) $^2\Pi_u$ $D_{\infty h}$
Ne AB[6] 335–347 nm

(2) $^2\Pi_u$ $D_{\infty h}$
T_0=26069(14) Ne AB[6] 372–384 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	2		755(20)	Ne	AB	6
Π_g	4		349(10)H	Ne	AB	6
Π_u	5		271(10)H	Ne	AB	6

$\tilde{C}\ ^2\Pi_u$ $D_{\infty h}$
T_0=21871.53 gas PD[4] $\tilde{C}-\tilde{X}$ 410–460 nm
21896(5) Ne AB[3]LF[5] $\tilde{C}-\tilde{X}$ 410–527 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		2241(5)T	Ne	AB	3
	2		752.4	gas	PD	4
			759(5)	Ne	AB	3
Π_u	5	Deformation	223H	gas	PD	4

A_0=−37(9) gas PD[4]
B_0=0.156 PD[4]

$\tilde{B}\ ^2\Sigma_u^+$ $D_{\infty h}$
T_0=10789(2) Ne AB[6] $\tilde{B}-\tilde{X}$ 672–927 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		2056(5)	Ne	AB	6
	2		930(4)	Ne	AB	6
Π_u	5		259(2)H	Ne	AB	6

$\tilde{A}\ ^2\Sigma_g^+$ $D_{\infty h}$
Ne AB[6] $\tilde{A}-\tilde{X}$ 907–1206 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	2		817(3)	Ne	AB	6
Π_u	5		275(2)	Ne	AB	6

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		2047(20)	Ne	LF	5
	2		936(20)	Ne	LF	5
Π_g	4		396(20)H	Ne	LF	5

A_0=−39(9) gas PD[4]
B_0=0.167 PD[4]

References

[1] S. Yang, K. J. Taylor, M. J. Craycraft, J. Conceicao, C. L. Pettiette, O. Cheshnovsky, and R. E. Smalley, Chem. Phys. Lett. **144**, 431 (1988).
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[4] Y. Zhao, E. de Beer, and D. M. Neumark, J. Chem. Phys. **105**, 2575 (1996).
[5] M. Schäfer, M. Grutter, J. Fulara, D. Forney, P. Freivogel, and J. P. Maier, Chem. Phys. Lett. **260**, 406 (1996).
[6] P. Freivogel, M. Grutter, D. Forney, and J. P. Maier, J. Chem. Phys. **107**, 22 (1997).

Si_4^-

Threshold for electron detachment from ground-state Si_4^- =17510(80) gas PE[1]TPE[2]

$^2B_{1u}$ D_{2h}
T_0=11460(3) Ne AB[3] $^2B_{1u}-\tilde{X}$ 780–875 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1		352(4)	Ne	AB	3
	2		278(4)	Ne	AB	3

$\tilde{X}$ $^2B_{2g}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2		365	gas	TPE	2

References

[1] T. N. Kitsopoulos, C. J. Chick, A. Weaver, and D. M. Neumark, J. Chem. Phys. **93**, 6108 (1990).
[2] C. C. Arnold and D. M. Neumark, J. Chem. Phys. **99**, 3353 (1993).
[3] J. Fulara, P. Freivogel, M. Grutter, and J. P. Maier, J. Phys. Chem. **100**, 18042 (1996).

CCCN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	5	Bend	179T	gas	MW	3

B_0=0.165 MW[1,2]

References

[1] M. Guélin, F. Friberg, and A. Mezaoui, Astron. Astrophys. **109**, 23 (1981).
[2] C. A. Gottlieb, E. W. Gottlieb, P. Thaddeus, and H. Kawamura, Astrophys. J. **275**, 916 (1983).
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cyc-$NaNO_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NO_2 s-stretch	1293.0	Ar	IR	2
	2	NO_2 scissors	825.6	Ar	IR	2
	3	ONaO s-stretch	306	Ar	IR	1
b_2	5	NO_2 a-stretch	1222.8	Ar	IR	1,2
	6	ONaO a-stretch	207	Ar	IR	1

References

[1] M. Barbeschi, L. Bencivenni, and F. Ramondo, Chem. Phys. **112**, 387 (1987).
[2] W.-J. Lo, M.-Y. Shen, C.-H. Yu, and Y.-P. Lee, J. Chem. Phys. **104**, 935 (1996).

t-NaONO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO stretch	1446.2	Ar	IR	1
		ON stretch	1159.1	Ar	IR	1
		ONO deform.	787.1	Ar	IR	1

Reference

[1] W.-J. Lo, M.-Y. Shen, C.-H. Yu, and Y.-P. Lee, J. Chem. Phys. **104**, 935 (1996).

cyc-KNO_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NO_2 s-stretch	1313.4	Ar	IR	2
	2	NO_2 scissors	807.3	Ar	IR	1,2
	3	OKO s-stretch	227	Ar	IR	1
b_2	5	NO_2 a-stretch	1217.3	Ar	IR	1,2

References

[1] M. Barbeschi, L. Bencivenni, and F. Ramondo, Chem. Phys. **112**, 387 (1987).
[2] W.-J. Lo, M.-Y. Shen, C.-H. Yu, and Y.-P. Lee, J. Chem. Phys. **104**, 935 (1996).

t-KONO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO stretch	1412.4	Ar	IR	1
		ON stretch	1171.0	Ar	IR	1
		ONO deform.	783.1	Ar	IR	1

Reference

[1] W.-J. Lo, M.-Y. Shen, C.-H. Yu, and Y.-P. Lee, J. Chem. Phys. **104**, 935 (1996).

OCBeO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	2189.5	Ar	IR	1
		BeO stretch	1498.2	Ar	IR	1

Reference

[1] L. Andrews and T. J. Tague, Jr., J. Am. Chem. Soc. **116**, 6856 (1994).

COBeO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	2056.5	Ar	IR	1
		BeO stretch	1533.9	Ar	IR	1

Reference

[1] L. Andrews and T. J. Tague, Jr., J. Am. Chem. Soc. **116**, 6856 (1994).

OTiCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1866.7	Ar	IR	1
		TiO stretch	952.8	Ar	IR	1

Reference

[1] G. V. Chertihin and L. Andrews, J. Am. Chem. Soc. **117**, 1595 (1995).

N_2FeO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NN stretch	2262.6	Ar	IR	1
			953.2	N_2	IR	2
		FeO stretch	887.3	Ar	IR	1,3
			853.9	N_2	IR	2

References

[1] G. V. Chertihin, W. Saffel, J. T. Yustein, L. Andrews, M. Neurock, A. Ricca, and C. W. Bauschlicher, Jr., J. Phys. Chem. **100**, 5261 (1996).
[2] L. Andrews, G. V. Chertihin, A. Citra, and M. Neurock, J. Phys. Chem. **100**, 11235 (1996).
[3] G. V. Chertihin, L. Andrews, and M. Neurock, J. Phys. Chem. **100**, 14609 (1996).

OUCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1799.6	Ar	IR	1
		UO stretch	804.4	Ar	IR	1

Reference

[1] T. J. Tague, Jr., L. Andrews, and R. D. Hunt, J. Phys. Chem. **97**, 10920 (1993).

$(AlO)_2$

$\tilde{B}$

T_0=25980(640) gas PE[3]

$\tilde{A}$

T_0=3950(160) gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Sym. stretch	730(80)	gas	PE	3

$\tilde{X}$ [a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1176.3T	Ar	IR	2
			945.4	Ar	IR	1,2
		Sym. stretch	660(80)	gas	PE	3

[a] *Ab initio* calculations cited in Ref. 2 suggest a linear structure, whereas those considered in Ref. 3 favor a rhombic, D_{2h} configuration. Isotopic substitution studies would be consistent with either structure. For the rhombic configuration, the absorption at 1176.3 may be contributed by a combination band.

References

[1] I. L. Rozhanskii, G. V. Chertikhin, L. V. Serebrennikov, and V. F. Shevel'kov, Zh. Fiz. Khim. **62**, 2351 (1988); Russ. J. Phys. Chem. **62**, 1215 (1988).
[2] L. Andrews, T. R. Burkholder, and J. T. Yustein, J. Phys. Chem. **96**, 10182 (1992).
[3] S. R. Desai, H. Wu, C. M. Rohlfing, and L.-S. Wang, J. Chem. Phys. **106**, 1309 (1997).

CNCN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡N s-stretch	2302.00	gas	IR	1,7
			2294.4	Ar	IR	2
	2	C≡N a-stretch	2059.73	gas	IR	1,7,8
			2053.7	Ar	IR	2
	3	N-C stretch	934.73[a]	gas	IR	6
			979.2[a]	Ar	IR	2
Π	4	Bend	463.69	gas	IR	2,5,6
			468.5	Ar	IR	2
			467.2			
	5	Bend	194.93	gas	IR	1,6
			200T[b]	Ar	IR	1

B_0=0.173 IR[1,3,8]MW[1,3-5]

[a] In Fermi resonance with $2\nu_4$.
[b] From combination bands.

References

[1] F. Stroh and M. Winnewisser, Chem. Phys. Lett. **155**, 21 (1989).
[2] F. Stroh, B. P. Winnewisser, M. Winnewisser, H. P. Reisenauer, G. Maier, S. J. Goede, and F. Bickelhaupt, Chem. Phys. Lett. **160**, 105 (1989); **162**, 253 (1989).
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[4] M. C. L. Gerry, F. Stroh, and M. Winnewisser, J. Mol. Spectrosc. **140**, 147 (1990).
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[6] F. Stroh, M. Winnewisser, and B. P. Winnewisser, J. Mol. Spectrosc. **162**, 435 (1993).
[7] F. Stroh, M. Winnewisser, and B. P. Winnewisser, Can. J. Phys. **72**, 1252 (1994).
[8] D. McNaughton, G. F. Metha, and R. Tay, Chem. Phys. **198**, 107 (1995).

CCCS

In an argon matrix, a weak absorption maximum at 26460 (378 nm) has been assigned[2] to CCCS.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1		2058.22	gas	DL	5
			2046.2vs	Ar	IR	2
	2		1533.2wm	Ar	IR	2
	3		725.6w	Ar	IR	2

B_0=0.096 MW[1,4]

References

[1] S. Yamamoto, S. Saito, K. Kawaguchi, N. Kaifu, H. Suzuki, and M. Ohishi, Astrophys. J. **317**, L119 (1987).
[2] G. Maier, J. Schrot, H. P. Reisenauer, and R. Janoschek, Chem. Ber. **124**, 2617 (1991).
[3] Y. Ohshima and Y. Endo, J. Mol. Spectrosc. **153**, 627 (1992).
[4] F. J. Lovas, R. D. Suenram, T. Ogata, and S. Yamamoto, Astrophys. J. **399**, 325 (1992).
[5] S. Takano, J. Tang, and S. Saito, J. Mol. Spectrosc. **178**, 194 (1996).

$NFeO_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	FeN stretch	980.5	N_2	IR	1
	2	FeO s-stretch	837.2	N_2	IR	1
a''	5	FeO a-stretch	928.0	N_2	IR	1

Reference

[1] L. Andrews, G. V. Chertihin, A. Citra, and M. Neurock, J. Phys. Chem. **100**, 11235 (1996).

NUO_2

$\tilde{X}$ C_1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		UO stretch	845.5	Ar	IR	1
		UO stretch	718.3	Ar	IR	1

Reference

[1] G. P. Kushto, P. F. Souter, L. Andrews, and M. Neurock, J. Chem. Phys. **106**, 5894 (1997).

SBCS

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1201.9	Ar	IR	1

Reference

[1] P. Hassanzadeh, L. Andrews, and R. D. Davy, J. Phys. Chem. **97**, 7412 (1993).

$(AlO)_2^-$

Threshold for electron detachment from ground-state $(AlO)_2^-$=15170(160) gas PE[1]

Reference

[1] S. R. Desai, H. Wu, C. M. Rohlfing, and L.-S. Wang, J. Chem. Phys. **106**, 1309 (1997).

$NSCN^+$

$\tilde{C}\ ^2A''$ C_s
T^a=29370(120) gas PE[1]

$\tilde{B}\ ^2A'$ C_s
T^a=21700(120) gas PE[1]

$\tilde{A}\ ^2A''$ C_s
T^a=17670(120) gas PE[1]

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

[a]From vertical ionization potentials.

Reference

[1] A. W. Allaf, R. L. Johnston, and R. J. Suffolk, Chem. Phys. Lett. **233**, 33 (1995).

N_4^+

$\tilde{A},\tilde{B}$

A broad, unstructured absorption[1–3] between 270 and 650 nm, with a maximum near 330 nm, leads to the formation of $N_2^+ + N_2$. Detection of the fluorescence of N_2^+ (B) at the higher energies in this range suggests that the potential energy surface for a bound excited state of N_4^+ which correlates with N_2^+ (B) has an avoided crossing with the surface for the dissociative $\tilde{A}$ state.[3]

$\tilde{X}\ ^2\Sigma_u$ $D_{\infty h}$ Structure: ESR,MO[4]DL[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	N≡N s-stretch	2283T[a]	Ne	IR	6
Σ_u^+	3	N≡N a-stretch	2234.51	gas	DL	7
			2237.6	Ne	IR	5,6

B_0=0.112 DL[7]

[a]Calculated using observed values for asymmetrically ^{15}N-substituted species.

References

[1] G. P. Smith and L. C. Lee, J. Chem. Phys. **69**, 5393 (1978).
[2] M. F. Jarrold, A. J. Illies, and M. T. Bowers, J. Chem. Phys. **81**, 214 (1984).
[3] S. C. Ostrander and J. C. Weisshaar, Chem. Phys. Lett. **129**, 220 (1986).
[4] L. B. Knight, Jr., K. D. Johannessen, D. C. Cobranchi, E. A. Earl, D. Feller, and E. R. Davidson, J. Chem. Phys. **87**, 885 (1987).
[5] M. E. Jacox and W. E. Thompson, Res. Chem. Intermed. **12**, 33 (1989).
[6] W. E. Thompson and M. E. Jacox, J. Chem. Phys. **93**, 3856 (1990).
[7] T. Ruchti, T. Speck, J. P. Connelly, E. J. Bieske, H. Linnartz, and J. P. Maier, J. Chem. Phys. **105**, 2591 (1996).

BeO_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		O_3 a-stretch	869.8	Ne	IR	1
			871.8	Ar	IR	1
			436.1	Ar	IR	1

Reference

[1] C. A. Thompson and L. Andrews, J. Chem. Phys. **100**, 8689 (1994).

OTiOO

$\tilde{X}$

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

Reference

[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. **99**, 6356 (1995).

OZrOO

$\tilde{X}$

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

Reference

[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. **99**, 6356 (1995).

OHfOO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			945.8T	Ar	IR	1

Reference

[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. **99**, 6356 (1995).

MoO_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	MoO stretch	976	Ne	IR	1
e	3	MoO stretch	922.2	Ne	IR	1

Reference

[1] W. D. Hewett, Jr., J. H. Newton, and W. Weltner, Jr., J. Phys. Chem. **79**, 2640 (1975).

WO_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	3	WO stretch	918.3	Ar	IR	1,2
			916	Kr	IR	1

References

[1] D. W. Green and K. M. Ervin, J. Mol. Spectrosc. **89**, 145 (1981).
[2] M. J. Almond and A. J. Downs, J. Chem. Soc. Dalton Trans. 809 (1988).

FeO_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			850(50)	gas	PE	2
			975.8T	Ar	IR	1

References

[1] G. V. Chertihin, W. Saffel, J. T. Yustein, L. Andrews, M. Neurock, A. Ricca, and C. W. Bauschlicher, Jr., J. Phys. Chem. **100**, 5261 (1996).
[2] H. Wu, S. R. Desai, and L.-S. Wang, J. Am. Chem. Soc. **118**, 5296 (1996).

(*cyc*-O_2Fe)O

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	OO stretch	1147.5	Ar	IR	1
		FeO stretch	928.1	Ar	IR	1

Reference

[1] G. V. Chertihin, W. Saffel, J. T. Yustein, L. Andrews, M. Neurock, A. Ricca, and C. W. Bauschlicher, Jr., J. Phys. Chem. **100**, 5261 (1996).

ONiOO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	1393.7	Ar	IR	1

Reference

[1] A. Citra, G. V. Chertihin, L. Andrews, and M. Neurock, J. Phys. Chem. A **101**, 3109 (1997).

cyc-(O_2Ni)O

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	OO stretch	1095.5T	Ar	IR	1

Reference

[1] A. Citra, G. V. Chertihin, L. Andrews, and M. Neurock, J. Phys. Chem. A **101**, 3109 (1997).

CuO_3

$\tilde{E}$
T_0=21060T gas PE[1]

$\tilde{D}$
T_0=9280(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			660(90)	gas	PE	1

$\tilde{C}$
T_0=6700(160) gas PE[1]

$\tilde{B}$
T_0=2580(160) gas PE[1]

$\tilde{A}$
T_0=1610(160) gas PE[1]

Reference

[1] H. Wu, S. R. Desai, and L.-S. Wang, J. Phys. Chem. A **101**, 2103 (1997).

UO_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	UO stretch	843.5	Ar	IR	1,2
	2	UO_2 s-stretch	745.6	Ar	IR	1–3
			740.7	Kr	IR	1
b_2	5	UO_2 a-stretch	852.6	Ar	IR	1–3
			848.1	Kr	IR	1

References

[1] S. D. Gabelnick, G. T. Reedy, and M. G. Chasanov, J. Chem. Phys. **58**, 4468 (1973).
[2] S. D. Gabelnick, G. T. Reedy, and M. G. Chasanov, J. Chem. Phys. **59**, 6397 (1973).
[3] R. D. Hunt and L. Andrews, J. Chem. Phys. **98**, 3690 (1993).

Ge_2O_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2	Ge-Ge breathing	400(60)	gas	PE	3
b_{2u}	5	GeO stretch	667.7	Ar	IR	1,2
			667	N_2	IR	1
b_{3u}	6	GeO stretch	600.0	Ar	IR	1,2
			599	N_2	IR	1

References

[1] J. S. Ogden and M. J. Ricks, J. Chem. Phys. **52**, 352 (1970).
[2] L. Andrews and M. McCluskey, J. Mol. Spectrosc. **154**, 223 (1992).
[3] J. B. Nicholas, J. Fan, H. Wu, S. D. Colson, and L.-S. Wang, J. Chem. Phys. **102**, 8277 (1995).

Sn_2O_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}	5		611.7	Kr	IR	1
			612.4	N_2	IR	1
b_{3u}	6		524.4	Kr	IR	1
			523	N_2	IR	1

Reference

[1] A. Bos and J. S. Ogden, J. Phys. Chem. **77**, 1513 (1973).

Pb_2O_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1		518T[a]	Ar	IR	3
			522T[a]	N_2	IR	3
b_{1g}	3		390T[a]	Ar	IR	3
			395T[a]	N_2	IR	3
b_{2u}	5		555.6	Ar	IR	1–3
			557.6	N_2	IR	1,3
b_{3u}	6		466.4	Ar	IR	1,3
			468.0	N_2	IR	1,3

[a]From combination band.

References

[1] J. S. Ogden and M. J. Ricks, J. Chem. Phys. **56**, 1658 (1972).
[2] S. A. Konnov, L. V. Serebrennikov, and A. A. Mal'tsev, Zh. Neorg. Khim. **27**, 323 (1982); Russ. J. Inorg. Chem. **27**, 184 (1982).
[3] G. V. Chertihin and L. Andrews, J. Chem. Phys. **105**, 2561 (1996).

$PbPb(O_2)$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			648.7	Ar	IR	1
			645.1			
			644.0	N_2	IR	1

Reference

[1] G. V. Chertihin and L. Andrews, J. Chem. Phys. **105**, 2561 (1996).

NSCN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	C≡N stretch	2225m	gas	IR	1
	2	N=S stretch	1374vs	gas	IR	1

Reference

[1] A. W. Allaf and R. J. Suffolk, J. Chem. Res., Synop. 186 (1994).

FeO_3^-

Threshold for electron detachment from ground-state FeO_3^-=26300(320) gas PE[1]

Reference

[1] H. Wu, S. R. Desai, and L.-S. Wang, J. Am. Chem. Soc. **118**, 5296 (1996).

CuO_3^-

Threshold for electron detachment from ground-state CuO_3^-=25740(320) gas PE[1]

Reference

[1] H. Wu, S. R. Desai, and L.-S. Wang, J. Phys. Chem. A **101**, 2103 (1997).

$Ge_2O_2^-$

Threshold for electron detachment from ground-state $Ge_2O_2^-$=5040(400) gas PE[1]

Reference

[1] J. B. Nicholas, J. Fan, H. Wu, S. D. Colson, and L.-S. Wang, J. Chem. Phys. **102**, 8277 (1995).

$BrCNO^+$

$\tilde{D}$
T^a=65110(200) gas PE[1]

$\tilde{C}$
T^a=57200(200) gas PE[1]

$\tilde{B}$
T^a=46400(200) gas PE[1]

$\tilde{A}$
T^a=23100(200) gas PE[1]

[a]From vertical ionization potentials.

Reference

[1] T. Pasinszki and N. P. C. Westwood, J. Phys. Chem. **99**, 6401 (1995).

$t\text{-}(NO)_2^+$

$\tilde{A}$

Dissociates into $NO+NO^+$, with onset at 10700(1000) and maximum at 16400(1000). AB[2–5,7]PE[8]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	NO s-stretch	2090	gas	PI,PE	6,8
					TPE	11,12
			2064.7[a]	Ne	IR	10
	2	NNO s-bend	323	gas	TPE	11
a_u	4	Torsion	118T	gas	TPE	11,12
b_u	5	NO a-stretch	1618	gas	TPE	12
			1619.2	Ne	IR	10,12
			1593.3	Ar	IR	1,9

[a]$(\nu_1+\nu_5)-\nu_5$.

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[2] J. A. Vanderhoff, J. Chem. Phys. **67**, 2332 (1977).
[3] R. R. Burke and R. P. Wayne, Int. J. Mass Spectrom. Ion Phys. **25**, 199 (1977).
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[8] F. Carnovale, J. B. Peel, and R. G. Rothwell, J. Chem. Phys. **84**, 6526 (1986).
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[11] I. Fischer, A. Strobel, J. Staecker, G. Niedner-Schatteburg, K. Müller-Dethlefs, and V. E. Bondybey, J. Chem. Phys. **96**, 7171 (1992).
[12] A. Strobel, N. Knoblauch, J. Agreiter, A. M. Smith, G. Niedner-Schatteburg, and V. E. Bondybey, J. Phys. Chem. **99**, 872 (1995).

$ArBeO_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1288.9	Ar	IR	1,2
			1264.1	Ar	IR	1,2

References

[1] C. A. Thompson and L. Andrews, J. Chem. Phys. **100**, 8689 (1994).
[2] L. Andrews, G. V. Chertihin, C. A. Thompson, J. Dillon, S. Byrne, and C. W. Bauschlicher, Jr., J. Phys. Chem. **100**, 10088 (1996).

FNCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NCO a-stretch	2174.8vs	Ne	IR	2
			2174.4s	Ar	IR	1,2
			2167s			
	2	NCO s-stretch	1245T	Ne	IR	2
	3	NF stretch	860.8wm	Ne	IR	2
			862.0m	Ar	IR	1,2
	4	NCO deform.	701.5wm	Ne	IR	2
			695wm	Ar	IR	1
	5	FNC deform.	203.5w	Ne	IR	2
a''	6	NCO deform.	533.8wm	Ne	IR	2
			529m	Ar	IR	1

References

[1] K. Gholivand, H. Willner, D. Bielefeldt, and A. Haas, Z. Naturforsch. B **39**, 1211 (1984).
[2] J. Jacobs, B. Jülicher, G. Schatte, H. Willner, and H.-G. Mack, Chem. Ber. **126**, 2167 (1993).

BrCNO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CNO a-stretch	2211	gas	IR	2
			2271.3	Ar	IR	1
			2252.5			
		CNO s-stretch	1321	gas	IR	2
			1305.6	Ar	IR	1

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[1] G. Maier and J. H. Teles, Angew Chem. **99**, 152 (1987); Angew. Chem. Int. Ed. Engl. **26**, 155 (1987).
[2] T. Pasinszki and N. P. C. Westwood, J. Phys. Chem. **99**, 6401 (1995).

SiO_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Si=O stretch	1363.5vs	Ar	IR	1
	2	OSiO s-stretch	877.1wm	Ar	IR	1
b_1	4	OPLA	287.8vs	Ar	IR	1
b_2	5	OSiO a-stretch	855.3ms	Ar	IR	1
	6	Deformation	292.0s	Ar	IR	1

Reference

[1] B. Tremblay, P. Roy, L. Manceron, M. E. Alikhani, and D. Roy, J. Chem. Phys. **104**, 2773 (1996).

$OPb(O_2)$

$\tilde{X}$

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

Reference

[1] G. V. Chertihin and L. Andrews, J. Chem. Phys. **105**, 2561 (1996).

c-$(NO)_2$

A diffuse gas-phase absorption with onset below 38500 (>260 nm) and maximum at 48800 (205 nm) has been assigned[4,7] to *c*-$(NO)_2$.

$\tilde{X}$ C_{2v} Structure: MW[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NO s-stretch	1868.25	gas	IR,DL	3,13,15
			1867.2	Ne	IR	14,16,17
			1866m	Ar	IR	1
			1867.0	N_2	IR	2,17
			1862m	CO_2	IR,Ra	1,8
			1866	NO	IR,Ra	5,6,10
	2	N⋯N stretch	262	CO_2	Ra	8
			266	NO	IR,Ra	5,6,10
	3	NNO s-bend	161	CO_2	Ra	8,10
			187	NO	Ra	5,6,10
a_2	4	Torsion	88.2[a]	gas	IR	11
			97	NO	IR,Ra	5,6,10
b_2	5	NO a-stretch	1789.09	gas	IR,DL	3,11,12
						13,18
			1780.6	Ne	IR	14,16,17
			1778.7			
			1776s	Ar	IR	1
			1781.2	N_2	IR	2,17
			1768s	CO_2	IR	1
			1762	NO	IR,Ra	6,10
	6	NNO a-bend	202	CO_2	Ra	8,10
			214	NO	Ra	5,6,10

$A_0=0.862$; $B_0=0.187$; $C_0=0.154$ MW[9]IR[15]

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

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[14] M. E. Jacox and W. E. Thompson, J. Chem. Phys. **93**, 7609 (1990).
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[18] A. Dkhissi, P. Soulard, A. Perrin, and N. Lacome, J. Mol. Spectrosc. **183**, 12 (1997).

t-$(NO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	Sym. stretch	1861.1vw	N_2	IR	4
b_u	5	Asym. stretch	1762.5	Ne	IR	3
			1760.6			
			1759.6	N_2	IR	2,4
			1740	CO_2	IR	1

References

[1] W. G. Fateley, H. A. Bent, and B. Crawford, Jr., J. Chem. Phys. **31**, 204 (1959).
[2] W. A. Guillory and C. E. Hunter, J. Chem. Phys. **50**, 3516 (1969).
[3] M. E. Jacox and W. E. Thompson, J. Chem. Phys. **93**, 7609 (1990).
[4] F. Legay and N. Legay-Sommaire, J. Chem. Phys. **102**, 7798 (1995).

NNO_2

$^3A_1$ C_{2v}
$T_0=x+8110$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	NO_2 scissors	540(40)	gas	PE	1

$^3A_2$ C_{2v}
$T_0=x^a$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NO_2 s-stretch	1240T	gas	PE	1
	2	NN stretch	880T	gas	PE	1
	3	NO_2 scissors	680T	gas	PE	1

[a]It is uncertain whether this or a $^1A'$ state which is calculated[1] to be nearly isoenergetic is the ground state of NNO_2.

Reference

[1] D. W. Arnold and D. M. Neumark, J. Chem. Phys. **102**, 7035 (1995).

SNNO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO stretch	1815.2	Ar	IR	1

Reference

[1] L. Andrews, P. Hassanzadeh, G. D. Brabson, A. Citra, and M. Neurock, J. Phys. Chem. **100**, 8273 (1996).

NSeNSe

$\tilde{X}$

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

Reference

[1] L. Andrews, P. Hassanzadeh, D. V. Lanzisera, and G. D. Brabson, J. Phys. Chem. **100**, 16667 (1996).

NO_3^+

$\tilde{B}\ ^1E'$ D_{3h}
T^a=24120(120) gas PE[1]

$\tilde{A}\ ^1E''$ D_{3h}
T^a=12100(120) gas PE[1]

$\tilde{b}\ ^3E'$ D_{3h}
T^a=8630(120) gas PE[1]

$\tilde{a}\ ^3E''$ D_{3h}
T^a=5080(120) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	1050(60)	gas	PE	1

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

[a]From vertical ionization potentials.

Reference

[1] D. Wang, P. Jiang, X. Zian, and G. Hong, J. Chem. Phys. **106**, 3003 (1997).

BF_3^+

$\tilde{E}\ ^2A_1'$ D_{3h}
T_0≅47800 gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	BF stretch	800T	gas	PE	3

τ=10 ns gas EM[5]

$\tilde{D}\ ^2E'$ D_{3h}
T_0=34860(160) gas PE[1,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	BF stretch	742(20)	gas	PE	1,4

Additional structure reported by Ref. 4 has been attributed to vibronic coupling.

$\tilde{C}\ ^2A_2''$ D_{3h}
T_0=27110(80) gas PE[1,2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	BF stretch	830(20)	gas	PE	2,4

$\tilde{B}\ ^2E'$ D_{3h}
T_0=10890(240) gas PE[1,2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	BF stretch	770(60)	gas	PE	1,4

$\tilde{A}\ ^2E''$ D_{3h}
T_0=5890(240) gas PE[1,4]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	3	BF_3 stretch	1661.6	Ne	IR	6

References

[1] P. J. Bassett and D. R. Lloyd, J. Chem. Soc. A 1551 (1971).
[2] C. F. Batten, J. A. Taylor, B. P. Tsai, and G. G. Meisels, J. Chem. Phys. **69**, 2547 (1978).
[3] E. Haller, H. Köppel, L. S. Cederbaum, W. von Niessen, and G. Bieri, J. Chem. Phys. **78**, 1359 (1983).
[4] G. Hagenow, K. Hottmann, and H. Baumgärtel, Chem. Phys. Lett. **164**, 395 (1989).
[5] J. C. Creasey, P. A. Hatherly, H. M. Jones, I. R. Lambert, and R. P. Tuckett, Mol. Phys. **78**, 837 (1993).
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BCl_3^+

$\tilde{E}\ ^2A_1'$ D_{3h}
T_0=49200(120) gas PE[1]TPE[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	BCl stretch	403(16)	gas	PE,TPE	1,6

$\tilde{D}\ ^2E'$ D_{3h}
T_0=29700(120) gas PE[1]TPE[6]

Emission which is observed between about 300 and 650 nm on excitation of BCl_3 by radiation of wavelength shorter than 81 nm (15.36 eV) arises from the $\tilde{D}$ state of BCl_3^+.[3–5] The emission between 330 and 420 nm has been attributed to the $\tilde{D}$–$\tilde{X}$ transition of BCl_3^+, and that between 420 and 580 nm, with vibrational spacings of ~445, to the $\tilde{D}$–$\tilde{A}$,$\tilde{B}$ transitions.[3] The T-PEPICO measurements of Ref. 6 indicate that the quantum yield for these emissions is ≤0.04 and that fragmentation into BCl_2^++Cl predominates.

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^+.

$A=1600(80)$ gas TPE[6]
$\tau=5.5(5)$ ns gas T-PEFCO[6]

$\tilde{C}\ ^2A_2''$ D_{3h}
$T_0=21780(120)$ gas PE[1]TPE[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	BCl stretch	403(16)	gas	PE,TPE	1,6

$\tilde{B}\ ^2E'$ D_{3h}
$T^a=9280(120)$ gas PE[1]TPE[6]
$A=800T$ gas TPE[6]

$\tilde{A}\ ^2E''$ D_{3h}
$T_0=5080(120)$ gas PE[1]TPE[6]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	3	BCl stretch	1103.8	Ne	IR	7
			1090	Ar	IR	2

[a]From vertical ionization potential.

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[1] P. J. Bassett and D. R. Lloyd, J. Chem. Soc. A 1551 (1971).
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FCO_2

$\tilde{B}\ ^2A_1$ C_{2v}
$T_0=13150$ gas AB[1,2] $\tilde{B}-\tilde{X}$ 500–795 nm
13103(5) Ne AB[4] $\tilde{B}-\tilde{X}$ 508–763 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	OCO s-stretch	1607(10)	Ne	AB	4
	2	CF stretch	1110	gas	AB	1
			1119(5)	Ne	AB	4
	3	OCO bend	610	gas	AB	1
			614(5)	Ne	AB	4
b_1	4	OPLA	840	gas	AB	1
			838(5)	Ne	AB	4

$\tilde{A}\ ^2A_2$ C_{2v}
$T_0=4670(40)$ gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	OCO s-stretch	1274(40)	gas	PE	3
	2	CF stretch	903(40)	gas	PE	3
	3	OCO bend	532(40)	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	OCO s-stretch	1465(70)	gas	PE	3
			1475Tvs	Ne	IR	4
	2	CF stretch	950(70)	gas	PE	3
			968.9m	Ne	IR	4
			975.1	Ar	IR	4
			975.5	N_2	IR	4
	3	OCO bend	520	gas	AB,PE	1,3
			518.5wm	Ne	IR	4
			521.6	Ar	IR	4
			522.8	N_2	IR	4
b_1	4	OPLA	735.2wm	Ne	IR	4
			730.6	Ar	IR	4
			728.5	N_2	IR	4
b_2	5	OCO a-stretch	1097.7ms	Ne	IR	4
			1113.6	Ar	IR	4
			1116.5	N_2	IR	4
	6	FCO bend	474.3wm	Ne	IR	4
			482.5	Ar	IR	4
			481.3	N_2	IR	4

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[1] M. M. Maricq, J. J. Szente, Z. Li, and J. S. Francisco, J. Chem. Phys. **98**, 784 (1993).
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[4] G. A. Argüello, H. Grothe, M. Kronberg, H. Willner, and H.-G. Mack, J. Phys. Chem. **99**, 17525 (1995).

NNO_2^-

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

Photoelectron spectra[2] of NNO_2^- indicate that at both 532 and 355 nm dissociation into N_2O+O^- occurs. Fast ion beam translational spectroscopy studies[6] indicate that a structured absorption with onset near 580 nm arises from excitation to the $\tilde{B}$ state. Two different dissociation channels occur in this energy range; dissociation on the ground-state potential surface leads to the formation of N_2O+O^-, and excited-state dissociation results in the formation of $NO+NO^-$. When 266 and 213 nm photons are used, the photoelectron spectra[5] suggest that electron detachment to form excited states of uncharged NNO_2 occurs.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NN stretch	1359.6wm	Ne	IR	4
			1355w	Ar	IR	1,3,4
	2	NO_2 s-stretch	950T	gas	PE	5
			1004.5wm	Ne	IR	4
			1008w	Ar	IR	1,3,4
b_2	5	NO_2 a-stretch	1199.3m	Ne	IR	4
			1205.5m	Ar	IR	1,3

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[1] D. E. Milligan and M. E. Jacox, J. Chem. Phys. **55**, 3404 (1971).
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t-$(NO)_2^-$

In gas-phase photoelectron spectra[1] taken at 532 nm, evidence was obtained for both electron detachment and photodissociation into $NO+NO^-$.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_u	5	Asym. stretch	1424.1T	Ne	IR	2

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[1] L. A. Posey and M. A. Johnson, J. Chem. Phys. **88**, 5383 (1988).
[2] M. E. Jacox and W. E. Thompson, J. Chem. Phys. **93**, 7609 (1990).

NO_3

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

$T_0=15089$ gas $AB^{1,2,4\text{-}7}LF^{8,9,17,21}$ $\tilde{B}-\tilde{X}$ 450–795 nm

All bands are diffuse.[2,7,21] The threshold for the production of $NO+O_2 \leqslant 16780$, and that for the production of $O+NO_2$ is 17090(20).[20] Above this second threshold, the predominant photodissociation products are $O(^3P)$ and NO_2.[19,20]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	930	gas	AB	2,6
			1450	gas	AB	6
			850	gas	AB	6

$\tau_0=340(20)\,\mu s$ gas LF^{10}

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

$T_0=7000(110)$ gas PE^{14}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	804(4)T	gas	PE	14
e'	4	Deformation	541(8)T	gas	PE	14

$\tilde{X}\ ^2A_2'$ D_{3h} Structure: DL^{11}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	1050	gas	LF,PE	8,9,14,17
a_2''	2	OPLA	762.33	gas	IR,LF	12,17
e'	3	NO stretch[a]	1492.39	gas	LF,DL IR	8,9,11,17 12
	4	Deformation[b]	360	gas	LF,PE	8,9,14,17

$B_0=0.459$ $DL^{11,13}IR^{12}$

[a]Anomalous structure appears in the high resolution spectrum of this band because of vibronic coupling with the $\tilde{B}\ ^2E'$ state.[16] Coupling with this state and with the $\tilde{A}\ ^2E''$ state leads to the appearance of infrared absorptions of several prominent overtone and combination bands between 1900 and 2600.[15,18] Among these bands, also observed in fluorescence,[8,17] is one near 2020, attributed by Ref. 17 to the occurrence of pseudorotation on the ground-state potential surface but by Ref. 15 to intensification of the fourth overtone of ν_4, which has appreciable ''negative'' anharmonicity, as a result of vibronic interaction with the $\tilde{A}$ and $\tilde{B}$ states.

[b]Coupled to the $\tilde{B}\ ^2E'$ state through this mode.[14]

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SSNO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO stretch	1772.5	Ar	IR	1
		SS stretch	670.9	Ar	IR	1

Reference

[1] L. Andrews, P. Hassanzadeh, G. D. Brabson, A. Citra, and M. Neurock, J. Phys. Chem. **100**, 8273 (1996).

SeSeNSe

$\tilde{X}$

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

Reference

[1] L. Andrews, P. Hassanzadeh, D. V. Lanzisera, and G. D. Brabson, J. Phys. Chem. **100**, 16667 (1996).

SeSeSeN

$\tilde{X}$

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

Reference

[1] L. Andrews, P. Hassanzadeh, D. V. Lanzisera, and G. D. Brabson, J. Phys. Chem. **100**, 16667 (1996).

t-O_4^+

In the gas phase, the high frequency tail of a photodissociation continuum, resulting in the formation of $O_2^+ + O_2$, has been observed[1–3] between 450 and 680 nm.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	O=O s-stretch	1644.1[a]	Ne	IR	4
b_u	5	O=O a-stretch	1164.4	Ne	IR	4
			1118	Ar	IR	5

[a] $(\nu_1+\nu_5)-\nu_5$.

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cyc-O_4^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		O=O s-stretch	1628.3[a]	Ne	IR	1,2
		O=O a-stretch	1320.3	Ne	IR	1,2

[a] $(\nu_1+\nu_5)-\nu_5$.

References

[1] W. E. Thompson and M. E. Jacox, J. Chem. Phys. **91**, 3826 (1989).
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CF_3^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	798.1	Ne	IR	5
e'	3	CF stretch	1662.4[a]	Ne	IR	3,5
			1667	Ar	IR	1,2,4

[a] Absorptions at 1650.6 and 1669.5 which appear in some neon-matrix experiments[3–5] are attributed to CF_3^+ in other trapping sites.

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[1] F. T. Prochaska and L. Andrews, J. Am. Chem. Soc. **100**, 2102 (1978).
[2] M. E. Jacox, Chem. Phys. **83**, 171 (1984).
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[5] D. Forney, M. E. Jacox, and K. K. Irikura, J. Chem. Phys. **101**, 8290 (1994).

SiF_3^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	3	SiF_3 stretch	1159.7	Ne	IR	1

Reference

[1] M. E. Jacox, K. K. Irikura, and W. E. Thompson, J. Chem. Phys. **103**, 5308 (1995).

FCO_2^-

Threshold for electron detachment from ground-state FCO_2^- = 34500(240) gas PE[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO stretch	1399[a]	gas	PE	2
			1316 Cs	Ar	IR	1
	2	OCO bend	899[a]	gas	PE	2
			883 Cs	Ar	IR	1
	3	CF stretch	596[a]	gas	PE	2
b_2	5	CO stretch	1749 Cs	Ar	IR	1

[a]From Franck–Condon simulation of observed photoelectron spectrum.

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[1] B. S. Ault, Inorg. Chem. **21**, 756 (1982).
[2] D. W. Arnold, S. E. Bradforth, E. H. Kim, and D. M. Neumark, J. Chem. Phys. **102**, 3493 (1995).

NO_3^-

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	3	NO_3 stretch	1356.2	Ne	IR	1

Reference

[1] D. Forney, W. E. Thompson, and M. E. Jacox, J. Chem. Phys. **99**, 7393 (1993).

$ClNO_2$

The onset of continuous absorption by gas-phase $ClNO_2$ occurs near 25000 (400 nm).[3] The maximum in this absorption is beyond the 185 nm limit of the observations.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NO_2 s-stretch	1267.3s	gas	IR	1,7
			1264.3	Ar	IR	4
	2	NO_2 scissors	792.76s	gas	IR	1,7,8
			787.0	Ar	IR	4
	3	Cl-N stretch	363.8vs	gas	IR	1,7
			365.0	Ar	IR	4
b_1	4	OPLA	651.7w	gas	IR	1,7
b_2	5	NO_2 a-stretch	1683.89s	gas	IR	1,6,7
			1674.8	Ar	IR	4
	6	NO_2 rock	408.1vw	gas	IR	1

$A_0 = 0.443$; $B_0 = 0.173$; $C_0 = 0.124$ MW[2,5]IR[6]

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[1] D. L. Bernitt, R. H. Miller, and I. C. Hisatsune, Spectrochim. Acta A **23**, 237 (1967).
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c-ClONO

$\tilde{X}$ C_s Structure: MW[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	N=O stretch	1715vs	gas	IR	2,3
			1714s	Ar	IR	1
			1717	N_2	IR	5
	2	ONO bend[a]	858w	gas	IR	2
			856m	Ar	IR	1
	3	ClO stretch[a]	644m	gas	IR	2
	4	O-N stretch[a]	406vs	gas	IR	2
			398m	Ar	IR	1
			390ms			
	5	ClON bend	270T	gas	IR	2
a''	6	Torsion[a]	344vw	gas	IR	2

$A_0 = 0.608$; $B_0 = 0.152$; $C_0 = 0.122$ MW[4]

[a]See Ref. 6.

References

[1] D. E. Tevault and R. R. Smardzewski, J. Chem. Phys. **67**, 3777 (1977).
[2] B. Janowski, N.-D. Knauth, and H. Martin, Ber. Bunsenges. Phys. Chem. **81**, 1262 (1977).
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t-ClONO[a]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		N=O stretch	1752ms	Ar	IR	1

[a]Originally believed to be OClNO. Reassigned by Ref. 2 to *t*-ClONO.

References

[1] D. E. Tevault and R. R. Smardzewski, J. Chem. Phys. **37**, 3777 (1977).
[2] T. J. Lee, J. Phys. Chem. **98**, 111 (1994).

$BrNO_2$

In the gas phase, unstructured absorption maxima have been observed[5] at 50250 (199 nm), 40490 (247 nm), and 26880 (372 nm).

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NO_2 s-stretch	1292	gas	IR	3–5
			1290.7	Ar	IR	1,2,5
			1291	O_2	IR	4
	2	NO_2 deform.	787	gas	IR	3–5
			782.9s	Ar	IR	2,5
			784	O_2	IR	4
	3	NBr stretch	281.8w	Ar	IR	5
b_1	4	OPLA	605	gas	IR	5
			605.6	Ar	IR	5
b_2	5	NO_2 a-stretch	1667	gas	IR	3–5
			1659.2vs	Ar	IR	2,5
			1655	O_2	IR	4
	6	NO_2 wag	290Tsh	Ar	IR	5

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[1] M. Feuerhahn, R. Minkwitz, and U. Engelhardt, J. Mol. Spectrosc. **77**, 429 (1979).
[2] D. E. Tevault, J. Phys. Chem. **83**, 2217 (1979).
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[4] A. Frenzel, V. Scheer, W. Behnke, and C. Zetzsch, J. Phys. Chem. **100**, 16447 (1996).
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t-BrONO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	N=O stretch	1727.9vs	Ar	IR	1–3
	2	ONO deform.	833.2ms	Ar	IR	2,3
	3	BrO stretch	584.8vs	Ar	IR	1–3
	4	O-N stretch	391.1wm	Ar	IR	2,3
	5	BrON deform.	197T	Ar	IR	3
a''	6	Torsion	150HT	Ar	IR	3

References

[1] M. Feuerhahn, R. Minkwitz, and U. Engelhardt, J. Mol. Spectrosc. **77**, 429 (1979).
[2] D. E. Tevault, J. Phys. Chem. **83**, 2217 (1979).
[3] D. Scheffler, H. Grothe, H. Willner, A. Frenzel, and C. Zetsch, Inorg. Chem. **36**, 335 (1997).

OSOO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OS stretch	1229.6	Ar	IR	1
		OO stretch	1041.3	Ar	IR	1
			597.6	Ar	IR	1

Reference

[1] S.-H. Jou, M.-Y. Shen, C.-H. Yu, and Y.-P. Lee, J. Chem. Phys. **104**, 5745 (1996).

S_4

$\tilde{A}$

gas AB[1,2,4] $\tilde{A}-\tilde{X}$ 425–575 nm

Unstructured absorption maximum at 19300 (518 nm) in an Ar matrix.[6]
Unstructured absorption maximum at 18870 (530 nm) in a Kr matrix.[1,2]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			680	gas	Ra	7
			661.6	Ar	IR	3,5,6
			660s	Kr	IR	3
			660	Xe	IR	3
			575	gas	Ra	7
			483wmT	Kr	IR	3
			303	gas	Ra	7
			320mT	Kr	IR	3
			270wmT	Kr	IR	3

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SeO_3

$\tilde{X}$ D_{3h} Structure: Ra[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	Deform.	356	Ar	IR	2
			358	N_2	IR	2
e'	3	SeO stretch	995	Ar	IR	2,3
			1005.5	N_2	IR	2

References

[1] N. J. Brassington, H. G. M. Edwards, D. A. Long, and M. Skinner, J. Raman Spectrosc. **7**, 158 (1978).
[2] A. K. Brisdon and J. S. Ogden, J. Mol. Struct. **157**, 141 (1987).
[3] G. D. Brabson, L. Andrews, and C. J. Marsden, J. Phys. Chem. **100**, 16487 (1996).

OSeOO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	1141.5	Ar	IR	1
			952.0	Ar	IR	1

Reference

[1] G. D. Brabson, L. Andrews, and C. J. Marsden, J. Phys. Chem. **100**, 16487 (1996).

cyc-(SeOSe)=O

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Se=O stretch	966.2	Ar	IR	1
			636.5	Ar	IR	1
			457	Ar	IR	1

Reference

[1] G. D. Brabson, L. Andrews, and C. J. Marsden, J. Phys. Chem. **100**, 16487 (1996).

BF_3^-

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	BF_3 stretch	847.2wm	Ne	IR	1
	2	Umbrella	595.3wm	Ne	IR	1
e	3	BF_3 stretch	1026.4m	Ne	IR	1
	4	Deformation	409T	Ne	IR	1

Reference

[1] M. E. Jacox and W. E. Thompson, J. Chem. Phys. **102**, 4747 (1995).

BCl_3^-

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	BCl_3 stretch	685.8	Ne	IR	1

Reference

[1] M. E. Jacox, K. K. Irikura, and W. E. Thompson, J. Chem. Phys. **104**, 8871 (1996).

CF_3

Rydberg state D_{3h}
gas AB[6]MPI[10] 139–165 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	820	gas	AB,MPI	6,10

$4s\ ^2A_1'$ D_{3h}
$T_0 \cong 51665$ gas AB[7]EM[11–14,16,20] $4s\,^2A_1'-\tilde{X}$ 180–300 nm
Calculations[14] suggest that this state is of mixed valence-Rydberg character, with increasing Rydberg contribution at large C–F distances.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	804T	gas	EM	12

$\tau = 12(3)$ ns gas EM[17,18]
Ref. 22 obtained a lifetime of 17.3(4) ns for this state, suggesting that it is identical to the upper state for the 450–750 nm emission bands of CF_3.

$3p\ ^2A_2'',^2E'$ D_{3h}
$T_0 \cong 51600$ gas EM[8,11,13,14] $3p-3s\,^2A_1'$ 450–750 nm
$\tau = 17.5(5)$ ns gas EM[17,18,22]EF[21]

The lower state of the visible emission of CF_3, calculated[14] to be the $3s\ ^2A_1'$ state, which assumes increasing valence character at large $C-F$ distances, is both observed and calculated to be dissociative.

$\tilde{X}\ ^2A_1$ C_{3v} Structure: ESR[1]MW[9]DL[15]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF stretch	1089	gas	IR,EM	2,12
					CARS	19
			1086	Ne	IR	5,23
			1087s	Ar	IR	3,4
	2	Umbrella	701(3)	gas	IR,EM	2,12
			701.4	Ne	IR	5,23
			703m	Ar	IR	3,4
e	3	CF stretch	1260.16	gas	IR,DL	2,15
			1253.8	Ne	IR	5,23
			1251vs	Ar	IR	3,4
	4	Deformation	508.7	Ne	IR	5,23
			512w	Ar	IR	4

$B_0 = 0.364$ MW[9]; $C_0 = 0.189$ DL[15]

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[1] R. W. Fessenden and R. H. Schuler, J. Chem. Phys. **43**, 2704 (1965).
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SiF_3

Unstructured emission bands between 290 and 340 nm and between 350 and 800 nm which appear with varying relative intensities on photoexcitation of SiF_4 by radiation at 99.1, 95.5, or 92.2 nm have been attributed[4] to SiF_3. The 350–800 nm band may correspond to the unstructured emission centered at 632 nm which has been observed[3,5] in the flowing afterglow of an SiF_4 discharge and in the reaction of F atoms with Si and which has been tentatively assigned to SiF_3. A third emission band, between 240 and 280 nm, becomes more prominent at higher excitation energies. This latter band occurs in the same spectral region as the 210–260 nm emission band system observed in a discharge through SiF_4. Although that band system was initially assigned[2] to SiF_3, subsequent studies[6] have demonstrated that it is entirely contributed by SiF_2.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiF stretch	834.9	Ne	IR	7
			832s	Ar	IR	1
	2	Umbrella	406s	Ar	IR	1
e	3	SiF stretch	958.6	Ne	IR	7
			954vs	Ar	IR	1
	4	Deformation	290wm	Ar	IR	1

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NF_3^+

$\tilde{E}$ ^2E C_{3v}
T^a=65920(900) gas PE[1]

$\tilde{D}$ $^2A_1$ C_{3v}
T_0=50600(560) gas PE[1]

$\tilde{C}$ ^2E C_{3v}
T_0=33800(560) gas PE[1]

$\tilde{B}$ $^2A_2$ C_{3v}
T^a=28900(720) gas PE[1]

$\tilde{A}$ ^2E C_{3v}
T_0=20330(650) gas PE[1]

$\tilde{X}$ $^2A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NF_3 stretch	967.0wm	Ne	IR	3
	2	Umbrella	565(40)	gas	PE	2
			658.6m	Ne	IR	3
e	3	NF_3 stretch	1233.5vs	Ne	IR	3
	4	Deformation	522.1wm	Ne	IR	3

Barrier to inversion ≅6000.[2]

[a]From vertical ionization potential.

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[1] P. J. Bassett and D. R. Lloyd, J. Chem. Soc. Dalton Trans. 248 (1972).
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[3] M. E. Jacox and W. E. Thompson, J. Chem. Phys. **102**, 6 (1995).

ClO_3

In a neon matrix,[1] bands between 300 and 440 nm have been attributed to ClO_3, and photodissociation of ClO_3 to produce OClO+O has been observed at wavelengths longer than 420 nm.

$\tilde{X}$ C_{3v} Structure: IR[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ClO stretch	905.0w	Ne	IR	1
	2	Deform.	566.6wm	Ne	IR	1
e	3	ClO stretch	1081.3vs	Ne	IR	1
	4	Deform.	475.8m	Ne	IR	1

Reference

[1] H. Grothe and H. Willner, Angew. Chem. **106**, 1581 (1994); Angew. Chem. Int. Ed. Engl. **33**, 1483 (1994).

CF_3^-

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1		1050.1wT	Ne	IR	1
e	3	CF_3 stretch	778.4mT	Ne	IR	1

Reference

[1] D. Forney, M. E. Jacox, and K. K. Irikura, J. Chem. Phys. **101**, 8290 (1994).

SiF_3^-

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiF_3 stretch	770.3	Ne	IR	1
	2	Umbrella	401H	Ne	IR	1
e	3	SiF_3 stretch	757.0	Ne	IR	1
			750.9			

Reference

[1] M. E. Jacox, K. K. Irikura, and W. E. Thompson, J. Chem. Phys. **103**, 5308 (1995).

ClOOCl

An unstructured gas-phase absorption with maximum at 40800 (245 nm) has been assigned[1,4–6,8] to ClOOCl. Cl atoms have been detected[6] on irradiation of ClOOCl in this band.

In an argon matrix, photodecomposition occurs at wavelengths shorter than 360 nm (27800).[7]

$\tilde{X}$ C_2 Structure: MW[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	OO stretch	750	gas	IR	4
			754.0m	Ar	IR	2,7
	2	ClO s-stretch	560	gas	IR	4
			543.0m	Ar	IR	7
b	5	ClO a-stretch	653	gas	IR	4
			647.7vs	Ar	IR	2,7
	6	Deformation	418.5w	Ar	IR	7

$A_0=0.437$; $B_0=0.080$; $C_0=0.071$ MW[3]

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$ClClO_2$

In the gas phase, prominent, unstructured absorption maxima appear[2–4] at 44200 and 33800 (226 and 296 nm). In a neon matrix, unstructured absorption maxima are observed[1,3,4] at 42700 and 34100 (234 and 293 nm), with half band widths of 40 and 45 nm, respectively.

In an argon matrix, the threshold[4] for photodecomposition into Cl+OClO, followed by cage recombination to form ClOClO, lies near 16400 (610 nm). The maximum for this process[5] lies near 33300 (300 nm).

$\tilde{X}$ C_s Structure: MW[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ClO_2 s-stretch	1041.5(5)s	gas	IR	2,3
			1041.2s	Ne	IR	1,3
			1040.7	Ar	IR	5
	2	ClO_2 scissors	522.7(5)wm	gas	IR	2,3
			522.5wm	Ne	IR	1,3
	3	ClCl stretch	440.5(5)s	gas	IR	2,3
			440.4s	Ne	IR	1,3
	4	Umbrella	271.4wm	Ne	IR	1,3
a''	5	ClO_2 a-stretch	1218.2(5)vs	gas	IR	2,3
			1216.4vs	Ne	IR	1,3
			1213.2	Ar	IR	5
	6	ClO_2 rock	251.4vw	Ne	IR	1,3

$A_0=0.315$; $B_0=0.120$; $C_0=0.093$ MW[6]

References

[1] H. S. P. Müller and H. Willner, Proceedings of the First European Workshop on Polar Stratospheric Ozone, Schliersee, Germany, 1990 (Air Pollution Research Report 34, CEC and BMFT, edited by J. A. Pyle and N. R. P. Harris).
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$BrClO_2$

In an argon matrix, an absorption maximum near 30800 (325 nm) is associated[1] with isomerization to BrOClO.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ClO_2 s-stretch	1019.2	Ar	IR	1
a''	5	ClO_2 a-stretch	1193.5	Ar	IR	1

Reference

[1] K. Johnsson, A. Engdahl, J. Kölm, J. Nieminen, and B. Nelander, J. Phys. Chem. **99**, 3902 (1995).

$IClO_2$

In an argon matrix, an absorption maximum near 28600 (350 nm) is associated[1] with photodissociation into $ICl+O_2$.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ClO_2 s-stretch	987.4	Ar	IR	1
a''	5	ClO_2 a-stretch	1161.2	Ar	IR	1

Reference

[1] K. Johnsson, A. Engdahl, J. Kölm, J. Nieminen, and B. Nelander, J. Phys. Chem. **99**, 3902 (1995).

ClOClO

In an argon matrix, an absorption maximum at 22200 (450 nm) is associated[2] with isomerization to $ClClO_2$.

In an argon matrix, photoisomerization into ClOOCl occurs between 488 and 665 nm.[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	ClO_t stretch	994.5vs	Ar	IR	1,2
	2	ClO stretch	695.9w	Ar	IR	1
	3	OCl stretch	440.3w	Ar	IR	1
	4	ClOCl deform.	338.7vw	Ar	IR	1

References

[1] J. Jacobs, M. Kronberg, H. S. P. Müller, and H. Willner, J. Am. Chem. Soc. **116**, 1106 (1994).
[2] K. Johnsson, A. Engdahl, J. Kölm, J. Nieminen, and B. Nelander, J. Phys. Chem. **99**, 3902 (1995).

BrOClO

In an argon matrix, an absorption maximum at 19000 (525 nm) is associated[1] with isomerization to $BrClO_2$.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	ClO_t stretch	991.1	Ar	IR	1

Reference

[1] K. Johnsson, A. Engdahl, J. Kölm, J. Nieminen, and B. Nelander, J. Phys. Chem. **99**, 3902 (1995).

ClOBrO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BrO_t stretch	834.4T	Ar	IR	1

Reference

[1] K. Johnsson, A. Engdahl, J. Kölm, J. Nieminen, and B. Nelander, J. Phys. Chem. **99**, 3902 (1995).

IOClO

In an argon matrix, an absorption maximum at 18200 (550 nm) is associated[1] with isomerization to $IClO_2$.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	ClO_t stretch	974.9	Ar	IR	1

Reference

[1] K. Johnsson, A. Engdahl, J. Kölm, J. Nieminen, and B. Nelander, J. Phys. Chem. **99**, 3902 (1995).

FSeSeF

$\tilde{X}$ C_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	SeF s-stretch	610.1	Ar	IR	1
b	5	SeF a-stretch	588.2	Ar	IR	1
	6	Deformation	202.9	Ar	IR	1

Reference

[1] A. Haas and H. Willner, Z. Anorg. Allg. Chem. **454**, 17 (1979).

$SeSeF_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SeF_2 s-stretch	599	Ar	IR	1
	2	Se=Se stretch	404	Ar	IR	1
	4	Deformation	220.5	Ar	IR	1
a''	5	SeF_2 a-stretch	570	Ar	IR	1

Reference

[1] A. Haas and H. Willner, Z. Anorg. Allg. Chem. **454**, 17 (1979).

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

TiH_4

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		TiH stretch	1663.8 1656.7	Ar	IR	1,2
			1657.8T	Kr	IR	1

TiD_4

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		TiD stretch	1205.6 1200.0	Ar	IR	1,2
			1201.1	Kr	IR	1

References

[1] Z. L. Xiao, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **95**, 2696 (1991).
[2] G. V. Chertihin and L. Andrews, J. Am. Chem. Soc. **116**, 8322 (1994).

ZrH_4

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ZrH stretch	1623.6	Ar	IR	1,2

ZrD_4

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ZrD stretch	1166.6	Ar	IR	1,2

References

[1] G. V. Chertihin and L. Andrews, J. Am. Chem. Soc. **117**, 6402 (1995).
[2] G. V. Chertihin and L. Andrews, J. Phys. Chem. **99**, 15004 (1995).

HfH_4

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		HfH stretch	1678.4	Ar	IR	1,2

HfD_4

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		HfD stretch	1201.7	Ar	IR	1,2

References

[1] G. V. Chertihin and L. Andrews, J. Am. Chem. Soc. **117**, 6402 (1995).
[2] G. V. Chertihin and L. Andrews, J. Phys. Chem. **99**, 15004 (1995).

ThH_4

$\tilde{X}$ T_d

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ThH stretch	1444.8 1443.3	Ar	IR	1

ThD_4

$\tilde{X}$ T_d

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ThD stretch	1032.1 1031.1	Ar	IR	1

Reference

[1] P. F. Souter, G. P. Kushto, L. Andrews, and M. Neurock, J. Phys. Chem. A **101**, 1287 (1997).

UH_4

$\tilde{X}$ T_d

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		UH stretch	1483.6 1481.7	Ar	IR	1

UD_4

$\tilde{X}$ T_d

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		UD stretch	1060.7T 1059.8	Ar	IR	1

Reference

[1] P. F. Souter, G. P. Kushto, L. Andrews, and M. Neurock, J. Am. Chem. Soc. **119**, 1682 (1997).

BH_4^-

$\tilde{X}$ T_d

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
t_2	3	BH stretch	2212.8	Ar	IR	1

Reference

[1] T. J. Tague, Jr. and L. Andrews, J. Am. Chem. Soc. **116**, 4970 (1994).

AlH_4^-

$\tilde{X}$ T_d

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	2	Deformation	750T	Ar	IR	1
f_2	3	AlH stretch	1609.3	Ar	IR	1
	4	Deformation	766.6	Ar	IR	1

AlD_4^-

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	2	Deformation	535T	Ar	IR	1
f_2	3	AlD stretch	1173.9	Ar	IR	1
	4	Deformation	566.6	Ar	IR	1

Reference

[1] P. Pullumbi, Y. Bouteiller, and L. Manceron, J. Chem. Phys. **101**, 3610 (1994).

NH_4^+

$\tilde{X}$ T_d Structure: LD[1,4]CC[2]TPE[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
f_2	3	NH stretch	3343.14	gas	LD,CC	1–3,6
	4	Deformation	1447.22	gas	DL	5,7

B_0=5.929 LD[1,4]CC[2]DL[7]

ND_4^+

$\tilde{X}$ T_d

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
f_2	3	ND stretch	2495.0	gas	LD	4

B_0=2.986(4) LD[4]TPE[8]

References

[1] M. Crofton and T. Oka, J. Chem. Phys. **79**, 3157 (1983).
[2] E. Schaeffer, M. H. Begemann, C. S. Gudeman, and R. J. Saykally, J. Chem. Phys. **79**, 3159 (1983).
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[4] M. W. Crofton and T. Oka, J. Chem. Phys. **86**, 5983 (1987).
[5] M. Polak, M. Gruebele, B. W. DeKock, and R. J. Saykally, Mol. Phys. **66**, 1193 (1989).
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[7] J. Park, C. Xia, S. Selby, and S. C. Foster, J. Mol. Spectrosc. **179**, 150 (1996).
[8] R. Signorell, H. Palm, and F. Merkt, J. Chem. Phys. **106**, 6523 (1997).

NH_4

$3p\ ^2F_2$ T_d
$T_0 \cong 15078$[ab] gas EM[1,2,4] $3p^2F_2$-$3s^2A_1$ 663.5 nm
Diffuse.

$3s\ ^2A_1$ T_d Structure: TPE[8]
gas $3p^2F_2$-$3s^2A_1$ 663.5 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NH stretch	2552T	gas	EM	1,4
e	2	Deformation	1581T	gas	EM	1,4

ND_4

$3p\ ^2F_2$ T_d
T_0[a]=14828.285(4) gas EM[1,2,4]AB[3,5] $3p^2F_2$-$3s^2A_1$ 675 nm
Three weak bands have been observed[4] 775, 1138, and 1722 cm^{-1} above the band origin. However, the assignment of these bands has not yet been established.
B_0=3.122 gas AB[5]

$3s\ ^2A_1$ T_d
gas $3p^2F_2$-$3s^2A_1$ 675 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ND stretch	1960T	gas	EM	1,4
e	2	Deformation	1080.25(7)	gas	EM	7

$\tau \cong 30\ \mu s$ gas AB[5]
B_0=2.856(4) gas TPE[8]

[a]Measured with respect to the lowest Rydberg state, $3s\ ^2A_1$. The ground state is dissociative.
[b]Estimated[5] by scaling of data for ND_4.

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[7] J. K. G. Watson, *Proceedings of the l7th International Symposium on Free Radicals*, Natl. Bur. Stand. (U.S.) Spec. Publ. No. 716, edited by K. M. Evenson (US GPO, Washington, DC, 1986), pp. 650–670.
[8] R. Signorell, H. Palm, and F. Merkt, J. Chem. Phys. **106**, 6523 (1997).

HBeHBeH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1493.4	Ar	IR	1
			1402.1	Ar	IR	1

Reference

[1] T. J. Tague, Jr. and L. Andrews, J. Am. Chem. Soc. **115**, 12111 (1993).

$MgCH_3$

$\tilde{A}\ ^2E$ C_{3v} Structure: LF[1]
T_0=20030.296(2) gas LF[1]
A_0=4.992; B_0=0.365 LF[1]

$\tilde{X}\ ^2A_1$ C_{3v} Structure: LF[1]MW[2]
B_0=0.367 LF[1]MW[2]

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[1] R. Rubino, J. M. Williamson, and T. A. Miller, J. Chem. Phys. **103**, 5964 (1995).
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$CaCH_3$

$\tilde{B}\ ^2A_1$ C_{3v}
T_0=16003(10) gas LF[1] $\tilde{B}-\tilde{X}$ 620–630 nm

$\tilde{A}\ ^2E$ C_{3v}
T_0=14743.382[a] gas LF[1,2,4] $\tilde{A}-\tilde{X}$ 630–730 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 umbrella	1048(10)	gas	LF	1
	3	CaC stretch	413(10)	gas	LF	1
e	6	CaCH deform.	391(5)H	gas	LF	1

A=72.71 gas LF[1,2,4]
A_0=5.386; B_0=0.254 LF[2,4]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 umbrella	1085(10)	gas	LF	1
	3	CaC stretch	419(10)	gas	LF	1
e	6	CaCH deform.	319(5)H	gas	LF	1

A_0=5.448; B_0=0.252 LF[2,4]MW[3]

[a]Predissociated above ~16200.[1]

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$SrCH_3$

$\tilde{B}\ ^2A_1$ C_{3v}
T_0=14777(10) gas LF[1] $\tilde{B}-\tilde{X}$ 670–680 nm

$\tilde{A}\ ^2E$ C_{3v}
T_0=13653(10)[a] gas LF[1] $\tilde{A}-\tilde{X}$ 670–740 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 umbrella	1054(10)	gas	LF	1
	3	SrC stretch	373(10)	gas	LF	1
e	6	SrCH deform.	342(5)H	gas	LF	1

A=273(20) gas LF[1]

$\tilde{X}\ ^2A_1$ C_{3v} Structure: MW[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 umbrella	1072(10)	gas	LF	1
	3	SrC stretch	362(10)	gas	LF	1
e	6	SrCH deform.	279(5)H	gas	LF	1

B_0=0.194 MW[2]

[a]Predissociated above ~15000.[1]

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$ZnCH_3$

$\tilde{C}\ ^2A_1$[a] C_{3v}
T_0=36510 gas AB[1] $\tilde{C}-\tilde{X}$ 260–274 nm

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

$\tilde{A}\ ^2E$ C_{3v} Structure: LF[6]
T_0=24082.82 gas AB[1]EM[2]LF[5,6] $\tilde{A}-\tilde{X}$ 379–437 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 deform.	1048	gas	AB,LF	1,4,5
	3	ZnC stretch	460	gas	LF	5

τ=40(3) ns gas EM[3]LF[4]
A=253 gas AB[1]EM[2,3]LF[4,5]
A_0=4.949; B_0=0.317 LF[6]

$\tilde{X}\ ^2A_1$ C_{3v} Structure: LF[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 deform.	1064	gas	EM,LF	3–5
	3	ZnC stretch	445	gas	LF	4,5
e	6	ZnCH deform.	315T	gas	LF	5

$A_0 \cong 5.15$; $B_0 = 0.310$ LF[6]

[a]Assignment to $\tilde{C}$ state suggested[4] by analogy with ZnH.

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$CdCH_3$

$\tilde{C}\ ^2A_1$ C_{3v}
$T_0 = 34916$ gas AB[1] $\tilde{C}-\tilde{X}$ 264–287 nm

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

$\tilde{A}\ ^2E$ C_{3v} Structure: LF[8]
$T_0 = 22835.22$ gas AB[1]EM[2–5]LF[6–9] $\tilde{A}-\tilde{X}$ 400–458 nm
Perturbations in the $^2E_{3/2}$ band origin suggest another nearby state of ^2E symmetry.[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 deform.	1019(3)	gas	LF	7,8
	3	CdC stretch	400(3)	gas	LF	6–8

$\tau = 70(4)$ ns gas EM[2,4]LF[7]
$A = 650$ gas LF[8]
$A_0 = 4.969$; $B_0 = 0.244$ LF[8]

$\tilde{X}\ ^2A_1$ C_{3v} Structure: LF[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 deform.	1000(3)	gas	EM,LF	5–7
	3	CdC stretch	355(3)	gas	EM,LF	5–7

$A_0 = 5.157$; $B_0 = 0.234$ LF[8]

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$H_2C{=}BH$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		BH stretch	2724.6	Ar	IR	1
		C=B stretch	1469.7	Ar	IR	1
b_1		H_2CB OPLA	705.7	Ar	IR	1
		Torsion	611.8	Ar	IR	1
b_2		HBC deform.	902.6	Ar	IR	1

$D_2C{=}BD$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		BD stretch	2070.2	Ar	IR	1
b_1		D_2CB OPLA	537.1	Ar	IR	1
b_2		DBC deform.	739.1	Ar	IR	1

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$AlCH_3$

$\tilde{X}\ ^1A_1$ C_{3v}
$B_0 = 0.393$ MW[1]

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$C_2H_3^+$

$\tilde{X}$ C_{2v} (bridged) Structure: LD[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
A_{1u}^+	6	CH a-stretch	3142.2	gas	LD	2,5

$A_0 = 13.341$; $B_0 = 1.142$; $C_0 = 1.046$ LD[1,2,5]MW[3,4,6]

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$HBNH_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NH stretch	3598.4	Ar	IR	1
			3588.4			
		BH stretch	2418.2	Ar	IR	1
		BN stretch	1556.4	Ar	IR	1
		OPLA	608.5	Ar	IR	1

$DBND_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ND stretch	2685.9	Ar	IR	1
			2678.7			

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C_2H_3

Rydberg state

T_0=59410 gas AB[3] 164–169 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1306	gas	AB	3

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

$T_0 \leq 20020$ gas AB[1] 500–400 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CC stretch	1200	gas	AB	1
		CCH bend	920	gas	AB	1

$\tilde{X}$ C_s[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a''	7	Mixed OPLA	895.16	gas	DL	4
			895.4	Ne	IR	5
			900	Ar	IR	2

A_0=7.913; B_0=1.083; C_0=0.949 DL[4]

C_2D_3

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a''	7	Mixed OPLA	704	Ar	IR	2

[a]Rapid tunneling, giving effective C_{2v} symmetry.[4]

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CH_3N

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

T_0=31830.913(12) gas AB[1],EM[1,2,4,5,7]LF[8,10] $\tilde{A}-\tilde{X}$ 288–356 nm

31576(20) N_2 AB[3,6] $\tilde{A}-\tilde{X}$ 281–317 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 stretch	2943	gas	LF	8,10
	2	CH_3 deform.	1239	gas	LF	8
			1166T	N_2	AB	6
	3	CN stretch	758(4)	gas	UV,LF	1,2,8
			755(22)	N_2	AB	3,6
e	5	CH_3 deform.	1500T[a]	gas	LF	8
	6	CH_3 rock	728(4)	gas	EM	5

τ_0=415(8) ns gas LF[9,10]
A=−22.52 gas EM[4,7]
A_0=5.423; B_0=0.845 EM[4,7]

$\tilde{X}$ $^3A_2$ C_{3v} Structure: EM[4,7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 s-stretch	2943(4)	gas	EM	2,5
	2	CH_3 deform.	1349(4)	gas	EM	2,5
	3	CN stretch	1040(4)	gas	EM,LF	2,5,10
			1029	N_2	AB	3
e	4	CH_3 a-stretch	2989(4)	gas	EM	5
	5	CH_3 deform.	1490(4)	gas	EM	5
	6	CH_3 rock	903(8)	gas	EM	2,5

A_0=5.61; B_0=0.929 EM[4,7]

CD_3N

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

T_0=31774.158(2)[b] gas AB[1],EM[2,4,5] $\tilde{A}-\tilde{X}$ 294–365 nm

31516(30) N_2 AB[3,6] $\tilde{A}-\tilde{X}$ 277–318 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_3 deform.	1044T	N_2	AB	6
	3	CN stretch	759(4)	gas	UV	1,2
			695T	N_2	AB	6
e		CD_3 rock	579(4)[c]	gas	EM	2

B_0=0.691 EM[4]

$\tilde{X}\ ^3A_2$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_3 deform.	941(4)	gas	EM	5
	3	CN stretch	1110(4)	gas	EM	2,5
e	6	CD_3 rock	749(8)	gas	EM	2,5

B_0=0.744 EM[4]

[a]From combination bands.
[b]Calculated assuming $A(CD_3N)=A(CH_3N)$.
[c]Observed as sequence band.

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SiH_2NH

In an argon matrix, an absorption maximum at 41700 (240 nm) has been assigned[1] to SiH_2NH.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SiH_2 stretch	2253	Ar	IR	1
		SiH_2 stretch	2175	Ar	IR	1
		Si=N stretch	1097	Ar	IR	1

SiD_2ND

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SiD_2 stretch	1638	Ar	IR	1
		SiD_2 stretch	1585	Ar	IR	1
		Si=N stretch	1063	Ar	IR	1

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CH_2OH^+

$\tilde{X}$ C_s Structure: MW[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3422.802	gas	LD	2
		CO stretch	1650(30)	gas	PE	1
		CH_2 deform.	1370(30)	gas	PE	1

A_0=6.591; B_0=1.146; C_0=0.973 LD[2]MW[3,4]

CD_2OD^+

$\tilde{X}$ C_s

A_0=3.407; B_0=0.903; C_0=0.711 MW[5]

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CH_3S^+

$\tilde{X}\ ^3A_2$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CS stretch	733(5)	gas	PI,TPE	1,2

CD_3S^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CS stretch	730(60)	gas	PI	1

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CH_3O

$\tilde{A}\ ^2A_1$ C_{3v} Structure: LF[22,23]

T_0=31644.2 gas EM[1,2,11,12]AB[5]LF[6,8,18,19,22–24,27–29,31] $\tilde{A}-\tilde{X}$ 271–421 nm
31291(3) Ar LF[21] $\tilde{A}-\tilde{X}$ 270–420 nm

Evidence for predissociation above 35437 (3793 above the origin of the $\tilde{A}$ state),[13,29,32] with CH_3+O the principal products.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 stretch	2947.8	gas	LF	31
	2	Umbrella	1289.3	gas	LF	19,27,31
			1308(4)	Ar	LF	21
	3	CO stretch	662.4	gas	AB,EM,LF	5,12,19,31
			657(2)	Ar	LF	21
e	4	CH_3 stretch	3077.8T	gas	LF	31
	5	CH_2 scissors	1403.0	gas	LF	19,31
			1410(3)	Ar	LF	21
	6	HCO deform.	929.5	gas	LF	31

τ=2.57(13) μs gas EM[2,9]LF[4,14,15,16,18,20,32]
A_0=4.981(3); B_0=0.743 LF[22–24,28]

$\tilde{X}\ ^2E$ C_{3v}[a] Structure: LMR[3,7]MW[10,17]LF[22]

High vibrational levels have been studied using SEP.[25,28,30]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 stretch	2840T[b]	gas	LF	19,27
	2	CH_3 umbrella	1412(4)T[c]	gas	LF	27
			1406(2)T	Ar	LF	21
	3	CO stretch	1047	gas	LF,EM	6,9,12, 19,27,30
			1044(2)	Ar	LF	21
e	4	CH_3 stretch	2778	gas	SEP	30
			2758(3)	Ar	LF	21
	5	CH_2 scissors	914	gas	SEP	30
	6	HCO deform.	651.5	gas	LF,SEP	19,26,27,30

A=−61.97(7) gas LMR[7]MW[10]EM[11,12]LF[19,22,23,27]
A_0=5.206(4); B_0=0.932 LMR[7]MW[10,17]LF[22,23]

CD_3O

$\tilde{A}\ ^2A_1$ C_{3v}
T_0=31554 gas LF[6,19]EM[12] $\tilde{A}-\tilde{X}$ 282–410 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_3 stretch	2015	gas	LF	19
	2	CD_3 umbrella	971	gas	LF	19
	3	CO stretch	663	gas	EM,LF	12,19
e	5	CD_2 scissors	1047	gas	LF	19

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CO stretch	1000T	gas	LF	19
	3	CD_3 umbrella	893T	gas	LF	19
e	5	CD_2 scissors	1174T	gas	LF,EM	6,12,19
	6	DCO deform.	496	gas	LF	19

A=−56(2) gas EM[12]
B_0=0.740 MW[17]

[a]Somewhat distorted by Jahn–Teller coupling.
[b]Ref. 30 indicates that reassignment is necessary.
[c]Ref. 30 favors assignment at 1359.

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CH_2OH

$\tilde{B}\ ^2A'(3p)$ C_s
T_0=41065(3) gas MPI[3,4,7]AB[5] $\tilde{B}-\tilde{X}$ 217–244 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	4	CO stretch	1621(7)	gas	MPI	3,4,7
	5	CH_2 scissors	1465(7)	gas	MPI	3,7
	6	HCOH deform.	1357(7)	gas	MPI	3,7
	7	HCOH deform.	1107(7)	gas	MPI	3,7
a''	9	Torsion	993(8)	gas	MPI	7

$\tilde{A}\ ^2A'(3s)$ C_s
T_0=35050 gas AB[5] $\tilde{A}-\tilde{X}$ 243–285 nm
Threshold for photodecomposition into H_2CO+H near 280 nm.[1,2]

$\tilde{X}\ ^2A''$ C_s[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3650m	Ar	IR	1,2
			3637m	N_2	IR	1
	4	CH_2 scissors	1459w	Ar	IR	2
	5	OH deform.	1334m	Ar	IR	1,2
	6	CO stretch	1176(7)	gas	MPI	7
			1183vs	Ar	IR	1,2
			1183s	N_2	IR	1
	7	HCOH deform.	1048s	Ar	IR	1,2
			1056m	N_2	IR	1
a''	8	Torsion	420m	Ar	IR	1,2
			482m	N_2	IR	1
	9	H_2CO OPLA	234(5)	gas	MPI	7

CD_2OD

$\tilde{B}\ ^2A'(3p)$ C_s
T_0=40913 gas MPI[3,7]AB[6] $\tilde{B}-\tilde{X}$ 216–244 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	4	CO stretch	1565	gas	MPI,AB	3,6,7
	5	CD_2 scissors	1109	gas	MPI,AB	3,6,7
a''	8	D_2CO OPLA	952(23)	gas	MPI	7
	9	Torsion	723(23)	gas	MPI	7

$\tilde{A}\ ^2A'(3s)$ C_s
T_0=35124 gas AB[6]
Threshold for photodecomposition into D_2CO+D near 280 nm.[1,2]

$\tilde{X}\ ^2A''$ C_s[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2694wm	Ar	IR	2
			2682m	N_2	IR	1
	4	CO stretch	1221(4)	gas	MPI	7
			1223m	Ar	IR	2
			1222m	N_2	IR	1
	5	CD_2 scissors	1020(5)	gas	MPI	7
			1041m	Ar	IR	2
	7		765wm	Ar	IR	2
a''	8	Torsion	329(23)	gas	MPI	7
	9	D_2CO OPLA	177(23)	gas	MPI	7

[a] Rapid interconversion of nonplanar forms.[7]

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CH_3S

A diffuse, unstructured absorption at 218.5 nm, observed on flash photolysis[1] of a number of sulfur-containing compounds or on pulse radiolysis[12] of CH_3SH in the presence of an F-atom source, has been attributed to CH_3S.

$\tilde{A}\ ^2A_1$ C_{3v} Structure: LF[9]
T_0=26396.8 gas EM[2]LF[6,9,11] $\tilde{A}-\tilde{X}$ 350–530 nm
Predissociation threshold $\geqslant$ 27885.[11] In an argon matrix, CH_2SH is formed.[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 umbrella	1098(2)	gas	LF	11
	3	CS stretch	401(2)	gas	EM,LF	2,6,9,11
e	6	HCS deform.	635(10)	gas	LF	11

τ_0=760(60) ns gas LF[8]; 1130(70) ns gas LF[10,11]
A_0=5.343(47); B_0=0.346 LF[9]

$\tilde{X}\ ^2E$ C_{3v} Structure: MW[7]LF[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 stretch	2776T	gas	LF	11
	2	CH_3 umbrella	1313(5)	gas	PD,LF	4,6,11
	3	CS stretch	727(3)	gas	EM,PE	2–4,6
					PD,LF	11
e	4	CH_3 stretch	2706T	gas	LF	11
	5	CH_3 deform.	1496(6)	gas	LF	11
	6	HCS deform.	586T	gas	LF	11

A=−259.1 gas LF[9,11]TPE[13]
A_0=5.68(4); B_0=0.450 MW[7]LF[9]

CD_3S

$\tilde{A}\ ^2A_1$ C_{3v}
T_0=26574 gas LF[6] $\tilde{A}-\tilde{X}$ 352–378 nm
Predissociation threshold ≤ 27728.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_3 umbrella	837(1)	gas	LF	6
	3	CS stretch	395(1)	gas	LF	6

τ_0=0.45(11) μs gas LF[6]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_3 umbrella	1100(50)	gas	PD	4
	3	CS stretch	667(1)	gas	PD,LF	4,6
e	5	DCS deform.	780(30)H	gas	PD	4

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H_2CFH^+

$\tilde{X}$ C_1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	FH stretch	3308.9 3291.0	Ne	IR	1
	7	HF wag	921.2	Ne	IR	1
	8	CF stretch	714.9	Ne	IR	1

D_2CFD^+

$\tilde{X}$ C_1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	FD stretch	2442.2 2429.4	Ne	IR	1

Reference

[1] C. L. Lugez, D. Forney, M. E. Jacox, and K. K. Irikura, J. Chem. Phys. **106**, 489 (1997).

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_0=20260(900) gas PE[1-4,7]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_3 deform.	1550(50)	gas	PE	3,4
			1503.3w	Ne	IR	8
		CH_3 deform.	1239.5wm	Ne	IR	8
		CH_3 umbrella	1073(50)	gas	PE	2,4
		CH_3 rock	870(50)	gas	PE	3,4
		CH_3 deform.	649.4wm 626.9wm	Ne	IR	8
		CCl stretch	654(50)	gas	PE	3,4

CD_3Cl^+

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD_3 stretch	2013.4m	Ne	IR	8
		CD_3 deform.	975.2w	Ne	IR	8
		CD_3 deform.	927.9wm	Ne	IR	8
		CCl stretch	628.9wm	Ne	IR	8

[a]From vertical ionization potential.

References

[1] D. W. Turner, Philos. Trans. R. Soc. London, Ser. A **268**, 7 (1970).
[2] A. W. Potts, H. J. Lempka, D. G. Streets, and W. C. Price, Philos. Trans. R. Soc. London, Ser. A **268**, 59 (1970).
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[8] C. L. Lugez, D. Forney, M. E. Jacox, and K. K. Irikura, J. Chem. Phys. **106**, 489 (1997).

H_2CClH^+

$\tilde{X}$ C_1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CH_2 a-stretch	3225.5wm	Ne	IR	1
	2	CH_2 s-stretch	3053.3m	Ne	IR	1
	3	ClH stretch	2626.1m	Ne	IR	1
	7	CCl stretch	798.8vw	Ne	IR	1
	8	Wag	655.0wm	Ne	IR	1

D_2CClD^+

$\tilde{X}$ C_1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CD_2 a-stretch	2444.2m	Ne	IR	1
	2	CD_2 s-stretch	2219.4w	Ne	IR	1
	3	ClD stretch	1909.9m	Ne	IR	1
	7	CCl stretch	575.6wm	Ne	IR	1

Reference

[1] C. L. Lugez, D. Forney, M. E. Jacox, and K. K. Irikura, J. Chem. Phys. **106**, 489 (1997).

CH_3Br^+

$\tilde{C}$ $^2A_1$ C_{3v}
T^a=75500(900) gas PE[1]

$\tilde{B}$ ^2E C_{3v}
T_0=31930(900) gas PE[1,3]
A Jahn–Teller splitting of ~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_0=19820(900) gas PE[1–3]
A broad absorption with maximum at 348 nm (28700) which appears on argon-resonance photolysis of CH_3Br isolated in an argon matrix and which has a photodecomposition threshold at a wavelength longer than 500 nm has been assigned[5] to the $\tilde{A}$–$\tilde{X}$ transition of CH_3Br^+.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	3130(100)	gas	PE	2,3
			3121.9wm	Ne	IR	6
	2	CH stretch	2930(120)	gas	PE	3
			2909.5s	Ne	IR	6
	3	Deformation	1417.3wm	Ne	IR	6
			1412.5wm			
	4	Deformation	1290(80)	gas	PE	1–3
			1296.7m	Ne	IR	6
	5	Deformation	850(80)	gas	PE	1–3
			815.0w	Ne	IR	6
	6	CBr stretch	468(80)	gas	PE	3
			549.7wm	Ne	IR	6
			537.7wm			
a''	7	CH_2 a-stretch	3055.3m	Ne	IR	6
	8	Deformation	1276.8wm	Ne	IR	6
	9	Deformation	650.8m	Ne	IR	6

CD_3Br^+

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CD stretch	2165(80)	gas	PE	2
	2	CD stretch	2091.6ms	Ne	IR	6
	4	Deformation	947(80)	gas	PE	2
			948.2wm	Ne	IR	6
a''	7	CD_2 a-stretch	2128.1m	Ne	IR	6
	8	Deformation	974.7ms	Ne	IR	6
	9	Deformation	491.8m	Ne	IR	6

[a]From vertical ionization potential.

References

[1] A. W. Potts, H. J. Lempka, D. G. Streets, and W. C. Price, Philos. Trans. R. Soc. London, Ser. A **268**, 59 (1970).
[2] J. L. Ragle, I. A. Stenhouse, D. C. Frost, and C. A. McDowell, J. Chem. Phys. **53**, 178 (1970).
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H_2CBrH^+

$\tilde{X}$ C_1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CH_2 a-stretch	3221.4w	Ne	IR	1
	2	CH_2 s-stretch	2979.3wm	Ne	IR	1
	3	BrH stretch	2395.6wm	Ne	IR	1

D_2CBrD^+

$\tilde{X}$ C_1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CD_2 a-stretch	2440.3wm	Ne	IR	1
	3	BrD stretch	1727.1wm	Ne	IR	1

Reference

[1] C. L. Lugez, D. Forney, M. E. Jacox, and K. K. Irikura, J. Chem. Phys. **106**, 489 (1997).

H_2PSH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SH stretch	2563.9	Ar	IR	1
		PH_2 wag	967.5	Ar	IR	1
		P-S stretch	484.1	Ar	IR	1

Reference

[1] Z. Mielke and L. Andrews, J. Phys. Chem. **97**, 4313 (1993).

8.9. Five-Atomic Dihydrides

HGa_3H

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		GaH stretch	1765.8	Ar	IR	1
			1753.2	Kr	IR	1
		GaH stretch	1752.8	Ar	IR	1
			1740.4	Kr	IR	1

DGa_3D

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		GaD stretch	1276.2	Ar	IR	1
			1267.2	Kr	IR	1
		GaD stretch	1262.9	Ar	IR	1
			1253.3	Kr	IR	1

Reference

[1] Z. L. Xiao, R. H. Hauge, and J. L. Margrave, Inorg. Chem. **32**, 642 (1993).

HBeCCH

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	BeH stretch	2119.4	Ar	IR	1
	4	BeC stretch	838.9	Ar	IR	1
Π	5	HCC bend	689.1	Ar	IR	1
	6	HBeC bend	550.0	Ar	IR	1

DBeCCD

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	BeD stretch	1535.0	Ar	IR	1
	4	BeC stretch	784.9	Ar	IR	1
Π	6	DBeC bend	450.0	Ar	IR	1

Reference

[1] C. A. Thompson and L. Andrews, J. Am. Chem. Soc. **118**, 10242 (1996).

HBCBH

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	4	BCB a-stretch	1872.0	Ar	IR	1,2

DBCBD

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

Vib sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	BD a-stretch	2190.9	Ar	IR	1,2
	4	BCB a-stretch	1727.4	Ar	IR	1,2

References

[1] P. Hassanzadeh and L. Andrews, J. Am. Chem. Soc. **114**, 9239 (1992).
[2] P. Hassanzadeh, Y. Hannachi, and L. Andrews, J. Phys. Chem. **97**, 6418 (1993).

HBeOBeH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BeH stretch	2092.4	Ar	IR	1
		BeOBe a-stretch	1403.1	Ar	IR	1
		Deformation	578.7	Ar	IR	1

DBeOBeD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BeD stretch	1642.7	Ar	IR	1
		BeOBe a-stretch	1279	Ar	IR	1
		Deformation	481	Ar	IR	1

Reference

[1] C. A. Thompson and L. Andrews, J. Phys. Chem. **100**, 12214 (1996).

cyc-HC=CHB

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BC_2 s-stretch	1170.6	Ar	IR	1,2
		HCC deform.	896.7	Ar	IR	2

cyc-DC=CDB

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BC_2 s-stretch	1169.4	Ar	IR	1,2
		DCC deform.	771.4	Ar	IR	2

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[1] J. M. L. Martin, P. R. Taylor, P. Hassanzadeh, and L. Andrews, J. Am. Chem. Soc. **115**, 2510 (1993).
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cyc-HC=CBH

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BH stretch	2651.4	Ar	IR	1
		Ring stretch	1119.7	Ar	IR	1

cyc-DC=CBD

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BD stretch	2004.0	Ar	IR	1

Reference

[1] L. Andrews, P. Hassanzadeh, J. M. L. Martin, and P. R. Taylor, J. Phys. Chem. **97**, 5839 (1993).

HCCBH

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	C≡C stretch	2080.4	Ar	IR	1

DCCBD

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		C≡C stretch	1940.3	Ar	IR	1

Reference

[1] L. Andrews, P. Hassanzadeh, J. M. L. Martin, and P. R. Taylor, J. Phys. Chem. **97**, 5839 (1993).

cyc-HC=CHAl

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		HCC deform.	609	Ar	IR	1,2

References

[1] T. R. Burkholder and L. Andrews, Inorg. Chem. **32**, 2491 (1993).
[2] G. V. Chertihin, L. Andrews, and P. R. Taylor, J. Am. Chem. Soc. **116**, 3513 (1994).

HCCAlH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C≡C stretch	2000.8	Ar	IR	1,2
		AlH stretch	1804.1	Ar	IR	1,2

DCCAlD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C≡C stretch	1882.7	Ar	IR	1
		AlD stretch	1314.8	Ar	IR	1

References

[1] T. R. Burkholder and L. Andrews, Inorg. Chem. **32**, 2491 (1993).
[2] G. V. Chertihin, L. Andrews, and P. R. Taylor, J. Am. Chem. Soc. **116**, 3513 (1994).

$(C_2H_2)Al$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		HCC deform.	569.0	Ar	IR	1,2
		AlC stretch	424.8	Ar	IR	1,2

$(C_2D_2)Al$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		DCC deform.	429.7	Ar	IR	1
		AlC stretch	405.8	Ar	IR	1

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[1] T. R. Burkholder and L. Andrews, Inorg. Chem. **32**, 2491 (1993).
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$(C_2H_2)Ga$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	2992	Ar	IR	1
		CC stretch	1682	Ar	IR	1
		HCC deform.	595	Ar	IR	1
		HCC deform.	566	Ar	IR	1
		GaC stretch	408	Ar	IR	1

$(C_2D_2)Ga$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD stretch	2242	Ar	IR	1
		CC stretch	1563	Ar	IR	1
		DCC deform.	486	Ar	IR	1
		DCC deform.	426	Ar	IR	1
		GaC stretch	375	Ar	IR	1

Reference

[1] T. R. Burkholder and L. Andrews, Inorg. Chem. **32**, 2491 (1993).

$(C_2H_2)In$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3062	Ar	IR	1
		CC stretch	1668	Ar	IR	1
		HCC deform.	595	Ar	IR	1
		HCC deform.	544	Ar	IR	1
		InC stretch	418	Ar	IR	1

$(C_2D_2)In$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD stretch	2312	Ar	IR	1
		CC stretch	1547	Ar	IR	1
		DCC deform.	436	Ar	IR	1
		DCC deform.	409	Ar	IR	1
		InC stretch	387	Ar	IR	1

Reference

[1] T. R. Burkholder and L. Andrews, Inorg. Chem. **32**, 241 (1993).

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

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

$\tilde{C}\ ^1A_1$ C_{2v}
T_0=38650(160) Ar AB[8] $\tilde{C}-\tilde{X}$ 213–259 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		C_3 s-stretch	900T	Ar	AB	8

$\tilde{B}\ ^1B_1$ C_{2v}
T_0=18720(80) Ar AB[8] $\tilde{B}-\tilde{X}$ 382–535 nm
In an argon matrix, randomization of carbon-13 labelling occurs on irradiation at wavelengths longer than 22500 (444 nm).[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		C_3 s-stretch	1000T	Ar	AB	8

$\tilde{A}\ ^1A_2$ C_{2v}
$T_0 \leqslant 13960$ Ar AB[8]

$\tilde{a}\ ^3B_1$ C_{2v}
T_0=10390(70) gas PE[6]

$\tilde{X}\ ^1A_1$ C_{2v} Structure: MW[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s-stretch	3059.6 3049.5	Ar	IR	1,2
	2	C_3 a-stretch	1963.2 1952.2	Ar	IR	1,2
	3	CH_2 scissors	1449.3 1446.9	Ar	IR	1,2
b_1	5	H_2CC OPLA	1003.0 999.2	Ar	IR	1,2
b_2	8	CH_2 rock	1025.0	Ar	IR	1

A_0=9.633; B_0=0.353; C_0=0.340 MW[3,5]

$D_2C{=}C{=}C$:

$\tilde{X}\ ^1A_1$ 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_0=4.842; B_0=0.314; C_0=0.294 MW[4]

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[1] G. Maier, H. P. Reisenauer, W. Schwab, P. Carsky, B. A. Hess, Jr., and L. J. Schaad, J. Am. Chem. Soc. **109**, 5183 (1987).
[2] J. W. Huang and W. R. M. Graham, J. Chem. Phys. **93**, 1583 (1990).
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HCCCH

In an argon matrix, a broad absorption near 31750 (315 nm) which shows some fine structure and bands between 38460 and 47600 (210–260 nm) have been attributed[8] to triplet HCCCH. Prolonged 313-nm irradiation of HCCCH isolated in solid argon leads both to its isomerization to $H_2C{=}C{=}C$:, which has a singlet ground state,[5,9] and to the randomization of carbon-13 substitution in HCCCH.[9]

An absorption band system of singlet HCCCH has also been identified[2] in the 310–370-nm spectral region, but a detailed analysis has not been reported. Beyond 28900 the bands are diffuse, and a continuous absorption is superposed on the short wavelength end of the band system. The molecule is linear in at least one of the states of the transition. A progression involving an upper-state vibrational frequency of 1094 has been tentatively identified. The preliminary analysis found B'=0.310 and B''=0.324.

$\tilde{X}\ ^3A$ C_2 Structure: ESR,IR[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3266.0s	Ar	IR	5–8
			3285	Kr	IR	3
		C_3 a-stretch	1619.4w	Ar	IR	6–8
		CCH s-bend	550.4m	Ar	IR	6,8
			402.6 401.5wm	Ar	IR	4–8
			408	Kr	IR	3
	7	HCC wag	248.5 245.9s	Ar	IR	4–8
			258	Kr	IR	3

DCCCD

$\tilde{X}\ ^3A$ C_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD stretch	2457.9s	Ar	IR	4,6,7
			2482	Kr	IR	3
		C_3 a-stretch	1529.0w	Ar	IR	6,7
		CCD, C_3 bend	384.0m	Ar	IR	6,7
			392	Kr	IR	3
	7	DCC wag	171m	Ar	IR	4

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cyc-HC=CHSi

In an argon matrix, *cyc*-HC=CHSi shows a weak, broad absorption between 260 and 320 nm, with maximum at 286 nm.[1,3] Irradiation in this spectral region results in rearrangement to form HCCSiH.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	3048.7wm	Ar	IR	1,3
	3	CH deform.	875.3m	Ar	IR	1,3
	4	SiC stretch	761.9ms	Ar	IR	1,3
b_1	6	CH deform.	677.2vs	Ar	IR	1,3
b_2	7	CH stretch	3026.5wm	Ar	IR	1,3
	8	CH deform.	1085.8s	Ar	IR	1,3
	9	SiC stretch	672.1s	Ar	IR	1,3

A_0=1.118; B_0=0.397; C_0=0.292 MW^2

cyc-DC=CDSi

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD stretch	2313.6w	Ar	IR	3
	4	SiC stretch	769.1vs	Ar	IR	3
b_1	6	CD deform.	518.4s	Ar	IR	3
b_2	7	CD stretch	2248.7w	Ar	IR	3
	8	CD deform.	938.6wm	Ar	IR	3
	9	SiC stretch	583.9s	Ar	IR	3

A_0=0.876; B_0=0.355; C_0=0.252 MW^2

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[1] G. Maier, H. P. Reisenauer, and H. Pacl, Angew. Chem. **106**, 1347 (1994); Angew. Chem. Int. Ed. Engl. **33**, 1248 (1994).
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HCCSiH

In an argon matrix, a broad absorption maximum at 500 nm is associated with isomerization to *cyc*-HC=CHSi and to $H_2C=C=Si$:.[1,2]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	3304.2m	Ar	IR	1,2
	2	C≡C stretch	1995.7m	Ar	IR	1,2
	3	SiH stretch	1969.9vs	Ar	IR	1,2
	4	SiH deform.	814.8ms	Ar	IR	1,2
	5	CH deform.	613.9m	Ar	IR	1,2
	6	SiC stretch	605.0m	Ar	IR	1,2
a''	8	CH deform.	722.8wm	Ar	IR	1,2

DCCSiD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CD stretch	2570.1w	Ar	IR	2
	2	C≡C stretch	1879.7ms	Ar	IR	2
	3	SiD stretch	1435.3vs	Ar	IR	2
	4	SiD deform.	641.6s	Ar	IR	2
	5	SiC stretch	575.5wm	Ar	IR	2
a''	8	CD deform.	479.9wm	Ar	IR	2

References

[1] G. Maier, H. P. Reisenauer, and H. Pacl, Angew. Chem. **106**, 1347 (1994); Angew. Chem. Int. Ed. Engl. **33**, 1248 (1994).
[2] G. Maier, H. Pacl, H. P. Reisenauer, A. Meudt, and R. Janoschek, J. Am. Chem. Soc. **117**, 12712 (1995).

$H_2C=C=Si$:

In an argon matrix, absorption maxima at 340, 325, and 310 nm have been assigned[1,2] to $H_2C=C=Si$:. Irradiation at 340 nm leads to isomerization to HCCSiH.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C=C stretch	1667.9s	Ar	IR	1,2
b_1	5	CH deform.	957.7s	Ar	IR	1,2

$D_2C=C=Si$:

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C=C stretch	1648.3	Ar	IR	2

References

[1] G. Maier, H. P. Reisenauer, and H. Pacl, Angew. Chem. **106**, 1347 (1994); Angew. Chem. Int. Ed. Engl. **33**, 1248 (1994).
[2] G. Maier, H. Pacl, H. P. Reisenauer, A. Meudt, and R. Janoschek, J. Am. Chem. Soc. **117**, 12712 (1995).

cyc-H_2SiCC

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiH_2 stretch	2214.4ms	Ar	IR	1,2
	2	CC stretch	1769.8w	Ar	IR	1,2
	3	SiH_2 scissors	1023.1vs	Ar	IR	1,2
	4	SiC_2 s-stretch	836.5ms	Ar	IR	1,2
b_1	6	SiH_2 stretch	2228.9ms	Ar	IR	1,2
	7	SiH deform.	676.4wm	Ar	IR	2
b_2	8	SiH deform.	757.4m	Ar	IR	2

cyc-D_2SiCC

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiD_2 stretch	1601.9m	Ar	IR	2
	2	CC stretch	1771.1w	Ar	IR	2
	3	SiC_2 s-stretch	842.3vs	Ar	IR	2
	4	SiD_2 scissors	722.2wm	Ar	IR	2
b_1	6	SiD_2 stretch	1626.3m	Ar	IR	2
	7	SiD deform.	500.5wm	Ar	IR	2
b_2	8	SiD deform.	604.2wm	Ar	IR	2

References

[1] G. Maier, H. P. Reisenauer, and H. Pacl, Angew. Chem. **106**, 1347 (1994); Angew. Chem. Int. Ed. Engl. **33**, 1248 (1994).
[2] G. Maier, H. Pacl, H. P. Reisenauer, A. Meudt, and R. Janoschek, J. Am. Chem. Soc. **117**, 12712 (1995).

$H_2C{=}C{=}C{:}^-$

Threshold for electron detachment from ground-state $H_2C{=}C{=}C{:}^-$ =14470(65) gas PE[1,2]

$^2A_1$ C_{2v}
(Dipole-Bound State)
T_0=14284.420(5) gas PD[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C_3 a-stretch	1965	gas	PD	4
	4	C_3 s-stretch	1117	gas	PD	4
b_1	6	H2CC OPLA	221.45	gas	PD	4
b_2	9		276.69	gas	PD	4

A_0=9.651; $\frac{1}{2}(B_0+C_0)$=0.346 PD[3]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_1	6	H_2CC OPLA	385.43	gas	PD	4
b_2	9		309.24	gas	PD	4

A_0=9.731; B_0=0.344; C_0=0.332 PD[3]

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H_2CCN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_1	5	H_2CC OPLA	663.79	gas	PE,DL	1,3

A_0=9.53; B_0=0.342; C_0=0.329 MW^2

D_2CCN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_1	5	D_2CC OPLA	538[a]	gas	PE	1

[a] From computer fit.

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H_2CCO^+

$\tilde{E}$ $^2A_1$ C_{2v}
T_0=68343(11) gas PE[2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CH_2 scissors	1177(4)[a]	gas	PE	2,4
			671(4)[a]	gas	PE	4
			397(4)[a]	gas	PE	4

$\tilde{D}$ $^2A_1$ C_{2v}
T_0=53414T gas PE[2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1488(4)[a]	gas	PE	4
			1164(4)[a]	gas	PE	4
			709(4)[a]	gas	PE	4

$\tilde{C}$ $^2B_2$ C_{2v}
T_0=52037(10) gas PE[1–4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		1697(4)[a]	gas	PE	4
	3	CH_2 scissors	1087(4)[a]	gas	PE	1,2,4

$\tilde{B}\ ^2B_1$ C_{2v}
T_0=40259(10) gas PE[1–4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCO a-stretch	2001(4)[a]	gas	PE	4
	4	CCO s-stretch	1001(4)[a]	gas	PE	1,2,4
			347(4)	gas	PE	4

$\tilde{A}\ ^2B_2$ C_{2v}
T_0=33706(6) gas PE[1–4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1528(4)[a]	gas	PE	4
			1164(4)[a]	gas	PE	4
			690(4)	gas	PE	4
b_1		OPLA	461(4)	gas	PE	4

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCO a-stretch	2263(4)[a]	gas	PE	2–4
	3		1379(4)	gas	PE	4
	4		1227(4)[a]	gas	PE	4

D_2CCO^+

$\tilde{E}\ ^2A_1$ C_{2v}
T_0=68261(11) gas PE[2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1133(4)[a]	gas	PE	4
			834(4)	gas	PE	2,4

$\tilde{D}\ ^2A_1$ C_{2v}
T_0=54117T gas PE[2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1267(4)	gas	PE	4
			1204(4)[a]	gas	PE	4
			1169(4)[a]	gas	PE	4

$\tilde{C}\ ^2B_2$ C_{2v}
T_0=52222(3) gas PE[1–4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1102(4)	gas	PE	4
			800(4)[a]	gas	PE	2,4

$\tilde{B}\ ^2B_1$ C_{2v}
T_0=39383(8) gas PE[2–4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1732(4)	gas	PE	4
			1056(4)[a]	gas	PE	4
			848(4)	gas	PE	4

$\tilde{A}\ ^2B_2$ C_{2v}
T_0=34077(9) gas PE[2–4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			2140(4)[a]	gas	PE	4
			1007(4)[a]	gas	PE	4
			106(4)	gas	PE	4
b_1		OPLA	299(4)	gas	PE	4

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			2286(4)[a]	gas	PE	2–4
			1091(4)[a]	gas	PE	2–4
			925(4)[a]	gas	PE	4

[a] ω.

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$Be(OH)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3805.9	Ar	IR	1
		OBeO a-stretch	1493.7	Ar	IR	1
		Deformation	456	Ar	IR	1

$Be(OD)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OD stretch	2805.4	Ar	IR	1
		OBeO a-stretch	1477.3	Ar	IR	1

Reference

[1] C. A. Thompson and L. Andrews, J. Phys. Chem. **100**, 12214 (1996).

$Mg(OH)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		MgO a-stretch	866.9	Ar	IR	1

Reference

[1] T. J. Tague, Jr. and L. Andrews, J. Phys. Chem. **98**, 8611 (1994).

HN=C=NH

$\tilde{X}$ C_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	2	NCN s-stretch	1285(20)[a]	gas	IR	2
			1275[a]	Ar	IR	1
	5	NCN deform.	537m	Ar	IR	1
b	7	NCN a-stretch	2104.7	gas	IR	2
			2097s	Ar	IR	1
	8	NH deform.	890(10)	gas	IR	2
			886vs	Ar	IR	1

A_0=12.650; B_0=0.346; C_0=0.346 IR,MW[3–5]

DN=C=ND

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	ND stretch	2545s[b]	Ar	IR	1
	5	NCN deform.	471m	Ar	IR	1
b	6	ND stretch	2545s[b]	Ar	IR	1
	7	NCN a-stretch	2107vs	Ar	IR	1
	8	ND deform.	752s	Ar	IR	1

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

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HCNNH

In an argon matrix, an absorption maximum at 41700 (240 nm) has been assigned[1] to HCNNH.

$\tilde{X}$ C_1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NH stretch	3250.1w	Ar	IR	1
	2	CH stretch	3142.5w	Ar	IR	1
	3	CNN a-stretch	2032.7vs	Ar	IR	1
	4	HNN bend	1278.1wm	Ar	IR	1
	5	CNN s-stretch	1187.5wm	Ar	IR	1
	6	Torsion	792.1w	Ar	IR	1
	7	HCN bend	606.5m	Ar	IR	1
	8	CNN bend	461.4w	Ar	IR	1

DCNND

$\tilde{X}$ C_1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	CD stretch	2398.1wm	Ar	IR	1
	3	CNN a-stretch	1958.4vs	Ar	IR	1
			1953.1vs			
	5	CNN s-stretch	984.5wm	Ar	IR	1
	7	DCN bend	569.4wm	Ar	IR	1
	8	CNN bend	425.7m	Ar	IR	1
			418.0m			

Reference

[1] G. Maier, J. Eckwert, A. Bothur, H. P. Reisenauer, and C. Schmidt, Liebigs Ann. **1996**, 1041.

H_2CCS

$\tilde{A}$ $^1A''$ C_s
$T_0 \cong 17995$ gas AB[10] $\tilde{A}-\tilde{X}$ 450–550 nm
Diffuse bands.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	2	C=C stretch	1402	gas	AB	10
	8	CCS bend	284T	gas	AB	10

$\tilde{X}\ ^1A_1$ C_{2v} Structure: MW[2–5]IR[9,11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s-stretch	3020	gas	IR	9
			3012w	Ar	IR	1,6,7
	2	C=C stretch	1757	gas	IR	9
			1755vs	Ar	IR	1,6–8
	3	CH_2 scissors	1331.67	gas	IR	9,11
			1323m	Ar	IR	1,6,7
	4	C=S stretch	850	gas	IR	9
			858	Ar	IR	7
b_1	5	H_2C=C OPLA	698.09	gas	IR	11
			692s	Ar	IR	1,6–8
	6	CCS bend	413.85	gas	IR	12
			404vw	Ar	IR	1,7
b_2	7	CH_2 a-stretch	3107.33	gas	IR	9,11
			3097	Ar	IR	7
			3068			
	8	CH_2 rock	921.60	gas	IR	9,11
			918	Ar	IR	7
	9	CCS bend	357.45	gas	IR	12
			356	Ar	IR	7

A_0=9.554; B_0=0.189; C_0=0.185 MW[2–5]IR[9,11,12]

D_2CCS

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

$T_0 \cong 18002$ gas AB[10] $\tilde{A}$–$\tilde{X}$ 450–550 nm

Diffuse bands.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	C=C stretch	1400	gas	AB	10
	8	CCS bend	256T	gas	AB	10

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_2 s-stretch	2237.48	gas	IR	11
			2229	Ar	IR	1,7
	2	C=C stretch	1740	gas	IR	11
			1738vs	Ar	IR	1,7
	3	CD_2 scissors	1030	Ar	IR	7
	4	C=S stretch	755	Ar	IR	7
b_1	5	D_2C=C OPLA	558.04	gas	IR	11
			555s	Ar	IR	1,7
	6	CCS bend	375	Ar	IR	7
b_2	7	CD_2 a-stretch	2330T	Ar	IR	7
	8	CD_2 rock	775	Ar	IR	7
	9	CCS bend	308	Ar	IR	7

A_0=4.784; B_0=0.168; C_0=0.162 IR[11]

References

[1] A. Krantz and J. Laureni, J. Am. Chem. Soc. **96**, 6768 (1974).
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[12] D. McNaughton, E. G. Robertson, and L. D. Hatherley, J. Mol. Spectrosc. **175**, 377 (1996).

H_2CCSe

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s-stretch	3032.3w	Ar	IR	3
	2	C=C stretch	1699.7vs	Ar	IR	3
	3	CH_2 scissors	1334.8w	Ar	IR	3
	4	C=Se stretch	662.1vw	Ar	IR	3
b_1	5	CH_2 wag	736.8m	Ar	IR	3
b_2	7	CH_2 a-stretch	3063.3vw	Ar	IR	3

A_0=9.35(25); B_0=0.129; C_0=0.127 MW[1,2]

References

[1] B. Bak, O. J. Nielsen, H. Svanholt, and A. Holm, Chem. Phys. Lett. **53**, 374 (1978).
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H_2CNO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C=N stretch	1664.0vs	Ar	IR	1
			1197.0s	Ar	IR	1
			1106.4m	Ar	IR	1
		CH_2 OPLA	792.9wm	Ar	IR	1

Reference

[1] M. McCluskey and H. Frei, J. Phys. Chem. **97**, 5204 (1993).

cyc-H_2CO_2

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

A_0=0.967; B_0=0.836; C_0=0.493 MW[1,2]

References

[1] F. J. Lovas and R. D. Suenram, Chem. Phys. Lett. **51**, 453 (1977).
[2] R. D. Suenram and F. J. Lovas, J. Am. Chem. Soc. **100**, 5117 (1978).

H_2CSO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH_2 a-stretch	3117vw	Ar	IR	5
	2	CH_2 s-stretch	2985w	gas	IR	6
			3013vw	Ar	IR	3,5
	3	CH_2 scissors	1355m	gas	IR	6
			1357m	Ar	IR	3,5
	4	SO stretch	1175.75s	gas	IR	1,4,6
			1165s	Ar	IR	3,5
	5	CS stretch	972w	Ar	IR	3,5
	6	CH_2 rock	866T[a]	gas	IR	7
			860w	Ar	IR	3,5
	7	CSO bend	397w	Ar	IR	3,5
a''	8	H_2CS OPLA	762.07s	gas	IR	1,4,7
			765s	Ar	IR	3,5

A_0=1.348; B_0=0.313; C_0=0.254 MW[1,2]IR[7]

D_2CSO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CD_2 a-stretch	2339w	Ar	IR	5
	2	CD_2 s-stretch	2137wT	gas	IR	6
			2180vw	Ar	IR	5
	3	SO stretch	1189s	gas	IR	6
			1181s	Ar	IR	5
	4	CD_2 scissors	1117wT	gas	IR	6
			1100m	Ar	IR	5
	5	CS stretch	835wT	gas	IR	6
			845w	Ar	IR	5
	6	CD_2 rock	719w	Ar	IR	5
	7	CSO bend	345m	Ar	IR	5
a''	8	D_2CS OPLA	602m	gas	IR	6
			607m	Ar	IR	5

A_0=1.148; B_0=0.277; C_0=0.223 MW[2]

[a]Estimated from analysis of perturbations.[7]

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$CH_2F_2^+$

$\tilde{G}$ $^2A_1$ C_{2v}
T_0=83900(1000) gas PE[1,3]

$\tilde{F}$ $^2B_2$ C_{2v}
T_0=44706(35) gas PE[1–3,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CF_2 stretch	708	gas	PE	5

$\tilde{E}$ $^2A_1$ C_{2v}
T_0=44432(35) gas PE[1–3,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CF_2 stretch	668	gas	PE	5

$\tilde{D}$ $^2B_1$ C_{2v}
T_0=44206(35) gas PE[1–3,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CF_2 stretch	711(5)	gas	PE	1–3,5

$\tilde{C}$ $^2A_2$ C_{2v}
T_0=23358(35) gas PE[1–3,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CF_2 stretch	1050(5)	gas	PE	1–3,5
	4	CF_2 scissors	500(80)	gas	PE	1,3

$\tilde{B}$ $^2A_1$ C_{2v}
T_0=22938(35) gas PE[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CF_2 stretch	1054(5)	gas	PE	5

$\tilde{A}$ $^2B_1$ C_{2v}
T_0=15185(35) gas PE[1–3,5]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 stretch	2744m	Ar	IR	4
	2	CH_2 scissors	1150(5)	gas	PE	1–3,5
	3	CF_2 stretch	1162(5)	gas	PE	5
	4	CF_2 scissors	527H	gas	PE	5
b_1	6	CH_2 stretch	2854wm	Ar	IR	4
b_2	8	CH_2 wag	1408s	Ar	IR	4
	9	CF_2 stretch	1255vs	Ar	IR	4

$CD_2F_2^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CF_2 stretch	970(80)	gas	PE	3
	4	CF_2 scissors	500(80)	gas	PE	3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_2 stretch	2062m	Ar	IR	4
b_1	7		980w	Ar	IR	4
b_2	8	CD_2 wag	1063s	Ar	IR	4
	9	CF_2 stretch	1262vs	Ar	IR	4

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[1] A. W. Potts, H. J. Lempka, D. G. Streets, and W. C. Price, Philos. Trans. R. Soc. London, Ser. A **268**, 59 (1970).
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$CH_2Cl_2^+$

$\tilde{G}\ ^2A_1$ 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_0=28530(35) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CCl_2 stretch	541(5)	gas	PE	2

$\tilde{C}\ ^2A_2$ C_{2v}
T_0=7673(35) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4	CCl_2 scissors	297(5)	gas	PE	2

$\tilde{B}\ ^2A_1$ C_{2v}
T_0=6713(35) gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4	CCl_2 scissors	276(5)	gas	PE	2

$\tilde{A}\ ^2B_1$ C_{2v}
T_0=300(35) gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CCl_2 stretch	677(5)	gas	PE	2
	4	CCl_2 scissors	400(5)	gas	PE	2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CCl_2 stretch	713(5)	gas	PE	1,2

[a]From vertical ionization potential.

References

[1] A. W. Potts, H. J. Lempka, D. G. Streets, and W. C. Price, Philos. Trans. R. Soc. London, Ser. A **268**, 59 (1970).
[2] T. Pradeep and D. A. Shirley, J. Electron Spectrosc. Relat. Phenom. **66**, 125 (1993).

t-HSSSH

$\tilde{X}$ C_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SH a-stretch	2542	gas	IR	1
		SSH a-bend	860	gas	IR	1
		S_3 a-stretch	480	gas	IR	1

A=0.470; B=0.092; C=0.079 MW[1]

Reference

[1] M. Liedtke, A. H. Saleck, K. M. T. Yamada, G. Winnewisser, D. Kremer, E. Kraka, A. Dolgner, J. Hahn, and S. Dobos, J. Phys. Chem. **97**, 11204 (1993).

c-HSSSH

$\tilde{X}$ C_s
Estimated[4] to be 87 cm^{-1} (0.25 kcal/mol) higher in energy than *t*-HSSSH.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SH s-stretch	2548	gas	IR	4
		SSH a-bend	865	gas	IR	4
		S_3 a-stretch	480	gas	IR	4
		S_3 bend	240(30)	gas	MW	3

A=0.470; B=0.092; C=0.079 MW[1–4]

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[1] D. Mauer, G. Winnewisser, K. M. T. Yamada, J. Hahn, and K. Reinartz, Z. Naturforsch. A **43**, 617 (1988).
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8.10. Five-Atomic Monohydrides

FeC=C=CH

$\tilde{A}$
T_0=7260(630) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Fe=C stretch	670(150)	gas	PE	1

Reference

[1] J. Fan, L. Lou, and L.-S. Wang, J. Chem. Phys. **102**, 2701 (1995).

FeCCCH[a]

$\tilde{A}$ $C_{\infty v}$
T_0=6860(760) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Fe≡C stretch	880(150)	gas	PE	1

[a]Acetylenic bonding.

Reference

[1] J. Fan, L. Lou, and L.-S. Wang, J. Chem. Phys. **102**, 2701 (1995).

FeC=C=CH$^-$

Threshold for electron detachment from ground-state FeC=C=CH$^-$ =12700(500) gas PE[1]

Reference

[1] J. Fan, L. Lou, and L.-S. Wang, J. Chem. Phys. **102**, 2701 (1995).

FeCCCH$^-$ [a]

Threshold for electron detachment from ground-state FeCCCH$^-$ = 10250(650) gas PE[1]

[a]Acetylenic bonding.

Reference

[1] J. Fan, L. Lou, and L.-S. Wang, J. Chem. Phys. **102**, 2701 (1995).

C_4H

Absorptions between 250 and 300 nm which were attributed by Ref. 1 to C_4H have since been reassigned (D. Forney and J. P. Maier, private communication) to C_6H_2. Groups of absorptions observed in an argon matrix[1] between 13408 and 13906, 17629 and 17939, 21972 and 25667, and 26867 and 32104 are tentatively attributed to C_4H.

$\tilde{X}\ ^2\Sigma$ $C_{\infty v}$ Structure: MW[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3307.4w	Ar	IR	7
	2	C≡C stretch	2083.9wm	Ar	IR	7
	3	C≡C stretch	2063.7	Ne	IR	8
			2060.6ms	Ar	IR	1,7
Π	7	Skel. bend	131T	gas	MW	6

B_0=0.165 MW[2–5]

C_4D

An absorption at 17685 and a group of bands between 26925 and 30883 in the argon-matrix observations[1] are tentatively attributed to C_4D.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2579.3w	Ar	IR	7
	2	C≡C stretch	2056.5wm	Ar	IR	7
	3	C≡C stretch	2052.9	Ne	IR	8
			2049.6ms	Ar	IR	1,7

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[1] K. I. Dismuke, W. R. M. Graham, and W. Weltner, Jr., J. Mol. Spectrosc. **57**, 127 (1975).
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HCCCO

$\tilde{X}\ ^2A'$ C_s Structure: MW[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2		2308.6	Ar	IR	3

A_0=8.709(2); B_0=0.153; C_0=0.150 MW[1,2]

DCCCO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2		2287.4	Ar	IR	3

A_0=8.488(3); B_0=0.142; C_0=0.139 MW[2]

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HCCCS

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$
B_0=0.090 MW[1]

DCCCS

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$
B_0=0.084 MW[1]

Reference

[1] Y. Hirahara, Y. Ohshima, and Y. Endo, J. Chem. Phys. **101**, 7342 (1994).

$HCSCN^+$

$\tilde{E}\ ^2A'$ C_s
T^a = 41100(1200) gas PE[1]

$\tilde{D}\ ^2A''$ C_s
T^a = 32300(1200) gas PE[1]

$\tilde{C}\ ^2A'$ C_s
T_0=29000(1200) gas PE[1]

$\tilde{B}\ ^2A'$ C_s
T_0=21800(1200) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1900T	gas	PE	1

$\tilde{A}\ ^2A''$ C_s
T^a=13700(1200) gas PE[1]

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

[a]From vertical ionization potential.

Reference

[1] G. Pfister-Guillouzo, F. Gracian, A. Senio, F. Bourdon, Y. Vallée, and J.-L. Ripoll, J. Am. Chem. Soc. **115**, 324 (1993).

HCOCN

$\tilde{A}\ ^1A''$ C_s
T_0=26283.396 gas LF[1,4,6]AB[4] $\tilde{A}-\tilde{X}$ 345–385 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CO stretch	1308	gas	LF	1,6
	4	HCO bend	1121	gas	LF	1,6
	5	CC stretch	943	gas	LF	1,6
	6	CCO bend	530	gas	LF	1,6
	7	CCN bend	217	gas	LF	1,6
a''	8	Bend	418	gas	LF	1,6
	9	Bend	376	gas	LF	1,6

A_0=1.957; B_0=0.169; C_0=0.154 AB,LF[4]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	2892m	gas	IR	5
	2	C≡N stretch	2229m	gas	IR,EM	2,5,6
	3	C=O stretch	1716s	gas	IR,EM	2,5,6
	4	CH rock	1383	gas	IR	5
	5	C-C stretch	914ms	gas	IR,EM	2,5,6
	6	CCO bend	626vw	gas	IR	5
	7	CCN bend	230	gas	LF,IR	1,2,6
a''	8	CH wag	960	gas	EM	6
	9	CCN bend	278	gas	LF,EM	1,6

A_0=2.251; B_0=0.167; C_0=0.155 MW[3,7]

DCOCN

$\tilde{A}\ ^1A''$ C_s
T_0=26335.6 gas LF[6] $\tilde{A}-\tilde{X}$ 345–380 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CD stretch	2232	gas	LF	6
	3	CO stretch	1279	gas	LF	6
	4	CC stretch	931	gas	LF	6
	5	CD rock	732	gas	LF	6
	6	CCO bend	527	gas	LF	6
	7	CCN bend	214	gas	LF	6
a''	8	Bend	406	gas	LF	6
	9	Bend	315	gas	LF	6

A^a=1.561; B^a=0.169; C^a=0.152 LF[6]

$\tilde{X}\ ^1A'$ C_s
A_0=1.737; B_0=0.168; C_0=0.152 LF[6]

[a]From analysis of 9_0^1 band.

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HCSCN

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CN stretch	2221	Ar	IR	2
	3	CH rock	1320	Ar	IR	2
	4	CS stretch	1103	Ar	IR	2
	5	CC stretch	889	Ar	IR	2
a''	8	CH wag	824	Ar	IR	2

A_0=1.445; B_0=0.107; C_0=0.099 MW[1]

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cyc-C_3HCl

In an argon matrix, weak absorption maxima at 37000 (270 nm) and 38500 (260 nm) have been attributed[1] to *cyc*-C_3HCl. Exposure of the molecule to 254 nm radiation results in its isomerization to HCCCCl and HClC=C=C:.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	3139.2w	Ar	IR	1
	2	Ring	1687.0m	Ar	IR	1
	3	Ring	1283.4wm	Ar	IR	1
	4	Ring	1059.7vs	Ar	IR	1
	5	CH deform.	897.2w	Ar	IR	1
	6	CCl stretch	580.5wm	Ar	IR	1
a''	8	CH deform.	883.7wm	Ar	IR	1

Reference

[1] G. Maier, T. Preiss, H. P. Reisenauer, B. A. Hess, Jr., and L. J. Schaad, J. Am. Chem. Soc. **116**, 2014 (1994).

HCCCCl

In an argon matrix, HCCCCl possesses broad, overlapping absorption maxima in the 270–300 nm spectral region.[1] Irradiation in that spectral region results in isomerization to ***cyc***-C_3HCl.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	3305.5s	Ar	IR	1
	2	C=C stretch	1983.0s	Ar	IR	1
	3	C-C stretch	1054.4vs	Ar	IR	1
	4	CCl stretch	725.1vs	Ar	IR	1
	5	CH deform.	475.4m	Ar	IR	1
a''	8	CH deform.	511.5wm	Ar	IR	1

Reference

[1] G. Maier, T. Preiss, H. P. Reisenauer, B. A. Hess, Jr., and L. J. Schaad, J. Am. Chem. Soc. **116**, 2014 (1994).

HClC=C=C:

In an argon matrix, HClC=C=C: possesses broad, overlapping absorption maxima in the 270–300 nm spectral region.[1] Irradiation in that spectral region results in isomerization to *cyc*-C_3HCl.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	3103.5vw	Ar	IR	1
	2	C_3 a-stretch	1967.6vs	Ar	IR	1
	3	CH deform.	1293.0w	Ar	IR	1
	4	C_3 s-stretch	1146.5w	Ar	IR	1
	5	CCl stretch	794.1ms	Ar	IR	1
a''	8	CH deform.	839.9vw	Ar	IR	1

Reference

[1] G. Maier, T. Preiss, H. P. Reisenauer, B. A. Hess, Jr., and L. J. Schaad, J. Am. Chem. Soc. **116**, 2014 (1994).

HFCCO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	3025.9	Xe	IR	3
	2	CO stretch	2142.2vs	Xe	IR	3
	3		1383.0m	Xe	IR	3
	4		1168.0m	Xe	IR	3
	5		1031.5w	Xe	IR	3
	7	Deformation	150(10)T	gas	MW	2
a''	8	HFCC OPLA	500(50)T	gas	MW	2
			755	Xe	IR	3
	9	CCO bend	380(40)T	gas	MW	2
			525.5w	Xe	IR	3

A_0=1.795; B_0=0.154; C_0=0.142 MW[1]

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$CF_2{=}NH^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		C=N stretch	1480(40)	gas	PE	1

Reference

[1] G. Pawelke, R. Dammel, and W. Poll, Z. Naturforsch. B **47**, 351 (1992).

$CF_2{=}NH$

$\tilde{X}$ C_s Structure: MW[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH stretch	3402.3m	gas	IR	1,5
			3388.4m	Ar	IR	5,6
	2	C=N stretch	1785.2vs	gas	IR	1,5
			1777.2vs	Ar	IR	5,6
	3	CF_2 a-stretch	1307vs	gas	IR	1,5
			1294.9vs	Ar	IR	5,6
	4	CNH deform.	1031.2s	gas	IR	1,5
			1027.0s	Ar	IR	5,6
	5	CF_2 s-stretch	947.2s	gas	IR	1,5
			941.9s	Ar	IR	5,6
	6	CF_2 scissors	572.7vw	Ar	IR	5,6
	7	CF_2 rock	542.0m	gas	IR	1,5
			541.4m	Ar	IR	5,6
a''	8	Torsion	831.65s	gas	IR	1,4,5
			827.8s	Ar	IR	5,6
	9	F_2CN OPLA	695.2w	gas	IR	1,5
			694.3w	Ar	IR	5,6

A_0=0.382; B_0=0.372; C_0=0.188 MW[2,3]

$CF_2{=}ND$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ND stretch	2519.3m	gas	IR	1,5
			2508.2m	Ar	IR	5,6
	2	CN stretch	1780.0vs	gas	IR	1,5
			1771.9vs	Ar	IR	5,6
	3	CF_2 a-stretch	1280vs	gas	IR	1,5
			1266.8vs	Ar	IR	5,6
	4	CF_2 s-stretch	954.0m	gas	IR	1,5
			951.5m	Ar	IR	5,6
	5	CND deform.	836.0s	gas	IR	1,5
			832.7s	Ar	IR	5,6
	6	CF_2 scissors	563.7vw	Ar	IR	5,6
	7	CF_2 rock	491.8m	gas	IR	1,5
			491.5m	Ar	IR	5,6
a''	8	F_2CN OPLA	705.1m	gas	IR	1,5
			702.4m	Ar	IR	5,6
	9	Torsion	613.9w	gas	IR	1,5
			612.1w	Ar	IR	5,6

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$HONO_2$

In the gas phase, continuous absorption begins near 330 nm, with a maximum near 38500 (260 nm), then increasing absorption out to the 190 nm observation limit.[4,5,31] Between 330 and 220 nm, photodissociation to $OH+NO_2$ predominates.[6,16,33,39] However, at 193 nm photodissociation to HONO+O is the major process.[33] Vacuum ultraviolet spectral observations[7,12] show an absorption maximum near 54900 (182 nm), a more prominent maximum near 73500 (136 nm), and overlapping absorption bands at higher energies. The onset of the photoproduction of OH ($A\ ^2\Sigma$)+NO_2 has been observed[12] at 68000 (147.5 nm).

$\tilde{X}$		C_s	Structure: MW[1,3,43]			
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3550.0m	gas	IR	2
			3522.3	Ar	IR	28
			3519.3			
			3491.8	N_2	IR	8,36
	2	NO_2 a-stretch	1709.57vs	gas	IR,DL LS	2,9,11,20, 21,23,35
			1699.4	Ar	IR	28
			1696.2			
			1698.3	N_2	IR	8,36
	3	Mixed	1325.74s	gas	IR,DL	2,19,26, 27,40,41
			1321.4	Ar	IR	28
			1318.7			
			1346.1	N_2	IR	8,36
	4	Mixed	1303.52vs	gas	IR,DL	2,26,27, 40,41
			1304.4	Ar	IR	28
			1311.9	N_2	IR	8,36
	5	ON stretch	879.11s	gas	IR,DL	2,18,32, 34,37,40, 41
			896.9	Ar	IR	2
			889.5			
			903.1	N_2	IR	8,36
	6	NO_2 scissors	646.83w	gas	IR	2,25,46
			656.6	Ar	IR	36
			664.1	N_2	IR	8,36
	7	NO_2 rock	580.30w	gas	IR	2,25,44
			588.0	Ar	IR	36
			597.5	N_2	IR	8,36
a''	8	ONO_2 OPLA	763.15s	gas	IR	2,25,44, 45
			763.6	Ar	IR	28
			767.7	N_2	IR	8,36
	9	Torsion	458.23m	gas	IR	2,15,24
			479	N_2	IR	8

A_0=0.434; B_0=0.404; C_0=0.209 MW[1,10,13,14,17,22]IR[11,24,25]

$DONO_2$

$\tilde{X}$		C_s				
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2621.5m	gas	IR	2
			2601.5	Ar	IR	36
			2599.1			
			2576.5	N_2	IR	8,36
	2	NO_2 a-stretch	1688.36vs	gas	IR	2,42
			1678.6	Ar	IR	36
			1674.9			
			1669.2	N_2	IR	8,36
	3	NO_2 s-stretch	1308.4vs	gas	IR	2
			1310.4	Ar	IR	36
			1311.1	N_2	IR	8,36
	4	DON bend	1013.6m	gas	IR	2
			1013.4	Ar	IR	36
			1012.2			
			1032.4	N_2	IR	8,36
	5	ON stretch	888.0s	gas	IR	2
			894.2	Ar	IR	36
			884.5			
			906.0	N_2	IR	8,36
	6	NO_2 scissors	642.14s	gas	IR	2,38
			660	N_2	IR	8
	7	NO_2 rock	541.58w	gas	IR	2,38
			559.9	N_2	IR	8,36
a''	8	ONO_2 OPLA	762.87s	gas	IR	2,29
			763.7	Ar	IR	36
			767.7	N_2	IR	8,36
	9	Torsion	343.85m	gas	IR	2,15,30
			361	N_2	IR	8

A_0=0.433; B_0=0.377; C_0=0.201 MW[1,43]IR[38]

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[46] T. L. Tan, W. F. Wang, E. C. Looi, and P. P. Ong, Spectrochim. Acta A **52**, 1315 (1996).

c,c-HOONO

In an argon matrix, an absorption maximum near 36400 (275 nm) nas been assigned[2] to *c,c*-HOONO.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OH stretch	3285.4	Ar	IR	1,2
	2	N=O stretch	1600.3	Ar	IR	1,2
	3	HOO bend	1395.0	Ar	IR	1,2
	4	OO stretch	927.2	Ar	IR	1,2
	5	ONO bend	794.3	Ar	IR	1,2
	6	N-O stretch	629.1	Ar	IR	1,2

c,c-DOONO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OD stretch	2434.4	Ar	IR	1
	2	N=O stretch	1594.1	Ar	IR	1
	3	DOO bend	1091.9	Ar	IR	1
	4	OO stretch	927.2	Ar	IR	1
	5	ONO bend	792.5	Ar	IR	1
	6	N-O stretch	630.8	Ar	IR	1

References

[1] W.-J. Lo and Y.-P. Lee, J. Chem. Phys. **101**, 5494 (1994).
[2] W.-J. Lo and Y.-P. Lee, Chem. Phys. Lett. **229**, 357 (1994).

t,perp-HOONO

In an argon matrix, an absorption maximum near 45500 (220 nm) nas been assigned[3] to *t,perp*-HOONO.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OH stretch	3545.5w	Ar	IR	1–3
			3563.3[a]	Ar	IR	1–3
			3541.7	N_2	IR	1,2
	2	N=O stretch	1703.6s	Ar	IR	1–3
			1708.3[a]	Ar	IR	1–3
			1701.4	N_2	IR	1,2
	3	HOO bend	1364.4m	Ar	IR	1–3
			1372.7[a]	Ar	IR	1–3
			1394.9	N_2	IR	1,2
	4	OO stretch	952.0m	Ar	IR	1–3
			957.4[a]	Ar	IR	1–3
			960.5	N_2	IR	1,2
	5	ONO bend	772.8m	Ar	IR	1–3
			782.9[a]	Ar	IR	1–3
			793.6	N_2	IR	1,2

t,perp-DOONO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OD stretch	2615.4	Ar	IR	1,2
			2633.5[a]	Ar	IR	1,2
			2622.3	N_2	IR	2
	2	N=O stretch	1703.7	Ar	IR	1,2
			1708.3[a]	Ar	IR	1,2
			1701.8	N_2	IR	2
	3	DOO bend	1089.7	Ar	IR	1,2
			1091.7[a]	Ar	IR	1,2
			1090.7	N_2	IR	2
	4	OO stretch	950.3	Ar	IR	1,2
			955.7[a]	Ar	IR	1,2
			957.3	N_2	IR	2
	5	ONO bend	772.1	Ar	IR	1,2
			782.0[a]	Ar	IR	1,2
			790.3	N_2	IR	2

[a]Less stable matrix site.

References

[1]B.-M. Cheng, J.-W. Lee, and Y.-P. Lee, J. Phys. Chem. **95**, 2814 (1991).
[2]W.-J. Chen, W.-J. Lo, B.-M. Cheng, and Y.-P. Lee, J. Chem. Phys. **97**, 7167 (1992).
[3]W.-J. Lo and Y.-P. Lee, Chem. Phys. Lett. **229**, 357 (1994).

$HSPS_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SH stretch	2571.3	Ar	IR	1
		Mixed	861.2	Ar	IR	1
		Mixed	765.7	Ar	IR	1
		Mixed	647.2	Ar	IR	1

$DSPS_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SD stretch	1860.3	Ar	IR	1
		Mixed	813.6	Ar	IR	1
		Mixed	687.4	Ar	IR	1

Reference

[1]Z. Mielke and L. Andrews, J. Phys. Chem. **97**, 4313 (1993).

$HCFClBr^+$

$\tilde{F},\tilde{G}$
T^a=51600(500) gas PE[1]

$\tilde{E}$
T^a=26700(400) gas PE[1]

$\tilde{D}$
T^a=23100(400) gas PE[1]

$\tilde{C}$
T^a=11600(400) gas PE[1]

$\tilde{B}$
T^a=7180(300) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1120(50)	gas	PE	1

$\tilde{A}$
T^a=2660(400) gas PE[1]

[a]From vertical ionization potentials.

Reference

[1]I. Novak, S. C. Ng, and A. W. Potts, Chem. Phys. Lett. **215**, 561 (1993).

8.11. Five-Atomic Nonhydrides

FeC_4^-

Threshold for electron detachment from ground-state $FeC_4^- \leqslant 17800(1600)$ gas PE[1]

Reference

[1]J. Fan, L. Lou and L.-S. Wang, J. Chem. Phys. **102**, 2701 (1995).

C_5

T_0=41967(35)T Ne AB[13] 220–240 nm
44228T Ar AB[8] 211–226 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1813	Ar	AB	8
			695(40)	Ne	AB	13
			654	Ar	AB	8

$^1\Pi_u$ $D_{\infty h}$
T_0=19599(8) Ne AB[13] $^1\Pi_u-\tilde{X}$ 490–510 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			697(10)	Ne	AB	13
			542(10)	Ne	AB	13
			286(10)	Ne	AB	13

$\tilde{X}$ $^1\Sigma_g^-$ $D_{\infty h}$ Structure: ESR[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	2	Sym. stretch	779(10)	gas	TPE	9,10
			776T	Ar	IR	15
Σ_u^+	3	Asym. stretch	2169.441	gas	IR,DL	4–7
			2166.4	Ne	IR	2,12,13
			2164	Ar	IR	1–3
			2157.0	Kr	IR	15
			2164.5	H_2	IR	14
	4	Asym. stretch	1444.3	Ne	IR	12
			1446.6	Ar	IR	11
			1443.2	Kr	IR	15
Π_g	5	Bend	218(13)T	gas	DL,TPE	7,9,10
Π_u	6	Bend	535(10)	gas	TPE	9,10
Π_u	7	Bend	118(3)T	gas	DL,TPE	7,9,10

B_0=0.0853 IR[4]DL[5–7]

References

[1]K. R. Thompson, R. L. DeKock, and W. Weltner, Jr., J. Am. Chem. Soc. **93**, 4688 (1971).
[2]W. R. M. Graham, K. I. Dismuke, and W. Weltner, Jr., Astrophys. J. **204**, 301 (1976).
[3]M. Vala, T. M. Chandrasekhar, J. Szczepanski, R. Van Zee, and W. Weltner, Jr., J. Chem. Phys. **90**, 595 (1989).
[4]P. F. Bernath, K. H. Hinkle, and J. J. Keady, Science **244**, 562 (1989).
[5]N. Moazzen-Ahmadi, A. R. W. McKellar, and T. Amano, Chem. Phys. Lett. **157**, 1 (1989).
[6]J. R. Heath, A. L. Cooksy, M. H. W. Gruebele, C. A. Schmuttenmaer, and R. J. Saykally, Science **244**, 564 (1989).

[7] N. Moazzen-Ahmadi, A. R. W. McKellar, and T. Amano, J. Chem. Phys. **91**, 2140 (1989).
[8] J. Szczepanski and M. Vala, J. Phys. Chem. **95**, 2792 (1991).
[9] T. N. Kitsopoulos, C. J. Chick, Y. Zhao, and D. M. Neumark, J. Chem. Phys. **95**, 5479 (1991).
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[11] R. H. Kranze and W. R. M. Graham, J. Chem. Phys. **96**, 2517 (1992).
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[14] M. Miki, T. Wakabayashi, T. Momose, and T. Shida, J. Phys. Chem. **100**, 12135 (1996).
[15] J. Szczepanski, S. Ekern, C. Chapo, and M. Vala, Chem. Phys. **211**, 359 (1996).

C_4Si

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CC stretch	2095.46	gas	DL	3
			2080.1	Ar	IR	2

B_0=0.051 MW[1]DL[3]

References

[1] M. Ohishi, N. Kaifu, K. Kawaguchi, A. Murakami, S. Saito, S. Yamamoto, S. Ishikawa, Y. Fujita, Y. Shiratori, and W. M. Irvine, Astrophys. J. **345**, L83 (1989).
[2] P. A. Withey and W. R. M. Graham, J. Chem. Phys. **96**, 4068 (1992).
[3] A. Van Orden, R. A. Provencal, T. F. Giesen, and R. J. Saykally, Chem. Phys. Lett. **237**, 77 (1995).

SiCCCSi

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	C_3 stretch	1968.19	gas	DL	2
			1955.2vs	Ar	IR	1
	4	SiC stretch	898.9w	Ar	IR	1

B_0=0.0316 DL[2]

References

[1] J. D. Presilla-Márquez and W. R. M. Graham, J. Chem. Phys. **100**, 181 (1994).
[2] A. Van Orden, T. F. Giesen, R. A. Provencal, H. J. Hwang, and R. J. Saykally, J. Chem. Phys. **101**, 10237 (1994).

Si_3C_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	''Breathing''	681.1	Ar	IR	1
b_2	7	SiC a-str.	956.7	Ar	IR	1
	8	CSiC a-stretch	597.8	Ar	IR	1

Reference

[1] J. D. Presilla-Márquez, C. M. L. Rittby, and W. R. M. Graham, J. Chem. Phys. **104**, 2818 (1996).

C_5^-

Threshold for electron detachment from ground-state C_5^-=23020(10) gas TPE[1]PE[2]

$\tilde{B}$ $^2\Pi_g$ $D_{\infty h}$
T_0=27847(15) Ne AB[6] $\tilde{B}-\tilde{X}$ 311–360 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		1756(17)	Ne	AB	6
	2		724(16)	Ne	AB	6

$\tilde{A}$ $^2\Pi_g$ $D_{\infty h}$
T_0=20200T gas MPD[3] $\tilde{A}-\tilde{X}$ 470–500 nm
20200(8) Ne AB[6] $\tilde{A}-\tilde{X}$ 457–495 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		1679(9)	Ne	AB	6
	2		718(43)	gas	MPD	3
			737(8)	Ne	AB	6

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	1822.3	Ne	IR	5
			1831.8	Ar	IR	4
Π_u	7	Bend	200T	gas	TPE	1

A=22T gas TPE[1]

References

[1] T. N. Kitsopoulos, C. J. Chick, Y. Zhao, and D. M. Neumark, J. Chem. Phys. **95**, 5479 (1991).
[2] D. W. Arnold, S. E. Bradforth, T. N. Kitsopoulos, and D. M. Neumark, J. Chem. Phys. **95**, 8753 (1991).
[3] M. Ohara, H. Shiromaru, Y. Achiba, K. Aoki, K. Hashimoto, and S. Ikuta, J. Chem. Phys. **103**, 10393 (1995).
[4] J. Szczepanski, S. Ekern, and M. Vala, J. Phys. Chem. A **101**, 1841 (1997).
[5] P. Freivogel, M. Grutter, D. Forney, and J. P. Maier, Chem. Phys. **216**, 401 (1997).
[6] D. Forney, M. Grutter, P. Freivogel, and J. P. Maier, J. Phys. Chem. A **101**, 5292 (1997).

$Be(CO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1975.3	Ar	IR	1
			609.6	Ar	IR	1

Reference

[1] L. Andrews, T. J. Tague, Jr., G. P. Kushto, and R. D. Davy, Inorg. Chem. **34**, 2952 (1995).

NNBeNN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NN stretch	1823.4	Ar	IR	1

Reference

[1] C. A. Thompson, L. Andrews, and R. D. Davy, J. Phys. Chem. **99**, 7913 (1995).

NN(*cyc*-BeN_2)

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1691.8	Ar	IR	1
			1682.9	N_2	IR	1
			928.4	N_2	IR	1

Reference

[1] C. A. Thompson, L. Andrews, and R. D. Davy, J. Phys. Chem. **99**, 7913 (1995).

OBeOBeO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1482.5T	Ne	IR	1,2
			1465.1T	Ar	IR	1,2

References

[1] C. A. Thompson and L. Andrews, J. Chem. Phys. **100**, 8689 (1994).
[2] L. Andrews, G. V. Chertihin, C. A. Thompson, J. Dillon, S. Byrne, and C. W. Bauschlicher, Jr., J. Phys. Chem. **100**, 10088 (1996).

Fe_2O_3

$\tilde{A}$

T_0=2020(400) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			650(80)	gas	PE	1

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			810(100)	gas	PE	1

Reference

[1] H. Wu, S. R. Desai, and L.-S. Wang, J. Am. Chem. Soc. **118**, 5296 (1996).

Cu_2O_3

$\tilde{B}$

T_0=6290(400) gas PE[1]

$\tilde{A}$

T_0=3870(400) gas PE[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			640T	gas	PE	1

Reference

[1] L.-S. Wang, H. Wu, S. R. Desai, and L. Lou, Phys. Rev. B **53**, 8028 (1996).

C_4O

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2221.7vs	Ar	IR	1
			1922.7s	Ar	IR	1
			1431.5wm	Ar	IR	1
			774.8w	Ar	IR	1
			484.0wm	Ar	IR	1

B_0=0.078 MW[2]

References

[1] G. Maier, H. P. Reisenauer, U. Schäfer, and H. Balli, Angew. Chem. **100**, 590 (1988); Angew. Chem. Int. Ed. Engl. **27**, 566 (1988).
[2] Y. Ohshima, Y. Endo, and T. Ogata, J. Chem. Phys. **102**, 1493 (1995).

C_4S

$\tilde{B}$

$T_0 \cong$ 41700 Ar AB[1]

$\tilde{A}$

T_0=22220 Ar AB[1] $\tilde{A}-\tilde{X}$ 380–450 nm

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1757	Ar	IR	1

B_0=0.051 MW[2]

References

[1] G. Maier, J. Schrot, and H. P. Reisenauer, Chem. Ber. **124**, 2613 (1991).
[2] Y. Hirahara, Y. Ohshima, and Y. Endo, Astrophys. J. **408**, L113 (1993).

$C(CN)_2$

In an argon matrix, two overlapping series of relatively sharp absorptions between 280 and 360 nm, with spacings of 1650–1870 cm^{-1}, as well as weak, broad absorptions at 21300 (470 nm) and 26500 (377 nm), have been attributed[2] to $C(CN)_2$.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1916w	Ar	IR	2
			1826w	Ar	IR	2
		CN a-stretch	1756m	Ar	IR	1,2
		C_3 a-stretch	1158wT	Ar	IR	1
		CCN deform.	392wT	Ar	IR	1

References

[1] W. H. Smith and G. E. Leroi, Spectrochim. Acta A **25**, 1917 (1969).
[2] I. R. Dunkin and A. McCluskey, Spectrochim. Acta A **50**, 209 (1994).

$Fe_2O_3^-$

Threshold for electron detachment from ground-state $Fe_2O_3^-$ =24690(320) gas PE[1]

Reference

[1] H. Wu, S. R. Desai, and L.-S. Wang, J. Am. Chem. Soc. **118**, 5296 (1996).

$Cu_2O_3^-$

Threshold for electron detachment from ground-state $Cu_2O_3^-$ =28560(240) gas PE[1]

Reference

[1] L.-S. Wang, H. Wu, S. R. Desai, and L. Lou, Phys. Rev. B **53**, 8028 (1996).

$NCCNO^+$

$\tilde{D}$ $^2\Sigma^+$ $C_{\infty v}$
T^a=60270(430) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+			1030(150)	gas	PE	1

$\tilde{C}$ $^2\Pi$ $C_{\infty v}$
T^a=46800(430) gas PE[1]

$\tilde{B}$ $^2\Sigma^+$ $C_{\infty v}$
T^a=22750(280) gas PE[1]

$\tilde{A}$ $^2\Pi$ $C_{\infty v}$
T^a=20740(280) gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+			2200(150)	gas	PE	1
			1630(150)	gas	PE	1

[a]From vertical ionization potentials.

Reference

[1] T. Pasinszki and N. P. C. Westwood, J. Phys Chem. **100**, 16856 (1996).

c-LiOONO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	N=O stretch	1423.4	Ar	IR	1
			1422.0			
	2	Mixed	966.2	Ar	IR	1
	3	NO stretch	874.2	Ar	IR	1
	4	OO stretch	792.3	Ar	IR	1
	5	LiO stretch	642.5	Ar	IR	1

Reference

[1] W.-J. Lo, Y.-P. Lee, J.-H. M. Tsai, H.-H. Tsai, T. P. Hamilton, J. G. Harrison, and J. S. Beckman, J. Chem. Phys. **103**, 4026 (1995).

t-LiOONO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	N=O stretch	1581.6	Ar	IR	1
			1580.4			
		Mixed	998.3	Ar	IR	1
			995.6			
		LiO stretch	647.7	Ar	IR	1
			645.0			
		OO stretch	600.4	Ar	IR	1

Reference

[1] W.-J. Lo, Y.-P. Lee, J.-H. M. Tsai, H.-H. Tsai, T. P. Hamilton, J. G. Harrison, and J. S. Beckman, J. Chem. Phys. **103**, 4026 (1995).

c-NaOONO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	N=O stretch	1437.4	Ar	IR	1
			1434.6			
	2	Mixed	961.4	Ar	IR	1
	3	NO stretch	840.7	Ar	IR	1
	4	OO stretch	770.9	Ar	IR	1
			768.7			

Reference

[1] W.-J. Lo, Y.-P. Lee, J.-H. M. Tsai, H.-H. Tsai, T. P. Hamilton, J. G. Harrison, and J. S. Beckman, J. Chem. Phys. **103**, 4026 (1995).

t-NaOONO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	N=O stretch	1549.3	Ar	IR	1
			1540.6			
		Mixed	996.3	Ar	IR	1
			994.1			
		OO stretch	609.4	Ar	IR	1
			607.4			

Reference

[1] W.-J. Lo, Y.-P. Lee, J.-H. M. Tsai, H.-H. Tsai, T. P. Hamilton, J. G. Harrison, and J. S. Beckman, J. Chem. Phys. **103**, 4026 (1995).

c-KOONO

In an argon matrix,[2] a broad absorption (~70 nm, fwhm) with maximum near 30800 (325 nm) has been assigned to *c*-KOONO. Irradiation in the spectral region of this band leads to the formation of KNO_3.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	N=O stretch	1444.5	Ar	IR	1
	2	Mixed	952.3	Ar	IR	1
	3	NO stretch	831.6	Ar	IR	1
	4	OO stretch	749.1	Ar	IR	1

References

[1] W.-J. Lo, Y.-P. Lee, J.-H. M. Tsai, H.-H. Tsai, T. P. Hamilton, J. G. Harrison, and J. S. Beckman, J. Chem. Phys. **103**, 4026 (1995).
[2] W.-J. Lo, Y.-P. Lee, J.-H. M. Tsai, and J. S. Beckman, Chem. Phys. Lett. **242**, 147 (1995).

t-KOONO

In an argon matrix,[2] a broad absorption (~70 nm, fwhm) with maximum near 26700 (375 nm) has been assigned to *t*-KOONO. Irradiation in the spectral region of this band leads to the formation of KNO_3.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	N=O stretch	1528.4	Ar	IR	1
		Mixed	987.4	Ar	IR	1
		OO stretch	602.2	Ar	IR	1

References

[1] W.-J. Lo, Y.-P. Lee, J.-H. M. Tsai, H.-H. Tsai, T. P. Hamilton, J. G. Harrison, and J. S. Beckman, J. Chem. Phys. **103**, 4026 (1995).
[2] W.-J. Lo, Y.-P. Lee, J.-H. M. Tsai, and J. S. Beckman, Chem. Phys. Lett. **242**, 147 (1995).

$NNBeO_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			928.9	N_2	IR	1

Reference

[1] L. Andrews, G. V. Chertihin, C. A. Thompson, J. Dillon, S. Byrne, and C. W. Bauschlicher, Jr., J. Phys. Chem. **100**, 10088 (1996).

O_2TiCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1887.7	Ar	IR	1

Reference

[1] G. V. Chertihin and L. Andrews, J. Am. Chem. Soc. **117**, 1595 (1995).

O_2TiN_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NN stretch	1901.3	Ar	IR	1
			909.4	Ar	IR	1

Reference

[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. **98**, 5891 (1994).

N_2FeO_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NN stretch	2271.3	Ar	IR	1
			1002.0	Ar	IR	1

Reference

[1] G. V. Chertihin, W. Saffel, J. T. Yustein, L. Andrews, M. Neurock, A. Ricca, and C. W. Bauschlicher, Jr., J. Phys. Chem. **100**, 5261 (1996).

O_2UCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1893.4	Ar	IR	1
		UO_2 a-stretch	870.9	Ar	IR	1

Reference

[1] T. J. Tague, Jr., L. Andrews, and R. D. Hunt, J. Phys. Chem. **97**, 10920 (1993).

Al_2O_3

$\tilde{B}$

T_0=9600(640) gas PE[2]

$\tilde{A}$

T_0=4920(160) gas PE[2]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1211.2	Ar	IR	1
		Sym. stretch	850(80)	gas	PE	2

References

[1] L. Andrews, T. R. Burkholder, and J. T. Yustein, J. Phys. Chem. **96**, 10182 (1992).
[2] S. R. Desai, H. Wu, C. M. Rohlfing, and L.-S. Wang, J. Chem. Phys. **106**, 1309 (1997).

Al_2S_3

$\tilde{X}$

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

Reference

[1] B. S. Ault, J. Phys. Chem. **98**, 77 (1994).

NCCNO

In the gas phase, absorption has been observed[3] between 210 and 290 nm, with a maximum at 251.7 nm (39730).

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ	1	CNO a-stretch	2328vs	gas	IR	3
			2356vs	Ar	IR	1
	2	CN stretch	2192m	gas	IR	3
			2192w	Ar	IR	1
	3	CNO s-stretch	1442s	gas	IR	3
			1445wm	Ar	IR	1
	4	CC stretch	714.75vw	gas	IR	2,3
			717vw	Ar	IR	1
Π	5	CNO bend	422T	gas	IR	3
	6	NCC bend	403.93w	gas	IR	2,3
			407vw	Ar	IR	1
	7	CCN bend	86T	gas	IR	3

B_0=0.077 IR^2MW^4

References

[1] G. Maier and J. H. Teles, Angew. Chem. **99**, 152 (1987); Angew. Chem. Int. Ed. Engl. **26**, 155 (1987).
[2] B. Guo, T. Pasinszki, N. P. C. Westwood, K. Zhang, and P. F. Bernath, J. Chem. Phys. **105**, 4457 (1996).
[3] T. Pasinszki and N. P. C. Westwood, J. Phys. Chem. **100**, 16856 (1996).
[4] Th. Brupbacher, R. K. Bohn, W. Jäger, M. C. L. Gerry, T. Pasinszki, and N. P. C. Westwood, J. Mol. Spectrosc. **181**, 316 (1997).

$Al_2O_3^-$

Threshold for electron detachment from ground-state $Al_2O_3^-$=29930(240) gas PE[1]

Reference

[1] S. R. Desai, H. Wu, C. M. Rohlfing, and L.-S. Wang, J. Chem. Phys. **106**, 1309 (1997).

O_2BeO_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1307.4	Ar	IR	1,2

References

[1] C. A. Thompson and L. Andrews, J. Chem. Phys. **100**, 8689 (1994).
[2] L. Andrews, G. V. Chertihin, C. A. Thompson, J. Dillon, S. Byrne, and C. W. Bauschlicher, Jr., J. Phys. Chem. **100**, 10088 (1996).

O_2MgO_2

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

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

References

[1] L. Andrews and J. T. Yustein, J. Phys. Chem. **97**, 12700 (1993).
[2] L. Andrews, G. V. Chertihin, C. A. Thompson, J. Dillon, S. Byrne, and C. W. Bauschlicher, Jr., J. Phys. Chem. **100**, 10088 (1996).

O_2CaO_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			494.4	Ar	IR	1,2
			449.5	N_2	IR	2

References

[1] L. Andrews, J. T. Yustein, C. A. Thompson, and R. D. Hunt, J. Phys. Chem. **98**, 6514 (1994).
[2] L. Andrews, G. V. Chertihin, C. A. Thompson, J. Dillon, S. Byrne, and C. W. Bauschlicher, Jr., J. Phys. Chem. **100**, 10088 (1996).

(*cyc*-O_2Fe)O_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1095.4	Ar	IR	1
			1097.6	O_2	IR	1
			968.9	Ar	IR	1
			970.2	O_2	IR	1

Reference

[1] G. V. Chertihin, W. Saffel, J. T. Yustein, L. Andrews, M. Neurock, A. Ricca, and C. W. Bauschlicher, Jr., J. Phys. Chem. **100**, 5261 (1996).

(*cyc*-O_2Fe)OO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1421	Ar	IR	1
			1413.4	O_2	IR	1
			1390	Ar	IR	1
			1368.4	O_2	IR	1
			1174.7	Ar	IR	1
			1166.6	O_2	IR	1

Reference

[1] G. V. Chertihin, W. Saffel, J. T. Yustein, L. Andrews, M. Neurock, A. Ricca, and C. W. Bauschlicher, Jr., J. Phys. Chem. **100**, 5261 (1996).

O_2RhO_2

$\tilde{X}$ D_{2d} Structure: IR[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	1048	Ar	IR	1
			1045	Xe	IR	1
			1038	O_2	IR	1

Reference

[1] A. J. L. Hanlan and G. A. Ozin, Inorg. Chem. **16**, 2848 (1977).

O_2NiO_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	1063.9	Ar	IR	1,2

References

[1] H. Huber, W. Klotzbücher, G. A. Ozin, and A. Vander Voet, Can. J. Chem. **51**, 2722 (1973).
[2] A. Citra, G. V. Chertihin, L. Andrews, and M. Neurock, J. Phys. Chem. A **101**, 3109 (1997).

O_2PdO_2

$\tilde{X}$ D_{2d} Structure: IR[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	1110.8	Ar	IR	1
		PdO stretch	504w	Ar	IR	1

Reference

[1] H. Huber, W. Klotzbücher, G. A. Ozin, and A. Vander Voet, Can. J. Chem. **51**, 2722 (1973).

O_2PtO_2

$\tilde{X}$ D_{2d} Structure: IR[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	1050.2	Ar	IR	1
			1047.2			

Reference

[1] H. Huber, W. Klotzbücher, G. A. Ozin, and A. Vander Voet, Can. J. Chem. **51**, 2722 (1973).

O_2CuO_2

T_0=15330(320) gas PE[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	1010(90)	gas	PE	1

Reference

[1] H. Wu, S. R. Desai, and L.-S. Wang, J. Phys. Chem. A **101**, 2103 (1997).

cyc-C_3F_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1		1930.5wm	Ar	IR	1
	3		797.4w	Ar	IR	1
b_2	7		1353.3vs	Ar	IR	1
	8		876.0w	Ar	IR	1
	9		543.8w	Ar	IR	1

Reference

[1] G. Maier, T. Preiss, and H. P. Reisenauer, Chem. Ber. **127**, 779 (1994).

FCCCF

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	C≡C stretch	2226.5vs	Ar	IR	1
	3		1115.7s	Ar	IR	1
	4		832.2wm	Ar	IR	1

Reference

[1] G. Maier, T. Preiss, and H. P. Reisenauer, Chem. Ber. **127**, 779 (1994).

$F_2C{=}C{=}C$:

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	C_3 a-stretch	2025.4vs	Ar	IR	1
	2		1436.3s	Ar	IR	1
	3		841.6wm	Ar	IR	1
	4		544.8w	Ar	IR	1
b_1	5		684.1w	Ar	IR	1
b_2	7	CF_2 a-stretch	1293.1m	Ar	IR	1
	8		568.4vw	Ar	IR	1

Reference

[1] G. Maier, T. Preiss, and H. P. Reisenauer, Chem. Ber. **127**, 779 (1994).

cyc-C_3Cl_2

In an argon matrix, weak absorption maxima at 37300 (268 nm) and 38800 (258 nm) have been attributed[1] to *cyc*-C_3Cl_2. Isomerization to ClCCCCl and $Cl_2C{=}C{=}C$: occurs when the molecule is exposed to radiation in the region of these absorptions.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Ring	1736.6wm	Ar	IR	1
	2	Ring	1263.2w	Ar	IR	1
	3	CCl stretch	527.5vw	Ar	IR	1
b_2	7	Ring	1095.9vs	Ar	IR	1
	8	CCl stretch	681.7w	Ar	IR	1

Reference

[1] G. Maier, T. Preiss, H. P. Reisenauer, B. A. Hess, Jr., and L. J. Schaad, J. Am. Chem. Soc. **116**, 2014 (1994).

ClCCCCl

In an argon matrix, ClCCCCl possesses strongly overlapping absorption bands between 275 and 320 nm.[1] Irradiation in that spectral region results in isomerization to *cyc*-C_3Cl_2.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	C=C stretch	2079.9vs	Ar	IR	1
	2	C-C stretch	1192.8wm	Ar	IR	1
	3	CCl stretch	743.0s	Ar	IR	1

Reference

[1] G. Maier, T. Preiss, H. P. Reisenauer, B. A. Hess, Jr., and L. J. Schaad, J. Am. Chem. Soc. **116**, 2014 (1994).

$Cl_2C{=}C{=}C$:

In an argon matrix, $Cl_2C{=}C{=}C$: possesses strongly overlapping absorption bands between 275 and 320 nm.[1] Irradiation in that spectral region results in isomerization to *cyc*-C_3Cl_2.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	C_3 a-stretch	1976.7vs	Ar	IR	1
	2	C_3 s-stretch	1238.1wm	Ar	IR	1
	3	ClCC deform.	542.9w	Ar	IR	1
b_2	7	CCl_2 a-stretch	890.5m	Ar	IR	1

Reference

[1] G. Maier, T. Preiss, H. P. Reisenauer, B. A. Hess, Jr., and L. J. Schaad, J. Am. Chem. Soc. **116**, 2014 (1994).

$Si_2O_3^-$

Threshold for electron detachment from ground-state $Si_2O_3^-$ =15330(800) gas PE[1]

There is evidence for the presence of a presumably less stable isomer of $Si_2O_3^-$ which has a threshold for electron detachment =7260(800) gas PE[1]

Reference

[1] L.-S. Wang, H. Wu, S. R. Desai, J. Fan, and S. D. Colson, J. Phys. Chem. **100**, 8697 (1996).

$Ge_2O_3^-$

Threshold for electron detachment from ground-state $Ge_2O_3^-$ =19610(800) gas PE[1]

Reference

[1] L.-S. Wang, H. Wu, S. R. Desai, J. Fan, and S. D. Colson, J. Phys. Chem. **100**, 8697 (1996).

O_2N-NO

In nitrogen- and neon-matrix studies,[4,8] excitation in the region of a weak absorption between 700 and 900 nm, with maximum near 720 nm, leads to isomerization forming O=N-O-N=O.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	N=O stretch	1829.54	gas	IR	1,5,7,10
			1830.2s	Ne	IR	8
			1830.0(2.5)	Ar	IR	11
			1840m	N_2	IR	4,11
			1867vs	O_2	IR	2
			1861	NO	IR,Ra	6
	2	NO_2 a-stretch	1652	gas	IR	5
			1643.3s	Ne	IR	8
			1630.0(2.5)	Ar	IR	11
			1630vs	N_2	IR	4,11
			1596s	O_2	IR	2
			1593	NO	IR,Ra	6
	3	NO_2 s-stretch	1304.25	gas	IR	1,5,9
			1302.5vs	Ne	IR	8
			1298.0(2.5)	Ar	IR	11
			1302s	N_2	IR	4,11
			1303	O_2	IR	2
			1298	NO	IR,Ra	6
	4	NO_2 deform.	773	gas	IR	1,5
			773.1wm	Ne	IR	8
			777.1(2.5)	Ar	IR	11
			776wm	N_2	IR	4,11
			788	O_2	IR	2
			787	NO	IR,Ra	6
	5	NO_2 rock	414	gas	IR	5
			420w	N_2	IR	4
			405	NO	Ra	6
	6	N-N stretch	241	gas	IR	5
			266	NO	Ra	6
	7	NO_2 wag	205	NO	Ra	6
a''	8	NNO_2 OPLA	627	NO	Ra	6
	9	Torsion	63	gas	IR	5
			70	NO	Ra	6

A_0=0.415; B_0=0.141; C_0=0.105 MW[3]IR[9,10]

References

[1] L. D'Or and P. Tarte, Bull. Soc. R. Sci. Liège **22**, 276 (1953).
[2] W. G. Fateley, H. A. Bent, and B. Crawford, Jr., J. Chem. Phys. **31**, 204 (1959).
[3] A. H. Brittain, A. P. Cox, and R. L. Kuczkowski, Trans. Faraday Soc. **65**, 1963 (1969).
[4] E. L. Varetti and G. C. Pimentel, J. Chem. Phys. **55**, 3813 (1971).
[5] C. H. Bibart and G. E. Ewing, J. Chem. Phys. **61**, 1293 (1974).
[6] E. M. Nour, L.-H. Chen, and J. Laane, J. Phys. Chem. **87**, 1113 (1983).
[7] L. A. Chewter, I. W. M. Smith, and G. Yarwood, Mol. Phys. **63**, 843 (1988).
[8] M. E. Jacox and W. E. Thompson, J. Chem. Phys. **93**, 7609 (1990).
[9] A. M. Andrews, J. L. Domenech, G. T. Fraser, and W. J. Lafferty, J. Mol. Spectrosc. **163**, 428 (1994).
[10] R. Georges, J. Liévin, M. Herman, and A. Perrin, Chem. Phys. Lett. **256**, 675 (1996).
[11] T. G. Koch and J. R. Sodeau, J. Chem. Soc. Faraday Trans. **92**, 2347 (1996).

O=N-O-N=O

In nitrogen-matrix studies,[1] absorption maxima were observed at 398, 381, and 363 nm. Excitation in the 370–480 nm spectral region resulted in photoisomerization into O_2N-NO.[1,3]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	N=O s-stretch	1740	NO	Ra	2
	2	N-O s-stretch	973.6m	Ne	IR	3
			968.4(2.5)	Ar	IR	4
			969w	N_2	IR	1
			973m	NO	IR,Ra	2
	3	NON bend	387m	N_2	IR	1
			395	NO	Ra	2
	4	Sym. O=NO bend	366s	N_2	IR	1
a_2	5	Torsion	140	NO	Ra	2
b_1	6	Torsion	105H	NO	Ra	2
b_2	7	N=O a-stretch	1697.2vs	Ne	IR	3
			1685.9(2.5)	Ar	IR	4
			1690s	N_2	IR	1
			1687vs	NO	IR	2
			1661w	N_2	IR	1
	8	N-O a-stretch	877vw	N_2	IR	1
			865vw	NO	IR	2
	9	Asym. O=NO bend	704vw	N_2	IR	1
			705vw	NO	IR	2

References

[1] E. L. Varetti and G. C. Pimentel, J. Chem. Phys. **55**, 3813 (1971).
[2] E. M. Nour, L.-H. Chen, and J. Laane, J. Phys. Chem. **87**, 1113 (1983).
[3] M. E. Jacox and W. E. Thompson, J. Chem. Phys. **93**, 7609 (1990).
[4] T. G. Koch and J. R. Sodeau, J. Chem. Soc. Faraday Trans. **92**, 2347 (1996).

$FONO_2^+$

T^a=48090(120) gas PE[1]

$\tilde{E}$ $^2A'$ C_s
T^a=40180(120) gas PE[1]

$\tilde{D}$ $^2A'$ C_s
T^a=30980(120) gas PE[1]

$\tilde{C}$ $^2A''$ C_s
T^a=24450(120) gas PE[1]

$\tilde{B}$ $^2A'$ C_s
T^a=3550(120) gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1090(40)	gas	PE	1

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

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

[a]From vertical ionization potentials.

Reference

[1]D. Wang, P. Jiang, and Q. Zhang, Chem. Phys. Lett. **262**, 771 (1996).

$ClONO_2^+$

T^a=58250(120) gas PE[1]

T^a=36630(120) gas PE[1]

$\tilde{E}$ $^2A''$ C_s
T^a=25170(120) gas PE[1]

$\tilde{D}$ $^2A'$ C_s
T^a=18640(120) gas PE[1]

$\tilde{B}$, $\tilde{C}$ $^2A''$,$^2A'$ C_s
T^a=11130(120) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			545(50)	gas	PE	1
			415(50)	gas	PE	1

$\tilde{A}$ $^2A'$ C_s
T^a=4680(120) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			770(50)	gas	PE	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1240(60)	gas	PE	1

[a]From vertical ionization potentials.

Reference

[1]D. Wang, Y. Li, P. Jiang, X. Wang, and B. Chen, Chem. Phys. Lett. **260**, 99 (1996).

$BrONO_2^+$

$\tilde{E}$ $^2A'$ C_s
T^a=24700(200) gas PE[1]

$\tilde{D}$ $^2A''$ C_s
T^a=20330(200) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		BrO stretch	670(60)	gas	PE	1

$\tilde{C}$ $^2A'$ C_s
T^a=15330(200) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		NO_2 a-stretch	1130(60)	gas	PE	1
		NO_2 s-stretch	1050(60)	gas	PE	1

$\tilde{B}$ $^2A'$ C_s
T^a=9520(200) gas PE[1]

$\tilde{A}$ $^2A'$ C_s
T^a=5240(200) gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			400(60)	gas	PE	1

A=2500(200) gas PE[1]

[a]From vertical ionization potential.

Reference

[1]D. Wang and P. Jiang, J. Phys. Chem. **100**, 4382 (1996).

cyc-F_2CO_2

$\tilde{X}$ C_{2v} Structure: IR[2,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO_2 s-stretch	1466.59vs	gas	IR	1,2
			1456[a]	Ar	IR	2
	2	CF_2 s-stretch	917.90m	gas	IR	1,2
			916[a]	Ar	IR	2
	3	CF_2 scissors	772m	gas	IR	1
	4	OCO deform.	511vw	gas	IR	1
b_1	6	CF_2 a-stretch	1259vs	gas	IR	1
			1249[a]	Ar	IR	2
	7	CF_2 rock	557w	gas	IR	1
b_2	8	CO_2 a-stretch	1062.10s	gas	IR	1,2
			1055[a]	Ar	IR	2
	9	CF_2 wag	617w	gas	IR	1

$A_0=0.266$; $B_0=0.211$; $C_0=0.163$ IR[2]

[a]Unpublished work cited in Ref. 2.

References

[1] A. Russo and D. D. DesMarteau, Angew. Chem. **105**, 956 (1993); Angew. Chem. Int. Ed. Engl. **32**, 905 (1993).
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[3] H. Bürger, P. Weinrath, G. A. Argüello, H. Willner, and J. Demaison, J. Mol. Spectrosc. **171**, 589 (1995).

$FONO_2$

$\tilde{X}$ C_s Structure: ED[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO_2 a-stretch	1760.9vs	gas	IR,Ra	1–4
			1758.4	Ne	IR	4
	2	NO_2 s-stretch	1301.2vs	gas	IR,Ra	1–4
			1300.9	Ne	IR	4
	3	OF stretch	927m	gas	IR,Ra	1–4
			929.8	Ne	IR	4
	4	NO_2 scissors	803.4s	gas	IR,Ra	1–4
			802.7	Ne	IR	4
	5	O-N stretch	632.9vw	gas	IR,Ra	1–4
			635.0	Ne	IR	4
	6	NO_2 rock	458.5ms	gas	IR,Ra	1–4
			459.9	Ne	IR	4
	7	OF rock	302.6vw	gas	IR,Ra	2,3
			300.0	Ne	IR	4
a''	8	NO_2 wag	707.3m	gas	IR	2,4
			710.0	Ne	IR	4
	9	Torsion	151.6vvw	gas	IR,Ra	2,3
			161.0	Ne	IR	4

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$ClONO_2$

The onset of continuous absorption by gas-phase $ClONO_2$ occurs near 25000 (400 nm).[3] Except for two possible shallow maxima, the absorption continues to rise out to the 185 nm cutoff of the observations.

$\tilde{X}$ C_s Structure: MW[5,10]IR[8]ED[17]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO_2 a-stretch	1736.9vs	gas	IR,Ra	1,2,4,13 21
			1727.6s	Ar	IR	9,11,16
			1734.0s	N_2	IR	11,16
			1730.0vs	O_2	IR	7,16
	2	NO_2 s-stretch	1292.7vs	gas	IR,Ra	1,2,4,13 18,21
			1285.8vs	Ar	IR	9,11,16
			1291.4vs	N_2	IR	11,16
			1289.7s	O_2	IR	7,16
	3	ClO stretch	809.4s	gas	IR,Ra	1,2,4,13 21
			801.6m	Ar	IR	9,11,16
			809.7wm	N_2	IR	11,16
			808.1m	O_2	IR	7,16
	4	Mixed	780.22ms	gas	IR,Ra DL	1,2,4 13–15,19 20,21
			775.6m	Ar	IR	9,11,16
			778.6m	N_2	IR	11,16
			776.3m	O_2	IR	7,16
	5	Mixed	563.1s	gas	IR,Ra	1,2,21
			560.9ms	Ar	IR	9,11,16
			563.2wm	N_2	IR	11,16
			559.0m	O_2	IR	7,16
	6	NO_2 rock	434.0m	gas	IR,Ra	1,2,21
			426	Ar	IR	9,11
			436.5w	N_2	IR	11
			435.0	O_2	IR	7
	7	ClO rock	273.3vvw	gas	IR,Ra	1,2,21
a''	8	NO_2 wag	711.0w	gas	IR	1,21
			710.8w	Ar	IR	9,11,16
			708.4w	N_2	IR	11,16
			704.6wm	O_2	IR	7,16
	9	Torsion	120.16	gas	IR,Ra	1,2,6,8 21

$A_0=0.404$; $B_0=0.093$; $C_0=0.075$ MW[5,10,22]
Torsional barrier = 1900(100) gas IR[6,8]

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$BrONO_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO_2 a-stretch	1714vs	gas	IR	1
			1709vs	Ne	IR	1
			1702vs	N_2	IR	1
	2	NO_2 s-stretch	1288vs	gas	IR	1
			1285vs	Ne	IR	1
			1285vs	N_2	IR	1
	3	NO_2 scissors	806vs	gas	IR	1
			802vs	Ne	IR	1
			805vs	N_2	IR	1
	4	OBr stretch	750w	Ne	IR	1
			750w	N_2	IR	1
	5	NO_2 rock	564s	gas	IR	1
			563s	Ne	IR	1
			574s	N_2	IR	1
			569s			
a''	8	ONO_2 OPLA	728wm	gas	IR	1
			723vw	Ne	IR	1
			725wm	N_2	IR	1

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CF_3O

$\tilde{A}$ $^2A_1$ C_{3v}
T_0=28531 gas LF[3–5] $\tilde{A}$–$\tilde{X}$ 330–400 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CO stretch	634(2)	gas	LF	5
e	6	FCO deform.	425(2)	gas	LF	3–5

τ_0=30.1 ns gas LF[3]
B_0=0.195 LF[5]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO stretch	1225T	gas	LF	3,4
	2	CF_3 s-stretch	907T	gas	LF	3,4
e	4	CF_3 a-stretch	1221.6	Ar	IR	1,2
	6	FCO deform.	483T	gas	LF	3,4

A=−41(5) LF[5]
B_0=0.198 LF[5]

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CF_3S

$\tilde{A}$ $^2A_1$ C_{3v}
gas LF,FD[1] $\tilde{A}$–$\tilde{X}$ 350–380 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CS stretch	313.8(4)[a]	gas	LF,FD	1

τ_0=2.7(4) μs gas LF[1]

[a] ω.

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CF_4^+

$\tilde{D}$ $^2A_1$ T_d Structure: PE,EF[7]EM[14]
T_0[a]=78830(160) gas PE[2,3,5]TPEPICO[15]
gas EF[6] $\tilde{D}$–$\tilde{C}$ 350–420 nm

Broad, unstructured emission maxima at 189 and 160 nm (52900 and 62500) which appear on He^+ or electron impact on CF_4 have been interpreted as arising from the $\tilde{D}$–$\tilde{B}$ and $\tilde{D}$–$\tilde{A}$ transitions of CF_4^+, respectively.[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF stretch	800(1)	gas	PE,EF	3,5,6

τ=2.1(2) ns gas EF[1]
B_0=0.180(3)[b] EF[7]

$\tilde{C}\ ^2F_2$ T_d Structure: PE,EF[7]EM[14]
T_0[a]=51230(160) gas PE[2,3,5]TPEPICO[15]
$T_0(\tilde{D}-\tilde{C})$=27662.2 gas EF[6]EM[14] $\tilde{D}-\tilde{C}$ 350–420 nm
Broad, unstructured emission maxima at 290 and 230 nm (34500 and 43500) which result from He^+ or electron impact[6] on CF_4 and from exposure of CF_4 to synchrotron radiation[10] of wavelength shorter than 57.4 nm have been interpreted as arising from the $\tilde{C}-\tilde{A}$ and $\tilde{C}-\tilde{X}$ transitions of CF_4^+, respectively.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF stretch	727.4	gas	PE,EF EM	2,3,5,6 14

$A=+16(1)$ EF[6–8]
τ=9.0(9) ns gas EF[1]EM[9,11]T-PEFCO[13]
B_0=0.169 EM[14]

$\tilde{B}\ ^2E$
T_0[a]=23800(1000) gas PE[2–5]
Dissociates into CF_3^+ + F, probably by internal conversion to the $\tilde{A}\ ^2F_2$ state. T-PEPICO[12]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF stretch	810(80)	gas	PE	3–5
e		Deformation	500(100)	gas	PE	3–5

$\tilde{A}\ ^2F_2$
T_0[a]=14100(1000) gas PE[2–5]
Direct dissociation into CF_3^+ + F. T-PEPICO[12]

$\tilde{X}\ ^2F_1$
Direct dissociation into CF_3^+ + F. T-PEPICO[12]

[a]Measured with respect to onset of first photoelectron band, estimated by Ref. 3 at 15.35 eV.
[b]From computer simulation of emission bands.

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$CF_2Cl_2^+$

$\tilde{H}$ C_{2v}
T[a]=68200(1000) gas PE[2–4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCl_2 stretch	565T	gas	PE	4

$\tilde{G}$ C_{2v}
T_0=56160(160) gas PE[1–4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCl_2 stretch	550(80)	gas	PE	4

$\tilde{E}$, $\tilde{F}\ ^2A_2$, $^2A_1$ C_{2v}
T[a]=36500(160) gas PE[1–4]
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[6] to the $\tilde{E},\tilde{F}-\tilde{X}$ transitions of $CF_2Cl_2^+$.

$\tilde{D}\ ^2B_2$ C_{2v}
T_0=19300(35) gas PE[1-4,8]
It has been proposed[7] that an unstructured emission in the 200–400 nm region, with its principal contribution at wavelengths longer than 300 nm, which appears on electron bombardment of CF_2Cl_2 at electron energies greater than that for the onset of the $\tilde{D}$ state of $CF_2Cl_2^+$ may be contributed by the $\tilde{D}-\tilde{X}$ transition of $CF_2Cl_2^+$.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CF_2 scissors	374(5)	gas	PE	1,3,4,8

$\tilde{C}\ ^2A_1$ C_{2v}
T[a]=13880(160) gas PE[1–4]

$\tilde{B}\ ^2B_1$ C_{2v}
T_0=10844(35) gas PE[1-4,8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF_2 stretch	1097(80)	gas	PE	3,4
	2	CCl_2 stretch	565(80)	gas	PE	4
	4	CCl_2 scissors	301(5)	gas	PE	4,8

$\tilde{A}\ ^2A_2$ C_{2v}
T[a]=6370(160) gas PE[1–4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF_2 stretch	1056(5)	gas	PE	8

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CF_2 scissors	609wm	Ar	IR	5
	4	CCl_2 scissors	457(5)	gas	PE	8
		CF_2 a-stretch	1234vs	Ar	IR	5
		CCl_2 a-stretch	1067m	Ar	IR	5
		FCCl deform.	424m	Ar	IR	5
		FCCl deform.	406m	Ar	IR	5

[a]From vertical ionization potential.

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CCl_4^+

$\tilde{D}\ ^2A_1$ T_d
$T^{a,b}$=68800(900) gas PE[2]
Fragments, producing CCl^+, in $<10^{-10}$ s. T-PEPICO[6]

$\tilde{C}\ ^2F_2$ T_d
$T_0{}^a$=39290(900) gas PE[2–4]
Fragments, producing CCl_2^+, in $<10^{-10}$ s. T-PEPICO[6]

$\tilde{B}\ ^2E$
$T^{a,b}$=15330(240) gas PE[2–4]
Dissociates into CCl_3^+ + Cl, probably by internal conversion to the $\tilde{A}\ ^2T_2$ state. PEPICO[5]

$\tilde{A}\ ^2F_2$ T_d
$T_0{}^a$=6450(320) gas PE[2–4]
Direct dissociation into CCl_3^+ + Cl. PEPICO[5]

$\tilde{X}\ ^2F_1$ T_d
Direct dissociation into CCl_3^+ + Cl. PEPICO[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.

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SiF_4^+

$\tilde{D}\ ^2A_1$ T_d Structure: PE,EF[9]
$T^{a,b}$=50800(200) gas PE[2]TPE[13]
EF[7]EM[8,10] $\tilde{D}-\tilde{C}$ 530–590 nm

$\tilde{D}-\tilde{C}$ band origin measured at 18146.8 in emission studies on a cooled beam.[7]

Continuous emission between 570 and 730 nm, with a maximum near 610 nm (16400), has been assigned to the $\tilde{D}-\tilde{C}$ transition.[8,10,12]

Broad, unstructured emission maxima at 370 and 304 nm (27000 and 32900) which appear on ion, electron, or photon impact on SiF_4 have been interpreted as arising from the $\tilde{D}-\tilde{B}$ and $\tilde{D}-\tilde{A}$ transitions of SiF_4^+, respectively.[6,8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiF stretch	743.4(5)	gas	EF,TPE	7,13
e	2	Deformation	258(40)	gas	TPE	13
f_2	3	SiF stretch	1178(40)	gas	TPE	13

τ=9.30(4) ns gas EF[1]EM[12]TPEFCO[13]
B_0=0.136(1)[c] EF[9]

$\tilde{C}\ ^2T_2$ T_d^d Structure: PE,EF[9]
$T_0{}^a$=33130(100) gas PE[2,3,5]TPE[13]
EF[7]EM[8,10] $\tilde{D}-\tilde{C}$ 530–590 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiF stretch	706.6(5)	gas	PE,EF	3,5,7,13
e	2	Deformation	159.0(5)	gas	EF	7
f_2	4	Deformation	431.0(5)	gas	PE,EF	3,5,7,13

A=+6.9(2) EF[7,9,11]
B_0=0.132[c] PE,EF[9]

$\tilde{B}\ ^2E$
$T_0{}^a$=22580(100) gas PE[2,3,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiF stretch	685(50)	gas	PE	5

$\tilde{A}\ ^2F_2$ T_d
$T_0{}^a$=17000(1000) gas PE[2,3,5]

$\tilde{X}\ ^2F_1$

[a]Measured with respect to a first ionization potential of 15.19 eV, estimated[4] by extrapolation of the photoionization efficiency curve for SiF_4.
[b]From vertical ionization potential.
[c]From Franck-Condon analysis of the photoelectron spectrum and computer simulation of the $\tilde{D}-\tilde{C}$ emission.
[d]Dynamic Jahn-Teller distortion, probably to C_{3v}.[7,9]

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$SiCl_4^+$

$\tilde{D}\ ^2A_1$ T_d
T_0=48900(400) gas PE[1,2]TPE[8]
Fragments to $SiCl_2^+$. T-PEPICO[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiCl stretch	379(16)	gas	TPE	8

$\tilde{C}\ ^2F_2$
T_0=26620(160) gas PE[1,2]TPE[8]
A broad, unstructured emission with maxima at 410 and 570 nm (24400 and 17500) has been assigned[5,6,9] to the $\tilde{C}-\tilde{X}$ and $\tilde{C}-\tilde{A}$ transitions, respectively, of gas-phase $SiCl_4^+$. Using pulsed synchrotron excitation[6] of $SiCl_4$, as well as TPEFCO measurements,[8] a radiative lifetime of 38.4(1) ns has been determined for the $\tilde{C}$ state of $SiCl_4^+$.

A broad absorption with maximum at 475 nm (21000) which appears on argon-resonance photolysis of $SiCl_4$ isolated in an argon matrix has been assigned[4] to the $\tilde{C}-\tilde{X}$ transition of $SiCl_4^+$. The energy difference is attributed to structural relaxation in the argon matrix. The absorption can be destroyed by exposure of the sample to 290–1000 nm radiation.

$\tilde{B}\ ^2E$
T^a=13880(400) gas PE[1,2]

$\tilde{A}\ ^2F_2$
T_0=7750(160) gas PE[1,2]

$\tilde{X}\ ^2F_1$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		$SiCl_2$ a-stretch	717T	Ar	IR	4

[a]From vertical ionization potential.

References

[1] J. C. Green, M. L. H. Green, P. J. Joachim, A. F. Orchard, and D. W. Turner, Philos. Trans. R. Soc. London, Ser. A **268**, 111 (1970).
[2] P. J. Bassett and D. R. Lloyd, J. Chem. Soc. A 641 (1971).
[3] R. G. Egdell, I. L. Fragala, and A. F. Orchard, J. Electron Spectrosc. Relat. Phenom. **17**, 267 (1979).
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[5] I. R. Lambert, S. M. Mason, R. P. Tuckett, and A. Hopkirk, J. Chem. Phys. **89**, 2675 (1988).
[6] I. R. Lambert, S. M. Mason, R. P. Tuckett, and A. Hopkirk, J. Chem. Phys. **89**, 2683 (1988).
[7] D. M. Smith, R. P. Tuckett, K. R. Yoxall, K. Codling, and P. A. Hatherly, Chem. Phys. Lett. **216**, 493 (1993).
[8] D. M. Smith, R. P. Tuckett, K. R. Yoxall, K. Codling, P. A. Hatherly, J. F. M. Aarts, and M. Stankiewicz, J. Chem. Phys. **101**, 10559 (1994).
[9] T. Ibuki, M. Kono, Y. Asari, A. Hiraya, and K. Shobatake, J. Chem. Phys. **106**, 4853 (1997).

$GeCl_4^+$

$\tilde{D}\ ^2A_1$ T_d
T_0=51070(400) gas PE[1,2]TPE[5]

$\tilde{C}\ ^2F_2$ T_d
T_0=21620(240) gas PE[1,2]TPE[5]

A broad, unstructured emission with maxima at 495 and 615 nm (20200 and 16300) has been assigned[3,4] to the $\tilde{C}-\tilde{X}$ and $\tilde{C}-\tilde{A}$ transitions, respectively, of gas-phase $GeCl_4^+$. Using pulsed synchrotron excitation of $GeCl_4$, a radiative lifetime of 65.4(4) ns has been determined[4] for the $\tilde{C}$ state of $GeCl_4^+$.

$\tilde{B}\ ^2E$
T_0=8880(1100) gas PE[1,2]TPE[5]

$\tilde{A}\ ^2F_2$
T_0=5650(1100) gas PE[1,2]TPE[5]

$\tilde{X}\ ^2F_1$

References

[1] J. C. Green, M. L. H. Green, P. J. Joachim, A. F. Orchard, and D. W. Turner, Philos. Trans. R. Soc. London, Ser. A **268**, 111 (1970).
[2] P. J. Bassett and D. R. Lloyd, J. Chem. Soc. A 641 (1971).
[3] I. R. Lambert, S. M. Mason, R. P. Tuckett, and A. Hopkirk, J. Chem. Phys. **89**, 2675 (1988).
[4] I. R. Lambert, S. M. Mason, R. P. Tuckett, and A. Hopkirk, J. Chem. Phys. **89**, 2683 (1988).
[5] D. M. Smith, R. P. Tuckett, K. R. Yoxall, K. Codling, P. A. Hatherly, J. F. M. Aarts, and M. Stankiewicz, J. Chem. Phys. **101**, 10559 (1994).

$OClO_3$

In a neon matrix, absorption between 380 and 510 nm, with a maximum at 23530 (425 nm) and with partially resolved structure, can be assigned[1] to $OClO_3$.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ClO_3 s-stretch	1161vs	Ne	IR	1
	2	ClO stretch	874w	Ne	IR	1
	3	Deform.	576m	Ne	IR	1
e	4	ClO_3 a-stretch	1234s	Ne	IR	1
	5	Deform.	646m	Ne	IR	1

Reference

[1] H. Grothe and H. Willner, Angew. Chem. **108**, 816 (1996); Angew. Chem. Int. Ed. Engl. **35**, 768 (1996).

Cl_2O_3

An unstructured gas-phase absorption between 220 and 320 nm, with maximum at 37450 (267 nm), has been assigned[2,4,5,8] to Cl_2O_3.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1225vs	gas	IR	1,4
			1216.0	Ne	IR	6
			1226.1	Ar	IR	3,6
			1213.5	Ar	IR	6
			1203.1	Ne	IR	6
			1200.7	Ar	IR	6
			1057s	gas	IR	4
			1060	Ne	IR	6
			1058.4	Ar	IR	3,6
			740w	gas	IR	4
			560wm	gas	IR	4

$A_0=0.288$; $B_0=0.070$; $C_0=0.059$ MW[7]

References

[1] A. J. Schell-Sorokin, D. S. Bethune, J. R. Lankard, M. M. T. Loy, and P. P. Sorokin, J. Phys. Chem. **86**, 4653 (1982).
[2] G. D. Hayman and R. A. Cox, Chem. Phys. Lett. **155**, 1 (1989).
[3] B.-M. Cheng and Y.-P. Lee, J. Chem. Phys. **90**, 5930 (1989).
[4] J. B. Burkholder, J. J. Orlando, and C. J. Howard, J. Phys. Chem. **94**, 687 (1990).
[5] J. B. Burkholder, R. L. Mauldin III, R. J. Yokelson, S. Solomon, and A. R. Ravishankara, J. Phys. Chem. **97**, 7597 (1993).
[6] H. S. P. Müller and H. Willner, J. Phys. Chem. **97**, 10589 (1993).
[7] R. R. Friedl, M. Birk, J. J. Oh, and E. A. Cohen, J. Mol. Spectrosc. **170**, 383 (1995).
[8] M. H. Harwood, D. M. Rowley, R. A. Freshwater, R. A. Cox, and R. L. Jones, J. Chem. Soc. Faraday Trans. **91**, 3027 (1995).

SF_4^+

T^a=51600(800) gas PE[1–3]

T^a=46800(400) gas PE[1–3]

T^a=43000(400) gas PE[1–3]

$\tilde{C},\tilde{D}\,^2B_2,^2A_1$ C_{2v}
T^a=31460(400) gas PE[1–3]

$\tilde{A},\tilde{B}\,^2A_2,^2B_1$ C_{2v}
T^a=25580(400) gas PE[1–3]

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

[a]From vertical ionization potential. The adiabatic first ionization potential of SF_4 is estimated to be 11.90 eV.[3]

References

[1] A. H. Cowley, M. Lattman, and M. L. Walker, J. Am. Chem. Soc. **101**, 4074 (1979).
[2] N. C. V. Costa, D. R. Lloyd, P. J. Roberts, D. W. J. Cruickshank, E. Avramides, A. Chablo, G. A. D. Collins, B. Dobson, and I. H. Hillier, J. Chem. Soc. Faraday Trans. 2 **77**, 899 (1981).
[3] H.-W. Jochims, E. Rühl, and H. Baumgärtel, Z. Naturforsch. B **44**, 13 (1989).

8.12. Six-Atomic Molecules

SiH_5^+

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	HH stretch	3693.97(6)	gas	PF	1

$A_0=2.519$[a]; $B_0=1.689(3)$; $C_0=1.639(3)$ PF[1]

[a]From *ab initio* calculations; fixed in the fit.

Reference

[1] D. W. Boo and Y. T. Lee, J. Chem. Phys. **103**, 514 (1995).

$LiBH_4$

$\tilde{X}$ C_{3v} Structure: MW[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			700(150)	gas	MW	1
e			400(150)	gas	MW	1

$B_0=0.769$ MW[1,2]

$LiBD_4$

$\tilde{X}$ C_{2v}
$B_0=0.625$ MW[2]

References

[1] Y. Kawashima and E. Hirota, J. Chem. Phys. **96**, 2460 (1992).
[2] Y. Kawashima and E. Hirota, J. Chem. Phys. **102**, 6961 (1995).

$NaBH_4$

$\tilde{X}$ C_{3v} Structure: MW[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			435T	gas	MW	1

$B_0=0.322$ MW[1]

$NaBD_4$

$\tilde{X}$ C_{3v}
$B_0=0.268$ MW[2]

References

[1] Y. Kawashima, C. Yamada, and E. Hirota, J. Chem. Phys. **94**, 7707 (1991).
[2] Y. Kawashima and E. Hirota, J. Chem. Phys. **102**, 6961 (1995).

KBH_4

$\tilde{X}$ C_{3v} Structure: MW[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			360T	gas	MW	1

B_0=0.210 MW[1]

Reference

[1] Y. Kawashima and E. Hirota, J. Chem. Phys. **102**, 6961 (1995).

$HBeH_2BeH$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BeH_t stretch	1982	Ar	IR	1
		BeHBe stretch	1536	Ar	IR	1
		BeHBe stretch	1420	Ar	IR	1
			872	Ar	IR	1
			558	Ar	IR	1

$DBeD_2BeD$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BeD_t stretch	1567	Ar	IR	1
		BeDBe stretch	1067	Ar	IR	1
			651	Ar	IR	1

Reference

[1] T. J. Tague, Jr. and L. Andrews, J. Am. Chem. Soc. **115**, 12111 (1993).

$HMgH_2MgH$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1531.0T	Ar	IR	1
			1164.2T	Ar	IR	1
			1013.7T	Ar	IR	1
			613.9T	Ar	IR	1

$DMgD_2MgD$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1127.7T	Ar	IR	1
			844.5T	Ar	IR	1
			736.9T	Ar	IR	1

Reference

[1] T. J. Tague, Jr. and L. Andrews, J. Phys. Chem. **98**, 8611 (1994).

U_2H_4

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		UH stretch	1547T	Ar	IR	1
		UH stretch	1495.0	Ar	IR	1

U_2D_4

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		UD stretch	1102.8	Ar	IR	1
		UD stretch	1067.9	Ar	IR	1

Reference

[1] P. F. Souter, G. P. Kushto, L. Andrews, and M. Neurock, J. Am. Chem. Soc. **119**, 1682 (1997).

CH_3CoH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_3 stretch	2982.0	Ar	IR	2
		CH_3 stretch	2942.1	Ar	IR	2
		CoH stretch	1722.6	Ar	IR	1,2
		Deformation	1168.5	Ar	IR	2
		Deformation	573.2	Ar	IR	2
			568.9			
		CoC stretch	530.8	Ar	IR	1,2

CD_3CoD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CoD stretch	1241.0	Ar	IR	1

References

[1] W. E. Billups, S.-C. Chang, R. H. Hauge, and J. L. Margrave, J. Am. Chem. Soc. **115**, 2039 (1993).
[2] W. E. Billups, S.-C. Chang, R. H. Hauge, and J. L. Margrave, J. Am. Chem. Soc. **117**, 1387 (1995).

CH_3ZnH

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 stretch	2919.8	Ar	IR	1
	2	ZnH stretch	1866.1	Ar	IR	1
	3	CH_3 deform.	1179.3	Ar	IR	1
	4	ZnC stretch	566.5	Ar	IR	1
e	7	CH_3 rock	689.4s	Ar	IR	1
			686.6			
	8	CZnH deform.	442.6	Ar	IR	1

CD_3ZnD

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	ZnD stretch	1344.7	Ar	IR	1
	3	CD_3 deform.	921.1	Ar	IR	1
	4	ZnC stretch	516.1	Ar	IR	1
e	7	CD_3 rock	530.5	Ar	IR	1
			527.9			
	8	CZnD deform.	317.2	Ar	IR	1

Reference

[1] T. M. Greene, L. Andrews, and A. J. Downs, J. Am. Chem. Soc. **117**, 8180 (1995).

CH_3CdH

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 stretch	2928.5	Ar	IR	1
	2	CdH stretch	1760.5	Ar	IR	1
	4	CdC stretch	508.6	Ar	IR	1
e	7	CH_3 rock	687.3	Ar	IR	1
			685.4			
	8	CCdH deform.	433.2	Ar	IR	1
			430.1			

CD_3CdD

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CdD stretch	1264.4	Ar	IR	1
	4	CdC stretch	465.3	Ar	IR	1
e	7	CD_3 rock	523.6	Ar	IR	1
			521.9			
	8	CCdD deform.	310.6	Ar	IR	1

Reference

[1] T. M. Greene, L. Andrews, and A. J. Downs, J. Am. Chem. Soc. **117**, 8180 (1995).

CH_3HgH

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 stretch	2921.2w	Ar	IR	1,2
	2	HgH stretch	1954.9vs	Ar	IR	1,2
	3	CH_3 deform.	1191.7vw	Ar	IR	1,2
	4	HgC stretch	534.0w	Ar	IR	1,2
e	5	CH_3 stretch	2990.6mT	Ar	IR	1
	6	CH_3 deform.	1425.0w	Ar	IR	1,2
	7	CH_3 rock	779.8	Ar	IR	1,2
			777.9			
	8	CHgH deform.	526.5	Ar	IR	1,2

CD_3HgD

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_3 stretch	2127.7w	Ar	IR	1,2
	2	HgD stretch	1400.7vs	Ar	IR	1,2
	3	CD_3 deform.	1024.5vwT	Ar	IR	1
	4	HgC stretch	487.0	Ar	IR	2
e	5	CD_3 stretch	2233.9m	Ar	IR	1
	6	CD_3 deform.	1041.1wT	Ar	IR	1,2
	7	CD_3 rock	593.5m	Ar	IR	1,2
			592.1			
	8	CHgD deform.	374.5	Ar	IR	2

References

[1] N. Legay-Sommaire and F. Legay, Chem. Phys. Lett. **217**, 97 (1994).
[2] T. M. Greene, L. Andrews, and A. J. Downs, J. Am. Chem. Soc. **117**, 8180 (1995).

H_2CBH_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CH_2 scissors	1414.7	Ar	IR	1
		BH_2 scissors	1239.8	Ar	IR	1
b_1		BH_2 OPLA	972.4	Ar	IR	1
b_2		BH_2 a-stretch	2560.6	Ar	IR	1

D_2CBD_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		BD_2 scissors	1177	Ar	IR	1
b_1		BD_2 OPLA	794.8	Ar	IR	1
b_2		BD_2 a-stretch	1923	Ar	IR	1

Reference

[1] P. Hassanzadeh, Y. Hannachi, and L. Andrews, J. Phys. Chem. **97**, 6418 (1993).

CH_3BH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	2979.2T	Ar	IR	1
		BH stretch	2560.6T	Ar	IR	1

CD_3BD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BD stretch	1935T	Ar	IR	1

Reference

[1] P. Hassanzadeh, Y. Hannachi, and L. Andrews, J. Phys. Chem. **97**, 6418 (1993).

CH_3GaH

In an argon matrix, an absorption with maximum at 45900 (218 nm) behaves appropriately for assignment to CH_3GaH.[1]

In an argon matrix, a weak, broad (100 nm FWHM) absorption at 16700 (600 nm) has also been attributed[1] to CH_3GaH. Irradiation of the sample in the region of this absorption leads to photodestruction of CH_3GaH.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	2970	Ar	IR	1
		CH stretch	2914	Ar	IR	1
		GaH stretch	1719.7	Ar	IR	1,2
			1712.5	Kr	IR	2
		CH_3 deform.	1432	Ar	IR	1
		CH_3 deform.	1176.4	Ar	IR	1,2
			1153.7	Kr	IR	2
		CH_3 rock	753.1	Ar	IR	1,2
			747.8	Kr	IR	2
		CH_3 rock	642	Ar	IR	1
		GaC stretch	528.6	Ar	IR	1,2
			520.0	Kr	IR	2

CD_3GaD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD stretch	2222	Ar	IR	1
		CD stretch	2137	Ar	IR	1
		GaD stretch	1243.6	Ar	IR	1,2
			1239.0	Kr	IR	2
		CD_3 deform.	1026	Ar	IR	1
		CD_3 deform.	747.0T[a]	Kr	IR	2
		CD_3 rock	578.2	Ar	IR	1,2
		GaC stretch	525.0T[b]	Ar	IR	2

[a]Ref. 1 gives 899 for an argon matrix.
[b]Ref. 1 gives 484.

References

[1] R. D. Lafleur and J. M. Parnis, J. Phys. Chem. **96**, 2429 (1992).
[2] Z. L. Xiao, R. H. Hauge, and J. L. Margrave, Inorg. Chem. **32**, 642 (1993).

$CH_2{=}SiH_2$

In an Ar or N_2 matrix, absorption maximum at 258 nm.[1–4] On irradiation at 254 nm, photoisomerizes to CH_3SiH.[2,4]

$\tilde{X}$ C_{2v} Structure: MW[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		SiH s-stretch	2219m	Ar	IR	1–3
			2214m	N_2	IR	2,4
		CH_2 scissors	1350w	Ar	IR	2,3
			1350w	N_2	IR	2,4
		Si=C stretch	985w	Ar	IR	1–3
			985w	N_2	IR	1,2,4
		SiH_2 scissors	927w	Ar	IR	1–3
			927w	N_2	IR	2,4
b_1		CH_2 wag	741s	Ar	IR	1–3
			747s	N_2	IR	2,4
b_2		SiH a-stretch	2239m	Ar	IR	1–3
			2235m	N_2	IR	2,4
		CH_2 rock	817s	Ar	IR	1–3
			817s	N_2	IR	2,4

A_0=3.493; B_0=0.493; C_0=0.432 MW[5]

$CH_2{=}SiD_2$

In an Ar matrix, absorption maximum at 259 nm.[1,4]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		SiD s-stretch	1600m	Ar	IR	1,3
			1600	N_2	IR	4
		CH_2 scissors	1335	Ar	IR	3
			1352	N_2	IR	4
		Si=C stretch	952w	Ar	IR	1,3
			952	N_2	IR	4
b_1		CH_2 wag	719s	Ar	IR	1,3
			725	N_2	IR	4
b_2		SiD a-stretch	1635m	Ar	IR	1,3
			1635	N_2	IR	4
		CH_2 rock	759s	Ar	IR	1,3
			760	N_2	IR	4
		SiD_2 rock	396w	Ar	IR	1,3
			396	N_2	IR	4

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[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).
[3] G. Maier, G. Mihm, and H. P. Reisenauer, Chem. Ber. **117**, 2351 (1984).

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[5] S. Bailleux, M. Bogey, J. Demaison, H. Bürger, M. Senzlober, J. Breidung, W. Thiel, R. Fajgar, and J. Pola, J. Chem. Phys. **106**, 10016 (1997).

H_2BNBH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BH stretch	2788.3	Ar	IR	1
		BH stretch	2426.5	Ar	IR	1
		BH stretch	2393.2	Ar	IR	1
		BNB a-stretch	1864.2	Ar	IR	1

Reference

[1] C. A. Thompson, L. Andrews, J. M. L. Martin, and J. El-Yazal, J. Phys. Chem. **99**, 13839 (1995).

CH_2CCH

In the gas phase, absorption between 230 and 280 nm, with a maximum at 41320 (242 nm), has been assigned[9] to CH_2CCH.

T_0=30109[a] gas AB[1] 290–345 nm
Ar AB[2] 288–359 nm
All bands in the gas-phase spectrum are diffuse.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C-C stretch	961(10)	gas	AB	1
			965(10)	Ar	AB	2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3322.29	gas	CC	5
			3308.8m	Ar	IR	2,4
		CH_2 wag	687.18	gas	DL	6,8
			686.5m	Ar	IR	2
		C_3 deformation	490T	gas	PE	3,7
			483.5m	Ar	IR	2,4

A_0=9.608; B_0=0.318; C_0=0.307 CC[5]DL[8]

CD_2CCD

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD stretch	2546.8m	Ar	IR	2,4
			552.9m	Ar	IR	2
			479.8	Ar	IR	4
			350T	gas	PE	7

[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.

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cyc-$(HC{=}NCH_2)^+$

$\tilde{D}\ ^2A'$ C_s
T^a=46200(800) gas PE[1–3]

$\tilde{C}\ ^2A''$ C_s
T^a=41200(800) gas PE[1–3]

$\tilde{B}\ ^2A'$ C_s
T^a=23240(160) gas PE[1–3]

$\tilde{A}\ ^2A''$ C_s
T^a=7900(160) gas PE[1–3]

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

[a]From vertical ionization potentials.

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CH_2CCH^-

Threshold for electron detachment from ground-state CH_2CCH^-=7410(65) gas PE[1,2]

CD_2CCD^-

Threshold for electron detachment from ground-state CD_2CCD^-=7380(65) gas PE[2]

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CH_3CC^-

Threshold for electron detachment from ground-state CH_3CC^-=21930(65) gas PE[1]

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

Reference

[1] M. S. Robinson, M. L. Polak, V. M. Bierbaum, C. H. DePuy, and W. C. Lineberger, J. Am. Chem. Soc. **117**, 6766 (1995).

$CH_2=C=NH$

$\tilde{B}$ C_s

T_0[a]=38900 gas AB[2,8]
38790 Ar AB[4]

$\tilde{A}$ C_s

T_0[a]=32840 gas AB[2,8] $\tilde{A}-\tilde{X}$ 273–317 nm
32680 Ar AB[4] $\tilde{A}-\tilde{X}$ 273–306 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			990	Ar	AB	4

$\tilde{X}$ C_s Structure: MO^3MW^6

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CCN a-stretch	2043.58	gas	IR	7
			2040vs	Ar	IR	1,4
	5	CCN s-stretch; NH deform.	1124wm	Ar	IR	1,4
	6	NH deform.	1000s	Ar	IR	1,4
	7	H_2CC OPLA	690m	Ar	IR	1,4
a''	11	Torsion	872m	Ar	IR	1,4

A_0=6.719; B_0=0.322; C_0=0.316 $MW^{5,6}IR^7$

$CD_2=C=ND$

$\tilde{B}$ C_s

T_0=38790 Ar AB[4]

$\tilde{A}$ C_s

T_0=32680 Ar AB[4] $\tilde{A}-\tilde{X}$ 272–306 nm

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CCN a-stretch	1998vs	Ar	IR	1,4
	5	CD_2 scissors	921m	Ar	IR	1,4
	6	ND deform.	800s	Ar	IR	1,4
a''	11	Torsion	648m	Ar	IR	1,4

[a]Bands originally tentatively assigned[2] to cyanoallyl.

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$HCNCH_2$

In an argon matrix, an intense absorption with maximum at 38800 (258 nm) and a weak, broad absorption with maximum near 31200 (320 nm) have been assigned[1] to $HCNCH_2$.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CNC a-stretch	1914.5s	Ar	IR	1
	5	CNC s-stretch	1183.6w	Ar	IR	1
	6	HCN deform.	866.3vs	Ar	IR	1
	8	CNC deform.	473.5wm	Ar	IR	1
a''	10	CH_2 deform.	1127.3w	Ar	IR	1

$DCNCD_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CNC a-stretch	1870.2vs	Ar	IR	1
			982.6w	Ar	IR	1
			900.1w	Ar	IR	1
			708.3ms	Ar	IR	1
			414.6w	Ar	IR	1

Reference

[1] G. Maier, C. Schmidt, H. P. Reisenauer, E. Endlein, D. Becker, J. Eckwert, B. A. Hess, Jr., and L. J. Schaad, Chem. Ber. **126**, 2337 (1993).

cyc-(HC=NCH$_2$)

(2H-Azirine)

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	3078.4w	Ar	IR	3
	2	CH stretch	3005.6w	Ar	IR	3
	3	C=N stretch	1669.1wm	Ar	IR	3
			1667.2wm			
	5		1240.5wm	Ar	IR	3
			1237.6wm			
	7		978.7vs	Ar	IR	3
			977.3			
			974.4			
			971.5			
			969.1			
a''	9	CH$_2$ a-stretch	3061.5vw	Ar	IR	3
	12		772.9wm	Ar	IR	3
			767.1wm			

A_0=1.188; B_0=0.741; C_0=0.503 MW[1,2]

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[3] G. Maier, C. Schmidt, H. P. Reisenauer, E. Endlein, D. Becker, J. Eckwert, B. A. Hess, Jr., and L. J. Schaad, Chem. Ber. **126**, 2337 (1993).

HCCAsH$_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CH stretch	3318	gas	IR	1
	2	CC stretch	2180	gas	IR	1
		AsH$_2$ stretch	2118	gas	IR	1

Reference

[1] J.-C. Guillemin, L. Lassalle, P. Dréan, G. Wlodarczak, and J. Demaison, J. Am. Chem. Soc. **116**, 8930 (1994).

CH$_3$CAs

$\tilde{X}$ C_{3v} Structure: MW[1]

B_0=0.117 MW[1]

CD$_3$CAs

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

B_0=0.100 MW[1]

Reference

[1] J.-C. Guillemin, L. Lassalle, P. Dréan, G. Wlodarczak, and J. Demaison, J. Am. Chem. Soc. **116**, 8930 (1994).

CH$_2$CHO

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

T_0=28784.09(1) gas AB[1]LF[2,4,6,12]FD[10]PF[13] $\tilde{B}-\tilde{X}$ 300–405 nm

The failure to detect fluorescence on excitation above 30000 suggests[2] the onset of predissociation near 330 nm. In the gas phase,[13] both CH$_3$ and H atoms are produced above 28700. In the argon matrix experiments,[5] the threshold for the photodecomposition of CH$_2$CHO to produce CH$_3$+CO was observed between 280 and 300 nm.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	4	CO stretch	1621	gas	FD,PF	10,12,13
					LF,DR	14
	5	CH$_2$ scissors	1405	gas	FD,PF	10,12,13
					LF,DR	14
	6	OCH bend	1274	gas	PF,LF,DR	13,14
	7	CH$_2$ rock	1122	gas	LF,FD	2,6,10,12
					PF,DR	13,14
	8	CC stretch	917	gas	LF,FD	2,6,10,12
					PF,DR	13,14
	9	CCO bend	449	gas	LF,FD	2,6,10,12
					PF,DR	13,14
a''	10	HCO wag	595H	gas	LF,DR	14
	11	CH$_2$ wag	436H	gas	PF,LF,DR	13,14
	12	Torsion	274H	gas	PF,LF,DR	13,14

τ_0=190(2) ns gas LF[11,14]

A_0=2.103(4); B_0=0.344(1); C_0=0.296(1) LF[6]

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

T_0=8006 gas AB[3] $\tilde{A}-\tilde{X}$ 1000–1250 nm

$\tilde{X}$ $^2A''$ C_s Structure: MW[8,9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	4	CCO stretch	1543	gas	LF	2,6,12,14
			1542m HF	Ar	IR	5
			1525m			
	5	CH$_2$ scissors	1486	gas	LF	14
	6	OCH deform.	1366	gas	LF	12,14
			1375m HF	Ar	IR	5
	7	CH$_2$ rock	1143	gas	LF,PD	2,6,7,14
	8	CC stretch	957	gas	LF	14
	9	CCO bend	500	gas	LF,PD	2,6,7,14
a''	10	CHO wag	703H	gas	LF	14
	11	CH$_2$ wag	557H	gas	LF	14
	12	Torsion	404H	gas	LF	14

A_0=2.224; B_0=0.382; C_0=0.326 LF[6]MW[8]

CD$_2$CDO

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

T_0=28840 gas LF[2]PF[13] $\tilde{B}-\tilde{X}$ 300–411 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			980	gas	LF	2
			768	gas	LF	2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		C=O stretch	1540	gas	LF	2
			1513ms HF	Ar	IR	5
			1223w HF	Ar	IR	5
		CC stretch	1050	gas	LF	2
		CCO bend	445	gas	LF	2

A_0=1.442; B_0=0.336; C_0=0.272 MW[9]

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CH_2CHO^-

Dipole-Bound State C_s
T_0=14712.747(5) gas PD[1–3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		C-C stretch	1143	gas	PD	2
		CCO bend	499	gas	PD	2
a''		Torsion	102H	gas	PD	2

A_0=2.221(2); B_0=0.376; C_0=0.320 PD[2,3]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CCO bend	525.82	gas	PD	2,3
a''		Torsion	375T	gas	PD	2

A_0=2.494; B_0=0.362; C_0=0.316 PD[2,3]

CD_2CDO^-

Dipole-Bound State C_s
T_0=14665.97(5) gas PD[1,2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1382(10)	gas	PD	1
			981(10)	gas	PD	1
		CCO bend	437(10)	gas	PD	1
a''		Torsion	80HT	gas	PD	1

A_0=1.419(3); B_0=0.330; C_0=0.268 PD[2,4]

$\tilde{X}$ C_s
A_0=1.554(1); B_0=0.319; C_0=0.264 PD[2]

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CH_2NOH

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3650.29vs	gas	IR	1,4,7
	2	CH_2 stretch	3109.72w	gas	IR	1,4,7
	3	CH_2 stretch	2973.17wm	gas	IR	1,4,7
	4	C=N stretch	1639.48wm	gas	IR	1,4,9
	5	CH_2 scissors	1410.48ms	gas	IR	1,4,9
	6	OH bend	1318.98vs	gas	IR	1,4,9
	7	CH_2 rock	1166m	gas	IR	1,4
	8	NO stretch	892.58s	gas	IR	1,4,6,9
	9	CNO deform.	530w	gas	IR	1,4
a''	10	CH_2 OPLA	952.61s	gas	IR	1,4,6
	11	CH_2 torsion	774.1m	gas	IR	1,4,6
	12	OH torsion	400T	gas	IR	1,4

A_0=2.258; B_0=0.396; C_0=0.336 MW[2,3,5,8]

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PH_3F_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	3	PH_3 deform.	1266.15m	gas	IR	1,3,5
	4	PF_2 a-stretch	755.99vs	gas	IR	1,3,5
			755	Ar	IR	2
e'	5	PH_3 a-stretch	2501.7s[a]	gas	IR	1,3,5
			2480w,br	Ar	IR	2
	6	PH_3 deform.	965.45s[b]	gas	IR	1,3,5
			974	Ar	IR	2
	7	PF_2 deform.	341.55m	gas	IR	4,5

A_0=2.868(15); B_0=0.159 gas IR[3,4]

PD_3F_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	3	PD_3 deform.	936m	gas	IR	5
	4	PF_2 a-stretch	745vs	gas	IR	5
			749	Ar	IR	2
e'	5	PD_3 a-stretch	1828s	gas	IR	5
	6	PD_3 deform.	719	Ar	IR	2
	7	PF_2 deform.	319m	gas	IR	5

[a]Effective value; deperturbed value = 2488.48.
[b]Deperturbed value.

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HNBBNH

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NH stretch	3682.8	Ar	IR	1
		BN stretch	1827.4	Ar	IR	1
		Deformation	413.3	Ar	IR	1

Reference

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H_2CCCC:

$\tilde{X}$ C_{2v} Structure: MW[2]
A_0=9.489; B_0=0.150; C_0=0.148 MW[1,2]

D_2CCCC:

$\tilde{X}$ C_{2v}
A_0=4.783; B_0=0.137; C_0=0.133 MW[2]

Reference

[1]T. C. Killian, J. M. Vrtilek, C. A. Gottlieb, E. W. Gottlieb, and P. Thaddeus, Astrophys. J. **365**, L89 (1990).

$HCCCNH^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NH stretch	3513.96	gas	LD	1
	3	CN stretch	2315.14	gas	DL	2

B_0=0.144 LD[1]MW[3]

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HOC≡COH

$\tilde{X}$ C_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b	8	OH stretch	3586.2wm	Ar	IR	1
	10	Deformation	1212.4vw	Ar	IR	1

DOC≡COD

$\tilde{X}$ C_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b	8	OD stretch	2591.1s	Ar	IR	1
	9	Deformation	1302.9vs	Ar	IR	1
	10	Deformation	950.9wm	Ar	IR	1

Reference

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CH_2NO_2

$^2B_1$ C_{2v}

In the gas phase, photodissociation into CH_2NO+O and into H_2CO+NO has been observed between 240 and 270 nm.[4]

In an Ar matrix, threshold for photodecomposition into H_2CO + NO near 290 nm.[1]

$^2A_2$ C_{2v}

T_0=12840(80) gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	NO_2 s-stretch	1444(25)	gas	PE	3
	4	CN stretch ?	936(25)	gas	PE	3
	5	NO_2 scissors	605(25)	gas	PE	3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s-stretch	3055 HF	Ar	IR	1,2
	2	CH_2 scissors	1419 HF	Ar	IR	1,2
	3	NO_2 s-stretch	1300(25)	gas	PE	3
			1297 HF	Ar	IR	1,2
	4	CN stretch	954(25)	gas	PE	3
			986 HF	Ar	IR	1,2
	5	NO_2 scissors	693 HF	Ar	IR	1,2
a_2	6	Torsion	205 H	gas	PE	3
b_1	7	CNO_2 OPLA[a]	719 HF	Ar	IR	1,2
	8	H_2CN OPLA[a]	606 HF	Ar	IR	1,2
b_2	9	CH_2 a-stretch	3200 HF	Ar	IR	1,2
	10	NO_2 a-stretch	1484[b] HF	Ar	IR	1,2
			1461			
	11	CH_2 rock	1095 HF	Ar	IR	1,2
	12	NO_2 rock	484T[c] HF	Ar	IR	1,2

CD_2NO_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	NO_2 s-stretch	1292(25)	gas	PE	3
			1296 DF	Ar	IR	1,2
	4	CN stretch + CD_2 scissors	906 DF	Ar	IR	1,2
	5	NO_2 scissors	668 DF	Ar	IR	1,2
a_2	6	Torsion	140 H	gas	PE	3
b_1	7	CNO_2 OPLA	694 DF	Ar	IR	1,2
b_2	10	NO_2 a-stretch	1460 DF	Ar	IR	1,2

[a]The two out-of-plane modes are strongly mixed.
[b]In Fermi resonance with $(\nu_4+\nu_{12})$.
[c]Estimated from $(\nu_4+\nu_{12})$.

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[4]D. R. Cyr, D. J. Leahy, D. L. Osborn, R. E. Continetti, and D. M. Neumark, J. Chem. Phys. **99**, 8751 (1993).

CH_2CFO

$\tilde{B}$ C_s

T_0=29874 gas LF[1] $\tilde{B}-\tilde{X}$ 307–335 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CO stretch	1790	gas	LF	1
	5	CF stretch	1253	gas	LF	1
	6	CH_2 rock	911	gas	LF	1
	7	CC stretch	874	gas	LF	1
	8	FCO bend	537	gas	LF	1
	9	CCO bend	421	gas	LF	1

τ_0=81.0(5) ns gas LF[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CO stretch	1724	gas	LF	1
	5	CF stretch	1211	gas	LF	1
	6	CH_2 rock	906T	gas	LF	1
	7	CC stretch	847	gas	LF	1
	8	FCO bend	584	gas	LF	1
	9	CCO bend	416T	gas	LF	1

Reference

[1]M. Furubayashi, I. Bridier, S. Inomata, N. Washida, and K. Yamashita, J. Chem. Phys. **106**, 6302 (1997).

$FeCCCCH^-$

Threshold for electron detachment from ground-state $FeCCCCH^-$ =13470(500) gas PE[1]

Reference

[1]J. Fan, L. Lou, and L.-S. Wang, J. Chem. Phys. **102**, 2701 (1995).

C_5H

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

A_{eff}=23.68; B_0=0.080 MW[1]

C_5D

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

A_{eff}=24.2; B_0=0.075 MW[2]

References

[1]C. A. Gottlieb, E. W. Gottlieb, and P. Thaddeus, Astron. Astrophys. **164**, L5 (1986).
[2]T. Hirota, H. Ozawa, Y. Sekimoto, and S. Yamamoto, J. Mol. Spectrosc. **174**, 196 (1995).

HCCCCO

$\tilde{X}$ C_s

B_{eff}=0.076 MW[1]

DCCCCO

$\tilde{X}$ C_s
B_{eff}=0.072 MW[1]

Reference

[1] H. Kohguchi, Y. Ohshima, and Y. Endo, J. Chem. Phys. **101**, 6463 (1994).

HCCCCS

$\tilde{X}$ $^2\Pi$ $C_{\infty v}$
B_0=0.048 MW[1]

DCCCCS

$\tilde{X}$ $^2\Pi$ $C_{\infty v}$
B_0=0.046 MW[1]

Reference

[1] Y. Hirahara, Y. Ohshima, and Y. Endo, J. Chem. Phys. **101**, 7342 (1994).

O=C=C=NOH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3583.2w	Ar	IR	1
	2	CCO stretch	2074.1vs	Ar	IR	1
	4	HON bend	1357.7wm	Ar	IR	1
	5	CNO stretch	889.1wT	Ar	IR	1
	6	CNO stretch	882.8m	Ar	IR	1
a''	10	HON deform.	512.5w	Ar	IR	1
	11	HON deform.	500.9vwT	Ar	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, B. Röther, and J. Eckwert, Liebigs Ann. **1996**, 303.

$HOONO_2$

In the gas phase, the threshold for unstructured absorption lies near 330 nm. This absorption increases steadily to a maximum at or beyond 190 nm.[4–7,10,12]

$\tilde{X}$ C_s Structure: MW[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3540.1wm	gas	IR	1,4,12
	2	NO_2 a-stretch	1728.3vs	gas	IR	1,3,7,12
	3	OH bend	1396.9wm	gas	IR	1,3,4,7,12,14
	4	NO_2 s-stretch	1304.2s	gas	IR	1–4,7,12
	5	O-O stretch	941.0w	gas	IR	1,3,11,12
			922.1w	gas	IR	1,3
			919.2w	gas	IR	1,3,11
	6	NO_2 scissors	802.54m	gas	IR,DL	1–4,7,9,12,13
	7	N-O stretch	648	gas	IR	13
	8	NO_2 rock	466	gas	IR	13
a''	10	NO_2 wag	722	gas	IR	11,13
	12	NO_2 torsion	145(6)	gas	MW	8

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

References

[1] H. Niki, P. D. Maker, C. M. Savage, and L. P. Breitenbach, Chem. Phys. Lett. **45**, 564 (1977).
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[13] R. R. Friedl, R. D. May, and G. Duxbury, J. Mol. Spectrosc. **165**, 481 (1994).
[14] S. Höjer, R. D. May, and C. E. Miller, J. Quant. Spectrosc. Radiat. Transfer **55**, 273 (1996).

NNBeBeNN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NN stretch	1804.1	Ar	IR	1
			1890.0	N_2	IR	1
			820.4	N_2	IR	1

Reference

[1] C. A. Thompson, L. Andrews, and R. D. Davy, J. Phys. Chem. **99**, 7913 (1995).

C_6

In an argon matrix, the growth behavior of the 1952.5 cm^{-1} infrared absorption on sample warmup has been tentatively correlated with that of an absorption maximum near 246 nm.[4]

$\tilde{A}$ $^3\Sigma_u^-$ $D_{\infty h}$
T_0=19558(5) Ne AB[10] $\tilde{A}$–$\tilde{X}$ 430–512 nm
19220 Ar AB[12]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		2096(5)	Ne	AB	10
	2		1566(5)	Ne	AB	10
	3		640(5)	Ne	AB	10

$\tilde{X}\ ^3\Sigma_g^-$ $D_{\infty h}$ Structure: ESR[2]DL[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	2061(10)	gas	TPE	6
			2050T	Ar	IR	11
	2	Sym. stretch	1322(10)	gas	TPE	5,6
	3	Stretch	489(10)	gas	TPE	6
Σ_u^+	4	Asym. stretch	1959.86	gas	DL	8
			1958.7	Ne	IR	9,10
			1952.0	Ar	IR	3,4,7
			1951.2	Kr	IR	11
	5	Asym. stretch	1199.4	Ne	IR	9
			1197.3	Ar	IR	1,3,7
			1197.0	Kr	IR	11
Π_g	7	Bend	240HT	gas	PE	5

B_0=0.048 DL[8]

References

[1] K. R. Thompson, R. L. DeKock, and W. Weltner, Jr., J. Am. Chem. Soc. **93**, 4688 (1971).
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[10] D. Forney, J. Fulara, P. Freivogel, M. Jakobi, D. Lessen, and J. P. Maier, J. Chem. Phys. **103**, 48 (1995).
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[12] J. Szczepanski, S. Ekern, and M. Vala, J. Phys. Chem. A **101**, 1841 (1997).

SiC_4Si

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	4	C=C stretch	1807.4	Ar	IR	1
	5	Si-C stretch	719.1	Ar	IR	1

Reference

[1] J. D. Presilla-Márquez, C. M. L. Rittby, and W. R. M. Graham, J. Chem. Phys. **106**, 8367 (1997).

Si_6

$\tilde{X}$ D_{4h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}			458	N_2	Ra	1
			300	N_2	Ra	1
b_{1g}			386	N_2	Ra	1
b_{2g}			252	N_2	Ra	1
e_g			404	N_2	Ra	1
e_u			462.9	Ne	IR	2
			460.9	Ar	IR	2
			458.5	Kr	IR	2

References

[1] E. C. Honea, A. Ogura, C. A. Murray, K. Raghavachari, W. O. Sprenger, M. F. Jarrold, and W. L. Brown, Nature (London) **366**, 42 (1993).
[2] S. Li, R. J. Van Zee, W. Weltner, Jr., and K. Raghavachari, Chem. Phys. Lett. **243**, 275 (1995).

C_6^-

Threshold for electron detachment from ground-state C_6^-=33725(10) gas PE[1,2]TPE[3]

$\tilde{F}$ $D_{\infty h}$
T_0=33680T gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		2058(5)	gas	PE	3
	2		1307(5)	gas	PE	3
	3		480(2)	gas	PE	3
Σ_u^+	5		837HT	gas	PE	3
Π_g	7		195HT	gas	PE	3
Π_u	8		313HT	gas	PE	3
	9		93HT	gas	PE	3

(3)$^2\Pi_g$ $D_{\infty h}$
T_0=22517(10) Ne AB[8] 401–445 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	2		1861(17)	Ne	AB	8
	3		626(15)	Ne	AB	8
Π_u	9		157(7)H	Ne	AB	8

(2)$^2\Pi_g$ $D_{\infty h}$
T_0=20064(8) Ne AB[8] 470–499 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	3		597(12)	Ne	AB	8
Π_g	7		237(6)H	Ne	AB	8
Π_u	9		152(6)H	Ne	AB	8

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

T_0=16476 gas PD[5] $\tilde{C}-\tilde{X}$ 445–629 nm

16458(5) Ne AB[4] $\tilde{C}-\tilde{X}$ 539–608 nm

16239 Ar AB[6] $\tilde{C}-\tilde{X}$ 573–616 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2052	gas	PD	5
			2064(5)	Ne	AB	4
	2	C≡C stretch	1767	gas	PD	5
			1817(5)	Ne	AB	4
	3	C-C stretch	602	gas	PD	5
			607(5)	Ne	AB	4
			605T	Ar	AB	6
Π_g	8		245H	gas	PD	5
Π_u	9		110H	gas	PD	5

$\tilde{A}\ ^2\Sigma_g^+$ $D_{\infty h}$

T_0=9352(2) Ne AB[8] $\tilde{A}-\tilde{X}$ 737–1070 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		2111(4)	Ne	AB	8
	2		1912(4)	Ne	AB	8
	3		651(3)	Ne	AB	8
Π_g	7		238(2)H	Ne	AB	8
Π_u	9		128(2)H	Ne	AB	8

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	3	C-C stretch	564	gas	PD	5
Σ_u^+	4	Asym. stretch	1938.5	Ne	IR	7
			1936.7	Ar	IR	6
Π_g	7		220T	gas	PE	3
	8		201H	gas	PD	5
Π_u	9		111T	gas	PE	3

A=−29(2) gas PE[3]

References

[1] S. Yang, K. J. Taylor, M. J. Craycraft, J. Conceicao, C. L. Pettiette, O. Cheshnovsky, and R. E. Smalley, Chem. Phys. Lett. **144**, 431 (1988).
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[6] J. Szczepanski, S. Ekern, and M. Vala, J. Phys. Chem. A **101**, 1841 (1997).
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C_5N

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

B_0=0.0468 MW[1]

Reference

[1] Y. Kasai, Y. Sumiyoshi, Y. Endo, and K. Kawaguchi, Astrophys. J. **477**, L65 (1997).

NCC≡CCN$^+$

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

T_0=25500(160) gas PE[1,3]

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

T_0=18720(160) gas PE[1,3]

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

T_0=17430(160) gas PE[1,3]

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

T_0=16781(1) gas EF[2]LF[3] $\tilde{A}-\tilde{X}$ 528–720 nm

16679 Ne LF[4] $\tilde{A}-\tilde{X}$ 530–816 nm

16709 Ne LF[4]AB[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡N stretch	2151(3)	gas	LF	3
			2154(2)	Ne	LF	4
	2	C≡C stretch	2099(3)	gas	LF	3
			2094(2)	Ne	LF	4
	3	C-C stretch	696(3)	gas	LF	3
			511(2)	Ne	LF	4
Π		Bend	440H	Ne	AB	5

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
			2220	Ne	LF	4
	2	C≡C stretch	1930(10)	gas	EF	2,3
			1942	Ne	LF	4
	3	C-C stretch	570(10)	gas	EF	2,3
			613	Ne	LF	4
Σ_u^+	4		2010[a]	Ne	LF	4
	5		1208[a]	Ne	LF	4

[a] From overtones and combination bands.

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$(NUO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}			823.3	Ar	IR	1
			674.1	Ar	IR	1
b_{3u}		UN stretch	479.5	Ar	IR	1

Reference

[1] G. P. Kushto, P. F. Souter, L. Andrews, and M. Neurock, J. Chem. Phys. **106**, 5894 (1997).

C_5O

$\tilde{X}$ $^1\Sigma^+$ $C_{\infty v}$ Structure: MW[1]
B_0=0.046 MW[1]

Reference

[1] T. Ogata, Y. Ohshima, and Y. Endo, J. Am. Chem. Soc. **117**, 3593 (1995).

NCCCNC

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡C stretch	2287.1s	Ar	IR	1,2
	2	-C≡N stretch	2203.6s	Ar	IR	1,2
	3	-N≡C stretch	2044.8vs	Ar	IR	1,2
	4	C-C,C-N a-stretch	1202.3vw	Ar	IR	1,2
	5	C-C,C-N s-stretch	610.1vwT	Ar	IR	1,2

References

[1] A. M. Smith, G. Schallmoser, A. Thoma, and V. E. Bondybey, J. Chem. Phys. **98**, 1776 (1993).
[2] A. M. Smith, V. E. Bondybey, M. Horn, and P. Botschwina, J. Chem. Phys. **100**, 765 (1994).

Fe_2O_4

$\tilde{A}$
T_0=1450(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			720(60)	gas	PE	1

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			710(60)	gas	PE	1

Reference

[1] H. Wu, S. R. Desai, and L.-S. Wang, J. Am. Chem. Soc. **118**, 5296 (1996).

Cu_2O_4

$\tilde{C}$
T_0=3630(400) gas PE[1]

$\tilde{B}$
T_0=2420(400) gas PE[1]

$\tilde{A}$
T_0=1290(400) gas PE[1]

Reference

[1] L.-S. Wang, H. Wu, S. R. Desai, and L. Lou, Phys. Rev. B **53**, 8028 (1996).

$Fe_2O_4^-$

Threshold for electron detachment from ground-state $Fe_2O_4^-$=28720(320) gas PE[1]

Reference

[1] H. Wu, S. R. Desai, and L.-S. Wang, J. Am. Chem. Soc. **118**, 5296 (1996).

$Cu_2O_4^-$

Threshold for electron detachment from ground-state $Cu_2O_4^-$=28240(240) gas PE[1]

Reference

[1] L.-S. Wang, H. Wu, S. R. Desai, and L. Lou, Phys. Rev. B **53**, 8028 (1996).

$ONCCNO^+$

$\tilde{C}$ $^2\Pi_u$ $D_{\infty h}$
T^a=54200(200) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+			1613(40)	gas	PE	1

$\tilde{B}$ $^2\Pi_g$ $D_{\infty h}$
T^a=47200(1000) gas PE[1]

$\tilde{A}$ $^2\Pi_u$ $D_{\infty h}$
T^a=16700(200) 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^+			2097(40)	gas	PE	1

[a]From vertical ionization potentials.

Reference

[1] T. Pasinszki and N. P. C. Westwood, J. Am. Chem. Soc. **117**, 8425 (1995).

Al_2O_4

$\tilde{A}$

T_0=9040(640) gas PE[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Sym. stretch	930(60)	gas	PE	1

Reference

[1] S. R. Desai, H. Wu, C. M. Rohlfing, and L.-S. Wang, J. Chem. Phys. **106**, 1309 (1997).

ONCCNO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u	4		2246.04	gas	IR	1,2
	5		1258.48	gas	IR	1,2

B_0=0.042 IR[2]

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[1] T. Pasinszki and N. P. C. Westwood, J. Am. Chem. Soc. **117**, 8425 (1995).
[2] B. Guo, T. Pasinszki, N. P. C. Westwood, and P. F. Bernath, J. Chem. Phys. **103**, 3335 (1995).

$Al_2O_4^-$

Threshold for electron detachment from ground-state $Al_2O_4^-$=32110(240) gas PE[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Sym. stretch	1090(60)	gas	PE	1

Reference

[1] S. R. Desai, H. Wu, C. M. Rohlfing, and L.-S. Wang, J. Chem. Phys. **106**, 1309 (1997).

Si_2O_4

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{1u}	7	Si=O stretch	1293.3	Ar	IR	1
	8	Si-O stretch	786.4	Ar	IR	1
b_{2u}	9		442w	Ar	IR	1
b_{3u}	11	Si-O stretch	889.2	Ar	IR	1
			285w	Ar	IR	1

Reference

[1] T. Mehner, H. J. Göcke, S. Schunck, and H. Schnöckel, Z. Anorg. Allg. Chem. **580**, 121 (1990).

F_2BNCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NCO a-stretch	2333vs	gas	IR	1
	2	Mixed	1569Ts 1553Ts	gas	IR	1
	3	BF_2 a-stretch	1413s	gas	IR	1
	4	BF_2 s-stretch	1213s	gas	IR	1
a''	10		659	gas	IR	1

Reference

[1] M. Alaee, E. G. Livingstone, and N. P. C. Westwood, J. Am. Chem. Soc. **115**, 2871 (1993).

$Si_2O_4^-$

Threshold for electron detachment from ground-state $Si_2O_4^-$=20980(800) gas PE[1]

Reference

[1] L.-S. Wang, H. Wu, S. R. Desai, J. Fan, and S. D. Colson, J. Phys. Chem. **100**, 8697 (1996).

N_2O_4

In the gas phase, absorption increases between 300 and 180 nm, with some indication of maxima near 265 and 190 nm.[7]

A broad gas-phase absorption with onset near 380 nm has its maximum near 340 nm.[7]

$\tilde{X}$ D_{2h} Structure: ED[1]IR[10,11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1		1383(3)	Ne	Ra	8
			1383	Ar	Ra	5
			1387(3)	Xe	Ra	8
	2		807(3)	Ne	Ra	8
			813	Ar	Ra	5
			815(3)	Xe	Ra	8
	3		265(3)	Ne	Ra	8
			262	Ar	Ra	5
			257(3)	Xe	Ra	8
a_u	4		82T	gas	IR[a]	6,12
b_{1g}	5		1718(3)	Xe	Ra	8
	6		480T	gas	IR[a]	6,12
			498(3)	Ne	Ra	8
			485(3)	Xe	Ra	8
b_{1u}	7		425	gas	IR	6
b_{2g}	8		657(3)	Xe	Ra	8
b_{2u}	9		1756.76	gas	IR,DL	6,10,13,14
			1749.2s	Ar	IR	2,3,9
			1735s			
			1761	N_2	IR	4
			1737			
			1750	O_2	IR	3
			1735			
	10		265T	gas	IR	11
b_{3u}	11		1261.08	gas	IR,DL	2,6,11,13,14
			1257.0s	Ar	IR	2,3,9
			1261	N_2	IR	4
			1261	O_2	IR	3
	12		755.37[b]	gas	IR	6,13
			747.85[b]	gas	IR	6,13
			755sh	Ar	IR	3
			745.8			
			751	N_2	IR	4
			755	O_2	IR	3
			746			

$A_0=0.218$; $B_0=0.122$; $C_0=0.078$ IR[10,11]DL[14]
Barrier to internal rotation = 1900(200) gas IR[12]

[a]From analysis of sequence bands near 540 cm^{-1}.
[b]Fermi resonance between ν_{12} and $\nu_6+\nu_{10}$.

References

[1] D. W. Smith and K. Hedberg, J. Chem. Phys. **25**, 1282 (1956).
[2] W. G. Fateley, H. A. Bent, and B. Crawford, Jr., J. Chem. Phys. **31**, 204 (1959).
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CF_3CO

$\tilde{A}$

$T_0=26023$ gas LF[2] $\tilde{A}-\tilde{X}$ 353–455 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			781(30)	gas	LF	2
		CCO bend	357(30)	gas	LF	2

$\tau=0.34$ μs gas LF[2]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1550(30)	gas	IR,LF	1,2
		CF_3 stretch	1338	gas	IR	1
		CF_3 stretch	1115	gas	IR	1
		CC stretch	1024	gas	IR	1
		CCO bend	633(30)	gas	LF	2

References

[1] M. Kozuka and T. Isobe, Bull. Chem. Soc. Jpn. **49**, 1766 (1976).
[2] Z. Li and J. S. Francisco, Mol. Phys. **79**, 1127 (1993).

$ClOClO_3$

An unstructured gas-phase absorption with maximum at 42740 (234 nm) has been assigned[4] to $ClOClO_3$.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ClO_2 s-stretch	1283vs	gas	IR	1–3,5
			1293.2	Ne	IR	6
			1287vs	Ar	IR	2
	2	Cl=O stretch	1040s	gas	IR	1,2
			1040.2	Ne	IR	6
			1039s	Ar	IR	2
	3	O-Cl stretch	749wm	gas	IR	1,2
			747.5	Ne	IR	6
			746m	Ar	IR	2
	4	Cl-O stretch	646vs	gas	IR	1,2
			652.1	Ne	IR	6
			647vs	Ar	IR	2
	5	O=Cl=O bend	580sh	gas	IR	2
			586.9	Ne	IR	6
			582m	Ar	IR	2
	6	ClO_3 deform.	511wm	gas	IR	2
			514.6	Ne	IR	6
			513m	Ar	IR	2
	7	O=Cl-O bend	355vw	Ar	IR	2
a''	9	ClO_2 a-stretch	1283vs	gas	IR	1–3,5
			1277.6	Ne	IR	6
			1271vs	Ar	IR	2
	10	O=Cl=O bend	561m	gas	IR	2
			565.3	Ne	IR	6
			561ms	Ar	IR	2
	11	O=Cl-O bend	382w	Ar	IR	2

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8.13. Seven-Atomic Molecules

C_2H_5

3*p* Rydberg state

In the gas phase, an absorption with maximum at 205 nm has been assigned[6,7] to the $3p-\tilde{X}$ transition of C_2H_5. The detection of this band in MPI studies[9] is consistent with the assignment to a Rydberg state.

3*s* Rydberg state

In the gas phase, a broad, unstructured absorption with maximum at 246 nm has been assigned[1,3,6,7] to the $3s-\tilde{X}$ transition of C_2H_5.

$\tilde{X}$ C_s Structure: MO[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CH_2 s-stretch	3033m	Ar	IR	2,4,5,8
			3032.6	H_2	IR	11
		CH_3 s-stretch	2920m	Ar	IR	4,5
		2-CH stretch	2842s	Ar	IR	2,4,5,8
		CH_2 deform.	1440m	Ar	IR	2,4,5,8
			1383	Ar	IR	8
		CH_3 deform.	1366m	Ar	IR	2,4,5,8
		CC stretch	1138w	Ar	IR	4,5,8
			1025	Ar	IR	8
		CCH_2 umbrella	528.1	gas	DL	10
			540vs	Ar	IR	2,4,5,8
a''		CH_2 a-stretch	3112s	Ar	IR	2,4,5,8
			3122.8	H_2	IR	11
		CH_3 a-stretch	2987s	Ar	IR	2,4,5
			2984.3	H_2	IR	11
		CH_3 deform.	1440m	Ar	IR	2,4,5,8
		H deform.	1175m	Ar	IR	4,5,8

C_2D_5

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CD_2 s-stretch	2199m	Ar	IR	4,5
		CD_3 s-stretch	2094m	Ar	IR	4,5
		2-CD stretch	2048m	Ar	IR	4,5
		CD_3 deform.	1070m	Ar	IR	4,5
		CD_3 deform.	1035m	Ar	IR	4,5
		CCD_2 umbrella	398vs	Ar	IR	4,5
a''		CD_2 a-stretch	2249m	Ar	IR	4,5
		CD_3 a-stretch	2170s	Ar	IR	4,5
		CD_3 deform.	1041m	Ar	IR	4,5

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[1] H. R. Wendt, D. Wyrsch, and H. E. Hunziker, Ber. Bunsenges. Phys. Chem. **78**, 201 (1974).
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$H_5O_2^+$

$\tilde{X}$ C_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		H_2O a-stretch	3684.4	gas	PF	1,2
		H_2O s-stretch	3608.8	gas	PF	1

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[1] L. I. Yeh, M. Okumura, J. D. Myers, J. M. Price, and Y. T. Lee, J. Chem. Phys. **91**, 7319 (1989).
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$H_2CCCH_2^+$

$\tilde{B}$

T^a=61400(800) gas PE[1]

$\tilde{A}$ ^2E D_2

T_0=35638(32) gas PE[1–4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_2 scissors	1320(6)	gas	PE	3,4
b_2	7	CH_2 deform.	1030(6)	gas	PE	3,4

$\tilde{X}$ ^2E D_2 Structure: PE[2,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_1	4	Torsion	745(5)	gas	PE	3,4
b_2	6	C_3 a-stretch	1802(10)	gas	PE	4

$D_2CCCD_2^+$

$\tilde{X}$ ^2E D_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_1	4	Torsion	565(50)	gas	PE	1

[a]From vertical ionization potential.

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[1] R. K. Thomas and H. Thompson, Proc. R. Soc. London, Ser. A **339**, 29 (1974).
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cyc-C_2SiH_4

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	3061.2w	Ar	IR	1
	2	SiH stretch	2166.7vs	Ar	IR	1
	3	CC stretch	1467.2m	Ar	IR	1
	4	SiH_2 deform.	975.9vs	Ar	IR	1
	5	CH deform.	900.6w	Ar	IR	1
	6	SiC stretch	778.5wm	Ar	IR	1
b_1	9	SiH stretch	2176.3s	Ar	IR	1
	10	Deformation	695.1ms	Ar	IR	1
	11	Deformation	589.2wm	Ar	IR	1
b_2	12	CH stretch	3041.6wm	Ar	IR	1
	13	CH deform.	1105.1m	Ar	IR	1
	14	SiC stretch	707.4m	Ar	IR	1
	15	SiH_2 deform.	655.4m	Ar	IR	1

Reference

[1] G. Maier, H. Pacl, and H. P. Reisenauer, Angew. Chem. **107**, 1627 (1995); Angew. Chem. Int. Ed. Engl. **34**, 1439 (1995).

$CH_2{=}CHOH^+$

$\tilde{D}$ $^2A'$ C_s
T^a=82300(400) gas PE[1,2]

$\tilde{C}$ $^2A'$ C_s
T^a=61200(400) gas PE[1,2]

$\tilde{B}$ $^2A''$ C_s
T^a=41300(400) gas PE[1,2]

$\tilde{A}$ $^2A'$ C_s
T^a=35400(400) gas PE[1,2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1400(50)	gas	PE,PI	2,3

[a]Values for syn- rotamer. From vertical ionization potential.

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[1] B. Albrecht, M. Allan, E. Haselbach, L. Neuhaus, and P. A. Carrupt, Helv. Chim. Acta **67**, 216 (1984).
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CH_3CHS

$\tilde{F}$ $^1A''$ C_s
T_0=51560(200) gas AB[2]

$\tilde{D}$ or $\tilde{E}$ $^1A'$ C_s
T_0=52770(100) gas AB[2]

$\tilde{C}$ $^1A'$ C_s
T_0=45260(100) gas AB[2]

$\tilde{B}$ $^1A'$ C_s
T^a=47600(100) gas AB[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		C=S stretch	1154	gas	AB	2

$\tilde{A}$ $^1A''$ C_s
T_0=17900(100) gas AB[2]
τ_0=0.40(5) μs gas LF[4]

$\tilde{a}$ $^3A''$ C_s
T_0=16294.9 gas AB[2,3]LF[7] $\tilde{a}-\tilde{X}$ 571–630 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	9	CS stretch	747.2	gas	AB,LF	3,7
	10	CCS deform.	283.9	gas	LF	7
a''	14	Wag	249.4	gas	LF	7
	15	Torsion	52.0	gas	LF	7

$\tau\sim$ 8.2 μs gas LF[4]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3010.4w	Ar	IR	6,8
		CH stretch	2982.0w	Ar	IR	6,8
		CH stretch	2944.4m	Ar	IR	6,8
		CH stretch	2908.7w	Ar	IR	6
			1435.3m	Ar	IR	6,8
			1433.4wm	Ar	IR	6
			1357.7s	Ar	IR	6,8
			1345.6vs	Ar	IR	6,8
		C=S stretch	1240	gas	AB	3
			1140.7s	Ar	IR	6,8
			1065.0wm	Ar	IR	6,8
			1020.2wm	Ar	IR	6,8
			820.1w	Ar	IR	6,8
			747.8s	Ar	IR	6,8
	15	Torsion	163.0	gas	LF	7

A_0=1.620; B_0=0.192; C_0=0.177 MW[1]

CD_3CDS

$\tilde{a}$ $^3A''$ C_s
T_0=16367.2 gas AB^3LF^7 $\tilde{a}-\tilde{X}$ 580–630 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	8	DCS deform.	751.8	gas	LF	7
	9	CS stretch	677.2	gas	AB,LF	3,7
a''	15	Torsion	29.6	gas	LF	7

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a''	15	Torsion	122.6	gas	LF	7

[a]Maximum of diffuse absorption with partially resolved structure.

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FCH_2CH_2

$\tilde{X}$ C_s Structure: MO[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_2 stretch	2885wm	Ar	IR	3
		CH_2 stretch	2856m	Ar	IR	2,3
		Deformation	1449w	Ar	IR	3
		Deformation	1426wm	Ar	IR	3
		CH_2 wag	1242vw	Ar	IR	3
		Mixed	1087s	Ar	IR	3
		CF stretch	1047s[a]	Ar	IR	2
		CCF deform.	427wm	Ar	IR	2

FCD_2CD_2

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		2-CD_2 stretch	2090wm	Ar	IR	2
		CF stretch + CD_2 scissors	1211s	Ar	IR	2
			1091m	Ar	IR	2
			1059wm	Ar	IR	2
		CF stretch + CD_2 scissors	969s	Ar	IR	2
		CCF deform.	424w	Ar	IR	2

[a]Ref. 3 proposes the assignment of this absorption to *t*-CH_2FCH_2F. Although that product is known to absorb near 1047 cm^{-1}, such an assignment is inconsistent with the infrared absorption pattern[2] obtained in a study of the reaction of F atoms with C_2H_4-1-^{13}C, as well as with the low yield of the more stable *gauche*-CH_2FCH_2F in the earlier work.[2]

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$CH_2(OH)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3637.6m[a]T	Ar	IR	1
		OH stretch	3564.4m[b]T	Ar	IR	1
		COH deform.	1424.4wmT	Ar	IR	1
		COH deform.	1358.7wT	Ar	IR	1
		CH_2 wag	1334.6wT	Ar	IR	1
		CO stretch	1056.5sT	Ar	IR	1
		CO torsion	547.7mT	Ar	IR	1

[a]Rotamer 1.
[b]Rotamer 2.

Reference

[1] C. Lugez, A. Schriver, R. Levant, and L. Schriver-Mazzuoli, Chem. Phys. **181**, 129 (1994).

$C_2H_3CN^+$

$\tilde{E}$ $^2A'$ C_s
T^a=42430(20) gas PE[1]

$\tilde{D}$ $^2A'$ C_s
T^a=27980(20) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		H deformation	1494T	gas	PE	1

$\tilde{C}\ ^2A''$ C_s
T_0=20340(60) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		H deformation	1363(32)	gas	PE	1
			678(32)	gas	PE	1

$\tilde{B}\ ^2A'$ C_s
T_0=16890(20) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		H deformation	1137(24)	gas	PE	1
			660(24)	gas	PE	1

$\tilde{A}\ ^2A'$ C_s
T_0=11530(20) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C≡N stretch	1903(16)	gas	PE	1
		H deformation	1194(24)	gas	PE	1
		C_3 deformation	492(32)	gas	PE	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C≡N stretch	2121(16)	gas	PE	1
		C=C stretch	1335(24)	gas	PE	1
			928(30)	gas	PE	1
			839(30)	gas	PE	1
			347(30)	gas	PE	1

[a]From vertical ionization potential.

Reference

[1]J. Delwiche, M. Gochel-Dupuis, J. E. Collin, and J. Heinesch, J. Electron Spectrosc. Relat. Phenom. **66**, 65 (1993).

$H_2C=(cyc\text{-}CN=CH)$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1818	Kr	IR	1

Reference

[1]K. Banert, M. Hagedorn, E. Knözinger, A. Becker, and E.-U. Würthwein, J. Am. Chem. Soc. **116**, 60 (1994).

CH_3OCN

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH_3 a-stretch	3042wT	gas	IR	1
	2	CH_3 s-stretch	2968	gas	IR	1
	3	OCN a-stretch	2263vs	gas	IR	1
	6	CH_3 rock	1213	gas	IR	1
	7	Skel. stretch	1112	gas	IR	1
	8	Skel. stretch	883T	gas	IR	1
a''	11	CH_3 a-stretch	3017	gas	IR	1
	12	CH_3 a-deform.	1462	gas	IR	1

Reference

[1]T. Pasinszki and N. P. C. Westwood, J. Phys. Chem. **99**, 1649 (1995).

$B(OH)_3$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3705	gas	Ra	2
	2	BOH deform.	1020	gas	Ra	2
	3	BO stretch	866	gas	Ra	2
a''	4	BO_3 OPLA	666.4	Ar	IR	3
			675.0	N_2	IR	1
	5	Torsion	436.0	Ar	IR	3
			513.8	N_2	IR	1
e'	6	OH stretch	3706	gas	IR	2
			3688.6	Ar	IR	3
			3668.5	N_2	IR	1
	7	BO stretch	1429	gas	IR	2
			1414.9	Ar	IR	3
			1426.2	N_2	IR	1
	8	HOB deform.	1017	gas	IR	2
			992.4	Ar	IR	3
			1009.9	N_2	IR	1
	9	BO_2 deform.	432.1	Ar	IR	3
			448.9	N_2	IR	1
e''	10	HOB deform.	520(5)[a]	Ar	IR	3

$B(OD)_3$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	BO stretch	887	gas	Ra	2
	3	BOD deform.	706	gas	Ra	2
a''	4	BO_3 OPLA	665.5	Ar	IR	3
	5	Torsion	317.6	Ar	IR	3
			376.0	N_2	IR	1
e'	6	OD stretch	2726	gas	IR	2
			2719.8	Ar	IR	3
			2704.6	N_2	IR	1
	7	BO stretch	1405	gas	IR	2
			1396.6	Ar	IR	3
	8	DOB deform.	810	gas	IR	2
			807.9	Ar	IR	3
			825.5	N_2	IR	1
	9	BO_2 deform.	385.9	Ar	IR	3
			404.7	N_2	IR	1
e''	10	DOB deform.	390(10)[a]	Ar	IR	3

[a]From combination bands.

References

[1] J. S. Ogden and N. A. Young, J. Chem. Soc. Dalton Trans. 1645 (1988).
[2] T. R. Gilson, J. Chem. Soc. Dalton Trans. 2463 (1991).
[3] L. Andrews and T. R. Burkholder, J. Chem. Phys. **97**, 7203 (1992).

CH_3CF_2

3*p* Rydberg state C_s
T_0=43275(40)U gas MPI[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	9	CF_2 wag	530	gas	MPI	1

Reference

[1] J. L. Brum, R. D. Johnson III, and J. W. Hudgens, J. Phys. Chem. **98**, 3645 (1994).

$C_5H_2^+$

$\tilde{A}$ $^2\Pi_g$ $D_{\infty h}$
T_0=20026(5)T Ne AB[1]

Reference

[1] P. Freivogel, J. Fulara, D. Lessen, D. Forney, and J. P. Maier, Chem. Phys. **189**, 335 (1994).

HC_5H

$^3\Sigma_u^-$ $D_{\infty h}$
T_0=23033(5) Ne AB[1] $^3\Sigma_u^- - \tilde{X}$ 390–435 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	2	C≡C s-stretch	1817(5)	Ne	AB	1
	3		751(5)	Ne	AB	1

$\tilde{X}$ $^3\Sigma_g^-$ $D_{\infty h}$
A_0=9.26; B_0=0.077; C_0=0.076 MW^2

References

[1] J. Fulara, P. Freivogel, D. Forney, and J. P. Maier, J. Chem. Phys. **103**, 8805 (1995).
[2] M. C. McCarthy, M. J. Travers, A. Kovács, W. Chen, S. E. Novick, C. A. Gottlieb, and P. Thaddeus, Science **275**, 518 (1997).

t-HCCCHOO

Irradiation at wavelengths longer than 590 nm leads to photodestruction and, in an argon matrix, to stabilization of HCC(*cyc*-CHOO).[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CH stretch	3313.5s	Ar	IR	1
		C≡C stretch	2093.8s	Ar	IR	1
		HCO bend	1401.5m	Ar	IR	1
		CO stretch	1221.2m	Ar	IR	1
		Mixed	1026.4s	Ar	IR	1
		OO stretch	933.3s	Ar	IR	1
		CCO bend	739.0m	Ar	IR	1
		HCC bend	655.6m	Ar	IR	1
a''		HCC bend	646.5m	Ar	IR	1
		Skel. OPLA	497.1w	Ar	IR	1

Reference

[1] S. Wierlacher, W. Sander, C. Marquardt, E. Kraka, and D. Cremer, Chem. Phys. Lett. **222**, 319 (1994).

c-HCCCHOO[a]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1412	Ar	IR	1
		CO stretch	1234	Ar	IR	1
		OO stretch	983	Ar	IR	1
			914	Ar	IR	1

[a]Tentative identification.

Reference

[1] S. Wierlacher, W. Sander, C. Marquardt, E. Kraka, and D. Cremer, Chem. Phys. Lett. **222**, 319 (1994).

HCC(*cyc*-CHOO)[a]

Photodecomposes into CO_2, C_2H_2, and propiolic acid on irradiation near 25000 (403(20) nm).[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3319	Ar	IR	1
			1397	Ar	IR	1
			1375	Ar	IR	1
			1247	Ar	IR	1
			950	Ar	IR	1
			873	Ar	IR	1
			676	Ar	IR	1

[a]Tentative identification.

Reference

[1] S. Wierlacher, W. Sander, C. Marquardt, E. Kraka, and D. Cremer, Chem. Phys. Lett. **222**, 319 (1994).

C_6H

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

T_0=18992.4 gas CR[8] $\tilde{A}-\tilde{X}$ 484–528 nm

18854(5) Ne AB[7] $\tilde{A}-\tilde{X}$ 444–530 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	C≡C stretch	2076(5)	Ne	AB	7
	5	C≡C stretch	1630.8	gas	CR	8
			1638(5)	Ne	AB	7
	6	C-C stretch	659.5	gas	CR	8
			658(5)	Ne	AB	7

A_0=−7.9 gas CR[8]
B_0=0.045 CR[8]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		C≡C stretch	1962.2T	Ne	IR	7
			1953.4	Ar	IR	6

A_{eff}=−15.1 gas MW[3–5]
B_0=0.046 MW[1–5]

C_6D

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

T_0=19043.9 gas CR[8] $\tilde{A}-\tilde{X}$ 524–526 nm

18900(10) Ne AB[8]

A_0=−8.2 gas CR[8]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		C≡C stretch	1862.4	Ar	IR	6

References

[1] H. Suzuki, M. Ohishi, N. Kaifu, S. Saito, and K. Kawaguchi, Publ. Astron. Soc. Jpn. **38**, 911 (1986).
[2] M. Guélin, J. Cernicharo, C. Kahane, J. Gómez-González, and C. M. Walmsley, Astron. Astrophys. **175**, L5 (1987).
[3] J. Cernicharo, M. Guélin, K. M. Menten, and C. M. Walmsley, Astron. Astrophys. **181**, L1 (1987).
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[5] J. C. Pearson, C. A. Gottlieb, D. R. Woodward, and P. Thaddeus, Astron. Astrophys. **189**, L13 (1988).
[6] T. J. Doyle, L. N. Shen, C. M. L. Rittby, and W. R. M. Graham, J. Chem. Phys. **95**, 6224 (1991).
[7] D. Forney, J. Fulara, P. Freivogel, M. Jakobi, D. Lessen, and J. P. Maier, J. Chem. Phys. **103**, 48 (1995).
[8] M. Kotterer and J. P. Maier, Chem. Phys. Lett. **266**, 342 (1997).

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

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

T_0=27350(160) gas PE[1]

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

T_0=21860(160) gas PE[1]

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

T_0=17190(5) gas EF[1] $\tilde{A}-\tilde{X}$ 580–670 nm

17098(20) Ne AB[2]LF[3] $\tilde{A}-\tilde{X}$ 494–820 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+			1870(160)	gas	EF	1
	3	C≡C stretch	2006(5)	Ne	AB	2
	4	CN stretch	1849(5)	Ne	AB	2
	5	C-C stretch	1187(5)	Ne	AB	2
	6	C-C stretch	600(160)	gas	EF	1
			584(5)	Ne	AB	2

τ_0=15(2) ns gas EF[1]
A=17T Ne LF[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	3403.4	Ne	LF	3
	2	C≡N stretch	2190(10)	gas	EF	1
			2194.6	Ne	LF	3
	3	C≡C stretch	2070(10)	gas	EF	1
			2070.2	Ne	LF	3
	4	C≡C stretch	1912.7	Ne	LF	3
	5	C-C stretch	1220(10)	gas	EF	1
			1213	Ne	LF	3
	6	C-C stretch	630(10)	gas	EF	1
			625	Ne	LF	3

A=91T Ne LF[3]

References

[1] G. Bieri, E. Kloster-Jensen, S. Kvisle, J. P. Maier, and O. Marthaler, J. Chem. Soc. Faraday Trans. 2 **76**, 676 (1980).
[2] D. Forney, P. Freivogel, J. Fulara, and J. P. Maier, J. Chem. Phys. **102**, 1510 (1995).
[3] A. M. Smith, J. Agreiter, and V. E. Bondybey, Chem. Phys. Lett. **244**, 379 (1995).

C_7

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

T_0=39556(30)T Ne AB[7] — $^1\Sigma_u^+-\tilde{X}$ 246–253 nm

40470 Ar AB[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			979(30)	Ne	AB	7
			428(30)	Ne	AB	7

T_0=32765(22)T Ne AB[7] — 246–306 nm

34360T Ar AB[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1256(25)	Ne	AB	7
			695(25)	Ne	AB	7

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

T_0=18440(7) Ne AB[7] — $^1\Pi_u-\tilde{X}$ 485–543 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2170(10)	Ne	AB	7
			1873(10)	Ne	AB	7
			568(10)	Ne	AB	7
			478(10)	Ne	AB	7

$\tilde{X}$ $D_{\infty h}$ Structure: DL[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	3	Sym. stretch	548(90)	gas	PE	5
			582T	Ar	IR	9
Σ_u^+	4	Asym. stretch	2138.315	gas	DL	1,2
			2134.6	Ne	IR	6,7
			2127.8	Ar	IR	8
			2120.4	Kr	IR	9
	5	Asym. stretch	1898.376	gas	DL	3
			1897.5	Ne	IR	6,7
			1894.3	Ar	IR	8
			1889.3	Kr	IR	9
Π_u	7	Bend	496(110)T	gas	PE	5

B_0=0.031 DL[1–3]

References

[1] J. R. Heath, R. A. Sheeks, A. L. Cooksy, and R. J. Saykally, Science **249**, 895 (1990).
[2] J. R. Heath and R. J. Saykally, J. Chem. Phys. **94**, 1724 (1991).
[3] J. R. Heath, A. Van Orden, E. Kuo, and R. J. Saykally, Chem. Phys. Lett. **182**, 17 (1991).
[4] J. Szczepanski and M. Vala, J. Phys. Chem. **95**, 2792 (1991).
[5] D. W. Arnold, S. E. Bradforth, T. N. Kitsopoulos, and D. M. Neumark, J. Chem. Phys. **95**, 8753 (1991).
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[8] R. H. Kranze, C. M. L. Rittby, and W. R. M. Graham, J. Chem. Phys. **105**, 5313 (1996).
[9] J. Szczepanski, S. Ekern, C. Chapo, and M. Vala, Chem. Phys. **211**, 359 (1996).

Si_7

$\tilde{X}$ D_{5h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'			435	N_2	Ra	1
			358	N_2	Ra	1
e_1'			422.4	Ar	IR	2
			420.4	Kr	IR	2
e_2'			340	N_2	Ra	1
			289	N_2	Ra	1

References

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[2] S. Li, R. J. Van Zee, W. Weltner, Jr., and K. Raghavachari, Chem. Phys. Lett. **243**, 275 (1995).

C_7^-

Threshold for electron detachment from ground-state C_7^-=27090(115) gas PE[1,2]

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

T_0=35231(25) Ne AB[6] — $\tilde{C}-\tilde{X}$ 278–284 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	3		491(25)	Ne	AB	6

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

T_0=20330(10) gas MPD[5]

20314(8) Ne AB[6] — $\tilde{B}-\tilde{X}$ 380–493 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1990(40)	gas	MPD	5
			2058(10)	Ne	AB	6
	2		1569(9)	Ne	AB	6
	3		575(8)	Ne	AB	6

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

T_0=15950(10) gas MPD[5]

15954(5) Ne AB[6] — $\tilde{A}-\tilde{X}$ 495–627 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1810(40)	gas	MPD	5
			1877(6)	Ne	AB	6
	2		1457(5)	Ne	AB	6
	3		500(40)	gas	MPD	5
			562(5)	Ne	AB	6

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	5	Asym. stretch	1736.4	Ne	IR	4
			1734.8	Ar	IR	3

References

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[6] D. Forney, M. Grutter, P. Freivogel, and J. P. Maier, J. Phys. Chem. A **101**, 5292 (1997).

C_6O

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+			2163.8	Ar	IR	1
			1447.8	Ar	IR	1

B_0=0.028 MW^2

References

[1] G. Maier, H. P. Reisenauer, and A. Ulrich, Tetrahed. Lett. **32**, 4469 (1991).
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C_5N_2

$\tilde{A}$

T_0=22762.9(2)T Ne AB^1LF^1
22737.3(2)T Ar AB^1LF^1
22731.8(2)T N_2 AB^1LF^1

$\tilde{A}-\tilde{X}$ 375–610 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1		1961.3(2)T	Ne	AB	1
			1960.5(2)T	Ar	AB	1
	8		601.2(2)T	Ar	AB	1
	9		508.5(2)T	Ar	AB	1

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1		2070.7(2)T	Ne	LF	1
			2071.4(2)T	Ar	LF	1
			2071.6(2)T	N_2	LF	1
	2		2030.7(2)T	Ne	LF	1
			2030.9(2)T	Ar	LF	1
			2032.0(2)T	N_2	LF	1
	3		1639.2(2)T	Ne	LF	1
			1639.5(2)T	Ar	LF	1
			1639.7(2)T	N_2	LF	1
	4		871.7(2)T	Ne	LF	1
			870.9(2)T	Ar	LF	1
	5		860.8(2)T	Ne	LF	1
			859.3(2)T	Ar	LF	1
	6		804.7(2)T	Ne	LF	1
			801.5(2)T	Ar	LF	1
	7		753.3(2)T	Ne	LF	1
			748.5(2)T	Ar	LF	1
	8		603.2(2)T[a]	Ne	LF	1
			609.6(2)T	Ar	LF	1
			601.9(2)T	Ar	LF	1
	9		527.7(2)T[a]	Ne	LF	1
			530.5(2)T	Ar	LF	1
			525.2(2)T	Ar	LF	1
			521.9(2)T	Ar	LF	1

[a]Center of split transition.

Reference

[1] A. M. Smith, C. Engel, A. Thoma, G. Schallmoser, B. E. Wurfel, and V. E. Bondybey, Chem. Phys. **184**, 233 (1994).

$(CN)_2CCO$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CCO a-stretch	2183	Ar	IR	1
			2185s	CO	IR	1
			1202w	CO	IR	1
			953w	CO	IR	1
			566w	CO	IR	1

Reference

[1] I. R. Dunkin and A. McCluskey, Spectrochim. Acta A **50**, 209 (1994).

$(CN)_2COO$

In an argon matrix, a weak, broad absorption at 26700 (375 nm) has been attributed[1] to $(CN)_2CCO$.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1290w	Ar	IR	1
			1275vw	Ar	IR	1
			1264vw	Ar	IR	1
			1245vw	Ar	IR	1

Reference

[1] I. R. Dunkin and A. McCluskey, Spectrochim. Acta A **50**, 209 (1994).

Al_2O_5

$\tilde{A}$

T_0=10890(640) gas PE[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Sym. stretch	900(60)	gas	PE	1

Reference

[1] S. R. Desai, H. Wu, C. M. Rohlfing, and L.-S. Wang, J. Chem. Phys. **106**, 1309 (1997).

O_2N-O-NO_2

In the gas phase, continuous absorption begins near 420 nm, and has its maximum beyond 200 nm.[11]

$\tilde{X}$ C_2[a] Structure: ED[6]MW[13]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	NO_2 a-stretch	1720vs	gas	IR	1,2,5,8
			1742.4vs	Ar	IR	12
			1745	N_2	IR	3
			1752	CO_2	IR	1
	2	NO_2 s-stretch	1338m	gas	IR	2,8
			1339.8wm	Ar	IR	12
			1305	N_2	IR	3
			1300	O_2	IR	4
			1316	CO_2	IR	1
	3		860m	gas	IR	2,8
			863.1w	Ar	IR	12
b	9	NO_2 a-stretch	1720vs	gas	IR	1,2,5,8
			1702.7s	Ar	IR	7,12
			1704	N_2	IR	3
			1704	O_2	IR	4
			1700	CO_2	IR	1
	10	NO_2 s-stretch	1245.9s	gas	IR	1,2,5,8,11
			1243.0m	Ar	IR	7,12
			1247	N_2	IR	3
			1241	O_2	IR	4
			1248	CO_2	IR	1
	11		743.4s	gas	IR	1,2,5,8,11
			737s	Ar	IR	7,12
			739	N_2	IR	3
			736	O_2	IR	4
			719	CO_2	IR	1
	12		614mT	gas	IR	2
			639.7w	Ar	IR	12
	13		557s	gas	IR	2,5
			569.4m	Ar	IR	12
	14		353vsT	gas	IR	2,9
			343.9vs	Ar	IR	12
	15		50w,brT	gas	IR	9

A_0=0.221; B_0=0.063; C_0=0.060 MW[10]

[a]Ref. 2 analyzed the spectrum in terms of a C_{2v} structure. However, the electron diffraction measurements of Ref. 6, analyzed using a dynamical model, and the low rotational temperature microwave spectral observations of Ref. 13 suggest instead a C_2 structure. The vibrational assignment has been revised to correspond with the results of *ab initio* calculations given in Ref. 13.

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SF_6^+

$\tilde{F}\ ^2A_{1g}$

T_0[a]=94450(100) gas PE[2,3,6]TPE[7]

Fragments into SF_2^+. T-PEPICO[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	690(40)	gas	PE	6,7
e_g	2		460T	gas	PE,TPE	6,7

$\tilde{E}\ ^2F_{1u}$

T_0[a]=57620(100) gas PE[2,3,6]TPE[7]

Fragments into SF_3^+. T-PEPICO[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	Sym. stretch	540(40)	gas	PE,TPE	6,7

$\tilde{D}\ ^2F_{2g}$

T_0[a]=33250(150) gas PE[1–3,6]TPE[7]

Fragments into SF_5^+, SF_4^+, and SF_3^+. T-PEPICO[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	Sym. stretch	590(40)	gas	PE,TPE	3,6,7

$\tilde{C}\ ^2E_g$

T_0[a]$\leqslant$24360(100) gas PE[1–3,6]TPE[7]

Low vibrational levels fragment into SF_5^++F, higher levels yield SF_4^+. T-PEPICO[5]

$\tilde{A},\tilde{B}\ ^2F_{1u}$, $^2F_{2u}$
T_0[a]=12780(240) gas PE[1–3,6]TPE[7]
Direct dissociation into SF_5^++F. T-PEPICO[4,5]

$\tilde{X}\ ^2F_{1g}$
Direct dissociation into SF_5^++F. T-PEPICO[4,5]
[a]Measured with respect to photoionization threshold, 15.116 eV, determined by Ref. 7.

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8.14. Eight-Atomic Molecules

$B_2H_6^+$

$\tilde{D}\ ^2B_{1u}$ D_{2h}
T_0=38650(100) gas PE[1–4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	BH_t stretch	2178(100)	gas	PE	2,4
			1000(140)	gas	PE	2

$\tilde{C}\ ^2B_{2u}$ D_{2h}
T^a=28000(100) gas PE[2–4]

$\tilde{B}\ ^2B_{3u}$ D_{2h}
T^a=21300(180) gas PE[2–4]

$\tilde{A}\ ^2A_g$ D_{2h}
T^a=11860(250) gas PE[2–4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g			1700(300)	gas	PE	2

$\tilde{X}\ ^2B_{2g}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g			900(60)	gas	PE	2

$B_2D_6^+$

$\tilde{D}\ ^2B_{1u}$ D_{2h}
T_0=38650(100) gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	BD_t stretch	1500(80)	gas	PE	2
			650(160)	gas	PE	2

$\tilde{C}\ ^2B_{2u}$ D_{2h}
T^a=28000(100) gas PE[2]

$\tilde{B}\ ^2B_{3u}$ D_{2h}
T^a=21300(180) gas PE[2]

$\tilde{A}\ ^2A_g$ D_{2h}
T^a=11860(250) gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g			1500(300)	gas	PE	2

$\tilde{X}\ ^2B_{2g}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g			800(120)	gas	PE	2

[a]From vertical ionization potential.

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$GaBH_6^+$

$\tilde{D}\ ^2A_1$ C_{2v}
T_0=34130(120) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		BH_t stretch	1950(100)	gas	PE	1
		GaH_t stretch	1480(100)	gas	PE	1

$\tilde{C}\ ^2B_2$ C_{2v}
T^a=20250(240) gas PE[1]

$\tilde{B}\ ^2B_1$ C_{2v}
T^a=14760(120) gas PE[1]

$\tilde{A}\ ^2A_1$ C_{2v}
T^a=10890(120) gas PE[1]

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

[a]From vertical ionization potential.

Reference

[1] J. M. Dyke, D. Haggerston, O. Warschkow, L. Andrews, A. J. Downs, and P. F. Souter, J. Phys. Chem. **100**, 2998 (1996).

$Ga_2H_6^+$

$\tilde{D}\ ^2B_{1u}$ D_{2h}
T_0=31550(120) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g		GaH_t stretch	1540(40)	gas	PE	1

$\tilde{C}\ ^2B_{2u}$ D_{2h}
T^a=14040(240) gas PE[1]

$\tilde{B}\ ^2B_{3u}$ D_{2h}
T^a=10970(240) gas PE[1]

$\tilde{A}\ ^2A_g$ D_{2h}
T^a=8630(240) gas PE[1]

$\tilde{X}\ ^2B_{2g}$ D_{2h}

$Ga_2D_6^+$

$\tilde{D}\ ^2B_{1u}$ D_{2h}
T_0=31470(120) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g		GaH_t stretch	1135(40)	gas	PE	1

$\tilde{C}\ ^2B_{2u}$ D_{2h}
T^a=13470(240) gas PE[1]

$\tilde{B}\ ^2B_{3u}$ D_{2h}
T^a=11050(240) gas PE[1]

$\tilde{A}\ ^2A_g$ D_{2h}
T^a=8550(180) gas PE[1]

$\tilde{X}\ ^2B_{2g}$ D_{2h}

[a]From vertical ionization potential.

Reference

[1] J. M. Dyke, D. Haggerston, O. Warschkow, L. Andrews, A. J. Downs, and P. F. Souter, J. Phys. Chem. **100**, 2998 (1996).

Ga_2H_6

$\tilde{X}$ D_{2h}[a] Structure: ED[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	GaH_t stretch	2000	Ar	Ra	3
			1986	N_2	Ra	3
	2	GaH_b stretch	1474	Ar	Ra	3
			1471	N_2	Ra	3
	3	GaH_2 deform.	736	Ar	Ra	3
			733	N_2	Ra	3
b_{2u}	8	GaH_t stretch	1993m	gas	IR	1,2
			2015m	Ar	IR	1,2
			1996m			
			2000m	N_2	IR	1,2
	9	GaH_2 rock	760w	gas	IR	1,2
			773m	Ar	IR	1,2
			761m			
			770m	N_2	IR	1,2
b_{1g}	11	GaH_t stretch	2011	Ar	Ra	3
			1997	N_2	Ra	3
b_{1u}	13	GaH_b stretch	1202s	gas	IR	1,2
			1213m	Ar	IR	1,2
			1208m			
			1195m			
			1220s	N_2	IR	1,2
	14	GaH_2 rock?	659m	Ar	IR	1,2
			655m			
			653m			
			648m			
			655s	N_2	IR	1,2
			647w			
b_{3g}	15	GaH_2 deform.	763	Ar	Ra	3
			761	N_2	Ra	3
b_{3u}	16	GaH_t stretch	1976m	gas	IR	1,2
			1985s	Ar	IR	1,2
			1968m			
			1985m	N_2	IR	1,2
	17	GaH_b stretch	1273s	gas	IR	1,2
			1283s	Ar	IR	1,2
			1278m			
			1253m			
			1282m	N_2	IR	1,2
	18	GaH_2 deform.	671vsT	gas	IR	1,2
			676vs	Ar	IR	1,2
			666s			
			673vs	N_2	IR	1,2

Ga_2D_6

$\tilde{X}$ D_{2h}[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	GaD_t stretch	1433	Ar	Ra	3
			1424	N_2	Ra	3
	2	GaD_b stretch	1060	Ar	Ra	3
			1059	N_2	Ra	3
	3	GaD_2 deform.	527	Ar	Ra	3
			525	N_2	Ra	3
b_{2u}	8	GaD_t stretch	1439m	gas	IR	1,2
	9	GaD_2 rock	555w	gas	IR	1,2
b_{1g}	11	GaD_b stretch	1451	Ar	Ra	3
			1442	N_2	Ra	3
b_{1u}	13	GaD_b stretch	860s	gas	IR	1,2
	14	GaD_2 rock	439wm	gas	IR	1,2
b_{3g}	15	GaD_2 deform.	543	Ar	Ra	3
			543	N_2	Ra	3
b_{3u}	16	GaD_t stretch	1416mT	gas	IR	1,2
	17	GaD_b stretch	923s	gas	IR	1,2
	18	GaD_2 deform.	484vsT	gas	IR	1,2

[a]As in Ref. 2, the axis definitions and vibrational numbering commonly used for diborane (J. L. Duncan, D. C. McKean, I. Torto, and G. D. Nivellini, J. Mol. Spectrosc. **85**, 16 (1981)) have been adopted.

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CH_2CHCH_2

$\tilde{D}$ $^2B_2$ C_{2v}
T_0=41557.8(5) gas MPI[13]Ra[14]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2	9	CH_2 a-twist	596	gas	Ra	14
b_1	12	CH_2 s-twist	564	gas	Ra	14

$\tilde{C}$ $^2B_1$ C_{2v} Structure: MPI[18]
T_0=40305.5(5) gas AB[2]MPI[11,13,18] $\tilde{C}-\tilde{X}$ 220–250 nm
In an argon matrix, a very prominent absorption maximum at 213 nm, with a shoulder at 220 nm, has been assigned[5] to this transition of CH_2CHCH_2.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	7	C_3 bend	385(2)	gas	MPI	11,18

$A_0 \cong 1.619$; $B_0 \cong 0.351$; $C_0 \cong 0.288$ MPI[11]

$\tilde{B}$ $^2A_1(3s)$ C_{2v}[a] Structure: MPI[18]
T_0=40056.5(5) gas MPI[7,8,13,18]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	7	C_3 bend	379(2)	gas	MPI	7,8,18
a_2	9	CH_2 a-twist	596(2)	gas	MPI	18
b_1	12	CH_2 s-twist	491(7)T	gas	MPI	8

$\tilde{A}$ $^2B_1$ C_{2v}
T_0=24485 gas AB[1] $\tilde{A}-\tilde{X}$ 370–410 nm
24480 Ar AB[5] $\tilde{A}-\tilde{X}$ 360–410 nm
Diffuse bands.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1241	gas	AB	1
			1005	gas	AB	1
			908	gas	AB	1
			359	gas	AB	1

$\tilde{X}$ $^2A_2$ C_{2v} Structure: DL[12]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH stretch	3048vw	Ar	IR	4–6
	4	CH_2 scissors	1488(4)	gas	Ra	10,15
			1477w	Ar	IR	4–6
	5	CH_2 rock	1245(3)	gas	Ra	10,15
			1242vw	Ar	IR	4–6
	6	C_3 stretch	1066(4)	gas	Ra	10,15
			990(20)	gas	PE	19
	7	C_3 bend	427(4)	gas	MPI,Ra	7,8,10,15
					PE	18,19
a_2	9	CH_2 a-twist	549(4)	gas	MPI,Ra	8,15,16
b_1	10	CH OPLA	968H	gas	Ra	10
			983.6s	Ar	IR	4–6,9
	11	CH_2 s-wag	801.72	gas	DL,PE	12,19
			801.1vs	Ar	IR	3–6,9
	12	CH_2 s-twist	518(4)	gas	MPI,Ra	7,8,10,15, 16,18
			510.1s	Ar	IR	4–6,9
b_2	13	CH_2 a-stretch	3105w	Ar	IR	4–6
	14	CH stretch	3016w	Ar	IR	4–6
	15	CH_2 scissors	1463vw	Ar	IR	4–6
	16	CH bend	1389m	Ar	IR	4–6
	17	C_3 stretch	1182	Ar	IR	6

A_0=1.802; B_0=0.346; C_0=0.290 DL[12]

CD_2CDCD_2

$\tilde{D}$ $^2B_2$ C_{2v}
T_0=41532.1(5) gas MPI[13]

$\tilde{C}$ $^2B_1$ C_{2v}
T_0=40286.7(5) gas MPI[13,18]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	7	C_3 bend	321(2)	gas	MPI	18

$\tilde{B}\ ^2A_1(3s)$ C_{2v}[a]
T_0=40096(2) gas MPI[7,13,18]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	7	C_3 bend	316(2)	gas	MPI	7,18
a_2	9	CD_2 a-twist	429(2)	gas	MPI	18

$\tilde{A}\ ^2B_1$ C_{2v}
T_0=24745 gas AB[1] $\tilde{A}-\tilde{X}$ 360–405 nm
Diffuse bands.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1155	gas	AB	1
			981	gas	AB	1
			823	gas	AB	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD stretch	2285	Ar	IR	6
	3	CD_2 stretch	2214	Ar	IR	6
	4	C_3 stretch	1272(8)	gas	Ra	17
			1263	Ar	IR	6
	5	CD_2 rock	1020(8)	gas	Ra	17
			1018	Ar	IR	6
			1007			
	6	Deform.	835(20)	gas	MPI,PE	7,19
	7	C_3 deform.	350(8)	gas	MPI,Ra PE	7,17–19
a_2	9	CD_2 torsion	372H	gas	Ra	17
b_1	10	Deform.	762H	gas	Ra	17
	11	Deform.	678(10)H	gas	PR	19
			646.5vs	Ar	IR	6,9
	12	Deform.	403(8)	gas	Ra,MPI	17,18
b_2	14	CD_2 stretch	2209	Ar	IR	6
	16	CD bend	1062	Ar	IR	6

[a]Evidence presented in Refs. 14 and 18 suggests that this state may be slightly nonplanar.

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$CH_2CHCH_2^-$

Threshold for electron detachment from ground-state $CH_2CHCH_2^-$ =3880(65) gas PE[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		C_3 bend	425(20)	gas	PE	1,2

$CD_2CDCD_2^-$

Threshold for electron detachment from ground-state $CD_2CDCD_2^-$ =3740(50) gas PE[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		C_3 bend	350(20)	gas	PE	1,2

References

[1] J. M. Oakes and G. B. Ellison, J. Am. Chem. Soc. **106**, 7734 (1984).
[2] P. G. Wenthold, M. L. Polak, and W. C. Lineberger, J. Phys. Chem. **100**, 6920 (1996).

H_2BSCH_3

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	BH_2 a-stretch	2603	Ar	IR	1
	4	BH_2 s-stretch	2526	Ar	IR	1
	5	CH_3 deform.	1496	Ar	IR	1
	6	CH_3 deform.	1320	Ar	IR	1
	7	BH_2 s-bend	1183	Ar	IR	1
	8	CH_3 rock	1161	Ar	IR	1
	9	B-S stretch	830	Ar	IR	1
	10	BH_2 rock	787	Ar	IR	1
	11	C-S stretch	693	Ar	IR	1
a''	14	CH_3 stretch	2945	Ar	IR	1
	15	CH_3 deform.	1448	Ar	IR	1
	16	CH_3 rock	1138	Ar	IR	1
	17	BH_2 OPLA	913	Ar	IR	1

Reference

[1] J. D. Carpenter and B. S. Ault, J. Phys. Chem. **97**, 3697 (1993).

c-$CH_3CH{=}NH$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	NH stretch	3247vvw	Ar	IR	1
	2	CH_3 a-stretch	3018m	Ar	IR	1
	3	CH stretch	2916	gas	IR	3
			2925ms	Ar	IR	1
			2920m			
	4	CH_3 s-stretch	2886	gas	IR	3
			2885m	Ar	IR	1
	5	C=N stretch	1655	gas	IR	3
			1652vs	Ar	IR	1
	6	CH_3 a-deform.	1438ms	Ar	IR	1
	7	CH_3 s-deform.	1412m	Ar	IR	1
	8	Mixed	1250	gas	IR	3
			1252vs	Ar	IR	1
	9	CH deform.	1107	gas	IR	3
			1114ms	Ar	IR	1
	10	CNH deform.	1052wm	Ar	IR	1
	11	CH_3 rock	950w	Ar	IR	1
	12	CCN deform.	485s	Ar	IR	1
a″	13	CH_3 a-stretch	2988	gas	IR	3
			2990m	Ar	IR	1
	14	CH_3 a-deform.	1454	gas	IR	3
			1435s	Ar	IR	1
			1433s			
	15	C=N torsion	1132vw	Ar	IR	1
	16	CH_3 wag	1045	gas	IR	3
			1045vs	Ar	IR	1
	17	CH wag	678	gas	IR	3
			674w	Ar	IR	1

A_0=1.772; B_0=0.326; C_0=0.290 MW[2]IR[4]

c-$CH_3CD{=}ND$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	ND stretch	2425vvw	Ar	IR	1
	2	CD_3 a-stretch	2256wm	Ar	IR	1
	3	CD stretch	2191m	Ar	IR	1
	4	CD_3 s-stretch	2062w	Ar	IR	1
	5	C=N stretch	1631s	Ar	IR	1
			1628vs			
	6	Mixed	1159ms	Ar	IR	1
	7	Mixed	1072m	Ar	IR	1
	8	CD_3 a-deform.	1032wm	Ar	IR	1
	9	Mixed	850w	Ar	IR	1
	10	CD rock	796s	Ar	IR	1
	11	CD_3 rock	736m	Ar	IR	1
	12	CCN bend	405m	Ar	IR	1
a″	13	CD_3 a-stretch	2216wm	Ar	IR	1
	14	CD_3 a-deform.	1039s	Ar	IR	1
	15	CD_3 wag	848ms	Ar	IR	1
	16	C=N torsion	811s	Ar	IR	1
	17	CD wag	527m	Ar	IR	1

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[1] I. Stolkin, T.-K. Ha, and H. H. Gunthard, Chem. Phys. **21**, 327 (1977).
[2] F. J. Lovas, R. D. Suenram, D. R. Johnson, F. O. Clark, and E. Tiemann, J. Chem. Phys. **72**, 4964 (1980).
[3] K. Hashiguchi, Y. Hamada, M. Tsuboi, Y. Koga, and S. Kondo, J. Mol. Spectrosc. **105**, 81 (1984).
[4] D. McNaughton and E. G. Robertson, J. Mol. Spectrosc. **163**, 80 (1994).

$C_2H_3NH_2$

$\tilde{X}$ C_1[a] Structure: MW[3–5]IR[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	5	CH stretch	2987	gas	IR	2
			2976			
	6	C=C stretch	1672	gas	IR	2
			1668			
	7	NH_2 scissors	1625T	gas	IR	2
	8	CH_2 scissors	1454	gas	IR	2
	10	NH_2 twist	1260	gas	IR	2
			1248			
	11	C-N stretch	1084	gas	IR	2
			1078			
	12	CH wag	1046	gas	IR	2
			1039			
	14	CH_2 wag	812s	gas	IR	2
			805s			
	15	NH_2 wag	615[b]	gas	IR	2,4,5
			570[c]	gas	IR	2,4,5
			470[d]	gas	IR	4,5
			425[e]	gas	IR	4,5
	16	C=C torsion	379[b]	gas	IR	4,5
			333[d]	gas	IR	4,5
			287[e]	gas	IR	4,5

A_0=1.879; B_0=0.335; C_0=0.286 MW[1,3,5]

[a] The barrier to inversion about the N atom is 356(3) cm^{-1},[3–5] leading to splittings in a number of the vibrational band centers. The $0^- - 0^+$ transition has been observed[5,6] in the far IR at 45.2 cm^{-1}. Ref. 5 has offered a tentative reassignment of the peaks associated with ν_{15} and ν_{16}.
[b] $1^- - 0^+$.
[c] $1^- - 0^-$.
[d] $1^+ - 0^+$.
[e] $1^+ - 0^-$.

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[1] F. J. Lovas, F. O. Clark, and E. Tiemann, J. Chem. Phys. **62**, 1925 (1975).
[2] Y. Hamada, K. Hashiguchi, M. Tsuboi, Y. Koga, and S. Kondo, J. Mol. Spectrosc. **105**, 93 (1984).
[3] R. D. Brown, P. D. Godfrey, and B. Kleibömer, J. Mol. Spectrosc. **124**, 21 (1987).
[4] Y. Hamada, N. Sato, and M. Tsuboi, J. Mol. Spectrosc. **124**, 172 (1987).
[5] R. D. Brown, P. D. Godfrey, B. Kleibömer, A. P. Pierlot, and D. McNaughton, J. Mol. Spectrosc. **142**, 195 (1990).
[6] D. McNaughton and E. G. Robertson, J. Mol. Spectrosc. **163**, 80 (1994).

$CH_3SCH_2^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			870(70)	gas	PE	1
			390(100)	gas	PE	1

Reference

[1] J. Baker and J. M. Dyke, Chem. Phys. Lett. **213**, 257 (1993).

C_2H_5O

$\tilde{B}$ $^2A'$ C_s
T_0=29210.207(6) gas EM[1,2,4]LF[3,5,6] $\tilde{B}-\tilde{X}$ 310–500 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CO stretch	585H	gas	LF	5,6

τ_0=1.7(2) μs gas LF[3]EM[4]
A_0=1.117(2); B_0=0.311(2); C_0=0.268(2) LF[6]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_2 wag	1370	gas	LF	3
		C-O stretch	1067	gas	LF,EM	3–5
		C-C stretch	875[a]	gas	LF	3
		CCO bend	442	gas	LF	3

A_0=1.318(2); B_0=0.321(2); C_0=0.284(3) LF[6]

[a]Assignment to overtone of CCO bend cannot be excluded.

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[1]D. W. G. Style and J. C. Ward, Trans. Faraday Soc. **49**, 999 (1953).
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$HOCH_2CH_2$

In the gas phase, the onset of continuous absorption has been reported[1] near 37700 (265 nm), with increasing absorption out to the 210 nm cutoff of the observations.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3625.8T	Ar	IR	2
		CH stretch	2991.0	Ar	IR	2
		CH stretch	2922.4T	Ar	IR	2
		CH stretch	2842.7	Ar	IR	2
			1355.4	Ar	IR	2
			1172.5	Ar	IR	2
		CO stretch	1040.1	Ar	IR	2
			873.9T	Ar	IR	2

References

[1]C. Anastasi, V. Simpson, J. Munk, and P. Pagsberg, J. Phys. Chem. **94**, 6327 (1990).
[2]Y.-P. Kuo, G.-H. Wann, and Y.-P. Lee, J. Chem. Phys. **99**, 3272 (1993).

C_2H_5S

$\tilde{B}$ C_s
T_0=23519.6 gas LF[1,2] $\tilde{A}-\tilde{X}$ 390–600 nm
Predissociation occurs.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CH_2 wag	1158.9	gas	LF	2
		CC stretch	1054.6	gas	LF	2
		CH_3 wag	862.8	gas	LF	2
		CS stretch	420.5	gas	LF	1,2
		CCS bend	256.0	gas	LF	2
a''		CH_2 twist	1203.3	gas	LF	2
		CH_2 rock	718.4	gas	LF	2

τ=75 ns gas LF[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CH_3 s-stretch	2950T	gas	LF	2
		CH_2 bend	1470(10)	gas	LF	2
		CH_2 wag	1257(10)	gas	LF	2
		CC stretch	1075(10)	gas	LF	2
		CH_3 wag	957(15)	gas	LF	2
		CS stretch	672.4	gas	LF	1,2
		CCS bend	296.0	gas	LF	2
a''		CH_3 a-stretch	3050T	gas	LF	2
		CH_2 twist	1290(10)	gas	LF	2
		CH_3 wag	890(10)	gas	LF	2
		CH_2 rock	478.3	gas	LF	2
		Torsion	271.9	gas	LF	2

References

[1]G. Black and L. E. Jusinski, Chem. Phys. Lett. **136**, 241 (1987).
[2]W.-C. Hung, M.-Y. Shen, C.-H. Yu, and Y.-P. Lee, J. Chem. Phys. **105**, 5722 (1996).

cyc-$C_4H_4^+$

$\tilde{F}$ ^2A_g D_{2h}
T^a=46500(1000) gas PE[1]

$\tilde{E}$ $^2B_{3u}$ D_{2h}
T^a=41600(1000) gas PE[1]

$\tilde{C}$ $^2B_{1u}$ D_{2h}
T^a=32000(1000) gas PE[1]

$\tilde{B}$ $^2B_{2u}$ D_{2h}
T^a=26300(1000) gas PE[1]

$\tilde{X}\ ^2B_{2g}$ D_{2h} Structure: PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g			1129(40)	gas	PE	1

[a]From vertical ionization potentials.

References

[1] J. Kreile, N. Münzel, A. Schweig, and H. Specht, Chem. Phys. Lett. **124**, 140 (1986).
[2] D. W. Kohn and P. Chen, J. Am. Chem. Soc. **115**, 2844 (1993).

cyc-C_4H_4

In an argon matrix,[8] absorption is weak between 420 and 250 nm and is accompanied by dissociation to form C_2H_2. Below 250 nm, the absorption rises abruptly.

$\tilde{X}$ D_{2h} Structure: IR[3–5]Ra[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g		CH stretch	3140(5)	Ne,Ar	Ra	7
		C=C stretch	1678(5)	Ne,Ar	Ra	7
		CH deform.	1059(5)	Ne,Ar	Ra	7
		CH deform.	989(5)	Ne,Ar	Ra	7
b_{1u}		CH stretch	3124wm	Ar	IR	5,6,8
		C=C stretch	1527	Ne	IR	6
			1526w	Ar	IR	4–6,8
		CH deform.	1028vw	Ar	IR	5
b_{2g}		CH OPLA deform.	531(5)	Ne,Ar	Ra	7
b_{2u}		CH stretch	3105wm	Ar	IR	5,6,8
		CH deform.	1244	Ne	IR	6
			1242s	Ar	IR	1–6,8
		Ring deform.	719wm	Ar	IR	4–6,8
b_{3g}		CH stretch	3093(5)	Ne,Ar	Ra	7
		Ring deform.	723(5)	Ne,Ar	Ra	7
b_{3u}		CH OPLA	576	Ne	IR	6
			569vs	Ar	IR	1–6,8

cyc-C_4D_4

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{1u}		C=C stretch	1456w	Ar	IR	4
b_{2u}		CD deform.	1043wm	Ar	IR	4
		Ring deform.	609wm	Ar	IR	4
b_{3u}		CD OPLA	421vs	Ar	IR	4

References

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$C_2H_3CH{=}C$:

$\tilde{b}\ ^3A''$ C_s
T_0=16420(240) gas PE[1]

$\tilde{a}\ ^3A'$ C_s
T_0=15520(120) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1250(50)	gas	PE	1
			500(50)	gas	PE	1
			360(50)	gas	PE	1

$\tilde{X}\ ^1A'$ C_s
Broadening in the first band of the photoelectron spectrum of the anion permits estimation of a lifetime between 20 and 200 fs for rearrangement to form vinylacetylene.[1]

Reference

[1] R. F. Gunion, H. Köppel, G. W. Leach, and W. C. Lineberger, J. Chem. Phys. **103**, 1250 (1995).

$C_2H_3CH{=}C{:}^-$

Threshold for electron detachment to form ground-state $C_2H_3CH{=}C{:}$
=7370(120) gas PE[1]

$C_2D_3CD{=}C{:}^-$

Threshold for electron detachment to form ground-state $C_2D_3CD{=}D{:}$
=7330(120) gas PE[1]

Reference

[1] R. F. Gunion, H. Köppel, G. W. Leach, and W. C. Lineberger, J. Chem. Phys. **103**, 1250 (1995).

CH_3CCOH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3430.0[a]	Ar	IR	1
		C≡C stretch	2192.7	Ar	IR	1

CD_3CCOH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OD stretch	2528.1[a]	Ar	IR	1

[a]Probably perturbed by interaction with NO trapped in an adjacent site.

Reference

[1] J. A. Harrison and H. Frei, J. Phys. Chem. **98**, 12142 (1994).

$H_2GaCl_2GaH_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}	8	GaH a-stretch	2020s	Ar	IR	1
	9	GaH_2 rock	480w	Ar	IR	1
b_{1u}	13	GaH_2 wag	578m	Ar	IR	1
	14	GaCl stretch	290w,sh	Ar	IR	1
b_{3u}	16	GaH s-stretch	1985m	Ar	IR	1
	17	GaH_2 scissors	690s	Ar	IR	1
	18	GaCl s-stretch	265s	Ar	IR	1

$D_2GaCl_2GaD_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}	8	GaD a-stretch	1450s	Ar	IR	1
	9	GaD_2 rock	355m	Ar	IR	1
b_{1u}	13	GaD_2 wag	410m	Ar	IR	1
	14	GaCl stretch	305w,sh	Ar	IR	1
b_{3u}	16	GaD s-stretch	1420m	Ar	IR	1
	17	GaD_2 scissors	495s	Ar	IR	1
	18	GaCl s-stretch	265s	Ar	IR	1

Reference

[1] C. R. Pulham, A. J. Downs, M. J. Goode, and I. M. Mills, Spectrochim. Acta A **51**, 769 (1995).

CH_3COO_2

A prominent gas-phase absorption with maximum near 207 nm has been attributed[4–6] to CH_3COO_2.

A weaker, broad gas-phase absorption with maximum near 245 nm has been attributed[2,4–6] to CH_3COO_2.

In an argon matrix, photodissociates in the 300–400 nm spectral region.[3]

$\tilde{A}$

T_0=5562(3) gas AB[1] $\tilde{A}$–$\tilde{X}$ 1348–1798 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	932(5)	gas	AB	1
			530	gas	AB	1

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1843s	Ar	IR	3
			1425w	Ar	IR	3
			1420w	Ar	IR	3
			1367m	Ar	IR	3
			1278vw	Ar	IR	3
			1169vw	Ar	IR	3
			1152m	Ar	IR	3
			1099m	Ar	IR	3
			1082vw	Ar	IR	3
			1030w	Ar	IR	3
			971m	Ar	IR	3
			736m	Ar	IR	3

References

[1] H. E. Hunziker and H. R. Wendt, J. Chem. Phys. **64**, 3488 (1976).
[2] M. C. Addison, J. P. Burrows, R. A. Cox, and R. Patrick, Chem. Phys. Lett. **73**, 283 (1980).
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[5] G. Moortgat, B. Veyret, and R. Lesclaux, J. Phys. Chem. **93**, 2362 (1989).
[6] C. M. Roehl, D. Bauer, and G. K. Moortgat, J. Phys. Chem. **100**, 4038 (1996).

$C_6H_2^+$

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

T_0=27350(160) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			650(80)	gas	PE	1

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

T_0=16658 gas EF[2,3]LF[3] $\tilde{A}$–$\tilde{X}$ 485–725 nm

16570 Ne LF[4]AB[5] $\tilde{A}$–$\tilde{X}$ 524–843 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	CH stretch	3243(2)T	gas	LF	3
	2	C≡C stretch	2053(2)	gas	LF	3
			2065.7	Ne	LF,AB	4,5
	3	C≡C stretch	1880(2)	gas	LF	3
			1890.2	Ne	LF,AB	4,5
	4	C-C stretch	617(2)	gas	LF,EF	2,3
			620	Ne	LF,AB	4,5
Π_g	10	Skel. bend	244T	gas	LF	3
			248H	Ne	LF	4

τ_0=17(2) ns gas EF[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	2	C≡C stretch	2182(2)	gas	EF	2,3
			2181.4	Ne	LF	4
	3	C≡C stretch	1903(2)	gas	EF	2,3
			1903.4	Ne	LF	4
	4	C-C stretch	632(2)	gas	EF	2,3
			635H	Ne	LF	4
Σ_u^+	6	C≡C stretch	2014T	Ne	LF	4
Π_g	10	Skel. bend	228(2)T	gas	LF	3
			230T	Ne	LF	4

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[2] M. Allan, E. Kloster-Jensen, and J. P. Maier, Chem. Phys. **17**, 11 (1976).
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HC_6H

$\tilde{X}$ $D_{\infty h}$
A_0=8.95; B_0=0.0450; C_0=0.0447 MW[1]

Reference

[1] M. C. McCarthy, M. J. Travers, A. Kovács, W. Chen, S. E. Novick, C. A. Gottlieb, and P. Thaddeus, Science **275**, 518 (1997).

cyc-(HOC=COHC)=O

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3506.3ms	Ar	IR	1
			1901.5m	Ar	IR	1
			1738.6s	Ar	IR	1
			1316.5vs	Ar	IR	1
			1279.4wm	Ar	IR	1
			1270.7wm	Ar	IR	1
			847.6wm	Ar	IR	1

Reference

[1] G. Maier and C. Rohr, Liebigs Ann. **1996**, 307.

C_7H

$\tilde{X}\ ^2\Pi_{1/2}$ $C_{\infty v}$
B_0=0.029 MW[1]

Reference

[1] M. J. Travers, M. C. McCarthy, C. A. Gottlieb, and P. Thaddeus, Astrophys. J. **465**, L77 (1996).

HC_5CN^+

$\tilde{A}$ $C_{\infty v}$
T_0=17548(5) Ne AB[1]

Reference

[1] D. Forney, P. Freivogel, J. Fulara, and J. P. Maier, J. Chem. Phys. **102**, 1510 (1995).

C_8

$^3\Sigma_u^-$ $D_{\infty h}$
T_0=15630(5) Ne AB[3] $^3\Sigma_u^- - \tilde{X}$ 550–640 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		2075(5)	Ne	AB	3
	4		471(5)	Ne	AB	3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	4	Sym. stretch	565T	gas	PE	2
Σ_u^-	5		2067.8	Ne	IR	3,6
			2063.9	Ar	IR	4
			2065.3	Kr	IR	5
	6		1707.8	Ne	IR	4–6
			1705.6	Ar	IR	4
			1706.0T	Kr	IR	5

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[5] J. Szczepanski, S. Ekern, C. Chapo, and M. Vala, Chem. Phys. **211**, 359 (1996).
[6] P. Freivogel, M. Grutter, D. Forney, and J. P. Maier, Chem. Phys. **216**, 401 (1997).

C_8^-

Threshold for electron detachment from ground-state C_8^-=35330(50) gas PE[1,2]

(2) $^2\Pi_u$ $D_{\infty h}$
T_0=16305 gas PD[4] 446–614 nm
16295(5) Ne AB[6] 438–614 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		2125(10)	Ne	AB	6
	2		1821(10)	Ne	AB	6
	4		469(8)	Ne	AB	6
Π_g	8		487(5)H	Ne	AB	6

$\tilde{C}\ ^2\Pi_u$ $D_{\infty h}$
T_0=12963 gas PD[4] $\tilde{C}-\tilde{X}$ 639–774 nm
12933(5) Ne AB[3] $\tilde{C}-\tilde{X}$ 665–775 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		2087	gas	PD	4
	2		2055(5)	Ne	AB	3
	3		959(5)	Ne	AB	3
	4		453	gas	PD	4
			475(5)	Ne	AB	3

$^2\Sigma_u^+$ $D_{\infty h}$
T_0=9545(2) Ne AB[6] 817–1048 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		2010(4)	Ne	AB	6
	2		1956(4)	Ne	AB	6

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	6		1796.0	Ne	IR	5

References

[1] S. Yang, K. J. Taylor, M. J. Craycraft, J. Conceicao, C. L. Pettiette, O. Cheshnovsky, and R. E. Smalley, Chem. Phys. Lett. **144**, 431 (1988).
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$NC(C{\equiv}C)_2CN^+$

$\tilde{E}\ ^2\Pi_u$ $D_{\infty h}$
T_0=30420(160) gas PE[1]

$\tilde{D}\ ^2\Pi_g$ $D_{\infty h}$
T_0=25580(160) gas PE[1]

$\tilde{B},\tilde{C}\ ^2\Sigma_g^+,\ ^2\Sigma_u^+$ $D_{\infty h}$
T_0=22190(160) gas PE[1]

$\tilde{A}\ ^2\Pi_u$ $D_{\infty h}$
T_0=15260(10) gas EF[1] $\tilde{A}-\tilde{X}$ 630–770 nm
15130[a] Ne AB[2]LF[3] $\tilde{A}-\tilde{X}$ 565–1510 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C s-stretch	2475(5)T	Ne	AB	2
	2	CN s-stretch	1940(80)	gas	PE	1
			2029	Ne	AB,LF	2,3
	3	C-C s-stretch	1726(5)	Ne	AB	2
	4	C-C s-stretch	449	Ne	AB,LF	2,3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡N s-stretch	2180(10)	gas	EF	1
			2185	Ne	LF	3
	2	C≡C s-stretch	2100(10)	gas	EF	1
			2094	Ne	LF	3
	3	C-C s-stretch	1360(10)	gas	EF	1
			1354	Ne	LF	3
	4	C-C s-stretch	460(10)	gas	EF	1
			458	Ne	LF	3

[a]Ref. 3 reported a second trapping site with T_0=15160.

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[1] E. Kloster-Jensen, J. P. Maier, O. Marthaler, and M. Mohraz, J. Chem. Phys. **71**, 3125 (1979).
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C_7O

$\tilde{X}$ $C_{\infty v}$
B_0=0.019 MW[1]

Reference

[1] T. Ogata, Y. Ohshima, and Y. Endo, J. Am. Chem. Soc. **117**, 3593 (1995).

$FB(NCO)_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NCO a-stretch	2296s	gas	IR	1
	2	NCO a-stretch	2233vs	gas	IR	1
		Mixed	1569Ts	gas	IR	1
			1560Ts	gas	IR	1
			1553Ts	gas	IR	1
	5	BF stretch	1276s	gas	IR	1

Reference

[1] M. Alaee, E. G. Livingstone, and N. P. C. Westwood, J. Am. Chem. Soc. **115**, 2871 (1993).

$FC(O)OONO_2$

In the gas phase, the onset of unstructured absorption with continuously increasing intensity out to the 190-nm observation limit occurs near 34500 (290 nm).[1]

$\tilde{X}$ C_1 Structure: ED[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	C=O stretch	1910	gas	IR	1
			1902.5wm	Ne	IR	1
	2		1763	gas	IR	1
			1762.6m	Ne	IR	1
	3		1302	gas	IR	1
			1302.0wm	Ne	IR	1
	4		1194	gas	IR	1
			1191.7vs	Ne	IR	1
	5		981	gas	IR	1
			983.3w	Ne	IR	1
	6		925	gas	IR	1
			926.0w	Ne	IR	1
	7		795	gas	IR	1
			792.0wm	Ne	IR	1
	8		712	gas	IR	1
			703.2vw	Ne	IR	1
	9		635	gas	IR	1
			631.3w	Ne	IR	1
	10		530	gas	IR	1
			530.0w	Ne	IR	1
	11		475T	gas	IR	1
	12		420	gas	IR	1
	13		395	gas	IR	1
	14		343	gas	IR	1
	15		331	gas	IR	1
	17		75T	gas	IR	1

Reference

[1] D. Scheffler, I. Schaper, H. Willner, H.-G. Mack, and H. Oberhammer, Inorg. Chem. **36**, 339 (1997).

CF_3ONO_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO_2 a-stretch	1744	gas	IR	2
			1735.5	Ar	IR	1
			1345.2	Ar	IR	1
		NO_2 s-stretch	1334	gas	IR	2
			1327.1	Ar	IR	1
		CF_3 stretch	1264	gas	IR	2
			1260.8s	Ar	IR	1
		CF_3 stretch	1244	gas	IR	2
			1249.5vs	Ar	IR	1
			1151	gas	IR	2
			1142.5vs	Ar	IR	1
		C-O stretch	924	gas	IR	2
			924.1w	Ar	IR	1
		NO_2 scissors	791	gas	IR	2
			785.2	Ar	IR	1
		ONO_2 OPLA	752.9	Ar	IR	1
			519.0	Ar	IR	1

References

[1] K. C. Clemitshaw and J. R. Sodeau, J. Phys. Chem. **91**, 3650 (1987).
[2] J. Chen, V. Young, T. Zhu, and H. Niki, J. Phys. Chem. **97**, 11696 (1993).

8.15. Hydrocarbons with More Than Eight Atoms

$t\text{-}H_2C{=}CH{-}CH{=}CH_2^+$

$\tilde{D}$

T^a=50180(120) gas PE[1]

$\tilde{C}$

T_0=31950(120) gas PE[1]

An absorption maximum which appears at 33890 (295 nm) in an argon matrix has been attributed[2] to *t*-butadiene cation.

$\tilde{B}$

T^a=26300(120) gas PE[1]

$\tilde{A}$

T^a=19850(120) gas PE[1]

A relatively weak absorption maximum which appears at 18720 (534 nm) in an argon matrix has been attributed[2] to *t*-butadiene cation.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_u	11		1000.9	Ar	IR	3,4
b_u	17		3125.3	Ar	IR	3,4
	18		3073.7	Ar	IR	3,4
	19		3026.3	Ar	IR	3,4
	20		1477.5	Ar	IR	3,4
	21		1330T	Ar	IR	3,4
	22		1251.1	Ar	IR	3,4
	23		1006.1	Ar	IR	3,4

$t\text{-}D_2C{=}CD{-}CD{=}CD_2^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_u	11		739.6	Ar	IR	3,4
b_u	17		2358.1	Ar	IR	3,4
	18		2276.1	Ar	IR	3,4
	19		2215.4	Ar	IR	3,4
	20		1319.1	Ar	IR	3,4
	21		1047.2	Ar	IR	3,4
	22		996.1	Ar	IR	3,4

[a]From vertical ionization potential.

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[1] J. H. D. Eland, Int. J. Mass Spectrom. Ion Phys. **2**, 471 (1969).
[2] T. Bally, S. Nitsche, K. Roth, and E. Haselbach, J. Am. Chem. Soc. **106**, 3927 (1984).
[3] W. Tang, X.-L. Zhang, and T. Bally, J. Phys. Chem. **97**, 4373 (1993).
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$C(CH_2)_3$

$\tilde{b}\ ^1A_1$
T_0=5640(50) gas PE[3]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''			758	Ar	IR	1
			755.5vs	Xe	IR	1,2
			500	Ar	IR	1
			499.0m	Xe	IR	1,2
e'			3115.1w	Xe	IR	1,2
			3100.1w			
			3031.2	Xe	IR	1,2
			3019.1w			
			1418.4wm	Xe	IR	1,2

$C(CD_2)_3$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''			671.1s	Xe	IR	2
			415.6vs	Xe	IR	2
e'			2204.9w	Xe	IR	2
			2192.5vw			
			1050.6wm	Xe	IR	2

References

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$C(CH_2)_3^-$

Threshold for electron detachment from ground-state $C(CH_2)_3^-$=3480(50) gas PE[1]

Reference

[1] P. G. Wenthold, J. Hu, R. R. Squires, and W. C. Lineberger, J. Am. Chem. Soc. **118**, 475 (1996).

$H_2CC(CH_3)CH_2^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			410(30)	gas	PE	1

Reference

[1] J. C. Schultz, F. A. Houle, and J. L. Beauchamp, J. Am. Chem. Soc. **106**, 7336 (1984).

cyc-$C_4H_7^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			990(100)	gas	PE	1

Reference

[1] J. C. Schultz, F. A. Houle, and J. L. Beauchamp, J. Am. Chem. Soc. **106**, 7336 (1984).

$CH_3CHCH{=}CH_2$

T_0=42039 gas AB[1] 227–238 nm

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			777.7	Xe	IR	2
a'		H deformation	1492	gas	Ra	3
	11	CH s-bend	1265	gas	Ra	3
	16	C—CH_3 s-stretch	872	gas	Ra	3
	17	C—C—C s-bend	499	gas	Ra	3
	18	Skel. s-bend	289	gas	Ra	3
a''	22	CH OPLA	952H	gas	Ra	3
	27	CH_3 torsion	103H	gas	Ra	3

References

[1] A. B. Callear and H. K. Lee, Trans. Faraday Soc. **64**, 308 (1968).
[2] G. Maier and S. Senger, Liebigs Ann. 1445 (1996).
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$H_2CC(CH_3)CH_2$

gas AB[1,5] 223–258 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CH stretch	2830T	gas	AB	1
		C_3 deformation	350T	gas	AB	1

$^2A_1$ (3*s*) C_{2v}
T_0=38369(30) gas MPI[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		C_3 deformation	432(30)	gas	MPI	2

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_2 stretch	3109	N_2	IR	3,4
		CH_2 stretch	3025	N_2	IR	3,4
			1000	N_2	IR	3,4
			475	N_2	IR	3,4
a'	5	CH_2 scissors	1492(4)	gas	Ra	6
			1498	N_2	IR	3,4
	7	CH_3 s-deform.	1392(4)	gas	Ra	6
			1394	N_2	IR	3,4
	8	CH_2 rock	1353(4)	gas	Ra	6
	9	C_3 stretch	1037(4)	gas	Ra,PE	6,7
	11	C-CH_3 stretch	865(4)	gas	Ra	6
	12	CCH_2 OPLA	780(10)H	gas	PE	7
			795	N_2	IR	3,4
	14	CH_2 twist	538HT	gas	Ra	6
	15	C_3 deformation	432(4)	gas	Ra,PE	6,7
a''	19	CH_2 scissors	1471	N_2	IR	3,4
	20	CH_3 deformation	1400	N_2	IR	3,4

$D_2CC(CD_3)CD_2$

$\tilde{X}$ C_s

Vib sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			845(20)	gas	PE	7
		C_3 deformation	350(20)	gas	PE	7

References

[1] A. B. Callear and H. K. Lee, Trans. Faraday Soc. **64**, 308 (1968).
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[7] P. G. Wenthold, M. L. Polak, and W. C. Lineberger, J. Phys. Chem. **100**, 6920 (1996).

$H_2CC(CH_3)CH_2^-$

Threshold for electron detachment from ground-state $H_2CC(CH_3)CH_2^-$ =4070(50) gas PE[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C_3 deform.	425(20)	gas	PE	1

$D_2CC(CD_3)CD_2^-$

Threshold for electron detachment from ground-state $D_2CC(CD_3)CD_2^-$ =3980(65) gas PE[1]

Reference

[1] P. G. Wenthold, M. L. Polak, and W. C. Lineberger, J. Phys. Chem. **100**, 6920 (1996).

n-C_4H_9

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		1-CH_2 a-stretch	3105	Ar	IR	1–3
		1-CH_2 s-stretch	3024	Ar	IR	1–3
			2886	Ar	IR	2
		2-CH_2 a-stretch	2835	Ar	IR	2,3
		2-CH_2 s-stretch	2809	Ar	IR	1–3
			1471	Ar	IR	2
		-CH_2- deform.	1463	Ar	IR	2,3
		2-CH_2 deform.	1425	Ar	IR	2,3
		2-CH_2 deform.	1183	Ar	IR	2,3
			1098	Ar	IR	2
		$(C_3H_7)CH_2$ OPLA	520s	Ar	IR	1,3

References

[1] J. Pacansky, D. E. Horne, G. P. Gardini, and J. Bargon, J. Phys. Chem. **81**, 2149 (1977).
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[3] J. Pacansky, R. J. Waltman, and L. A. Barnes, J. Phys. Chem. **100**, 16828 (1996).

cyc-C_5H_5

$\tilde{A}$ $^2A_2''$ D_{5h} Structure: LF[9]
T_0=29572.166(2) gas AB[1,3,4]LF[6,8,11] $\tilde{A}-\tilde{X}$ 306–395 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1125T	gas	LF	11
			1058	gas	LF	11
			1020	gas	LF	11
e_2'			798	gas	AB,LF	4,9,11
e_2''		CH bend	331	gas	AB,LF	1,3,4,9,11

τ_0=64.9(5) ns gas LF[7,11]
B_0=0.286; C_0=0.144 LF[8,9]

$\tilde{X}$ $^2E_1''$ D_{5h} Structure: ESR[2]AB[4]LF[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3079wm	Ar	IR	10
			1383m	Ar	IR	10
			661vs	Ar	IR	10
e_2'	10	C-C stretch	1690(40)[a]	gas	PD	5
	11	CH deform.	1170(40)	gas	PD	5
	12		880	gas	PD,LF	5,6,9
	13	Ring deform.	475	gas	LF	6
e_2''	14	Ring deform.	380	gas	LF	6

B_0=0.296; C_0=0.148 LF[8,9]

cyc-C_5D_5

$\tilde{A}\ ^2A_2''$ D_{5h}
T_0=29819.434(2) gas AB[4]LF[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e_2''		CD bend	233	gas	AB	4

B_0=0.233; C_0=0.117 LF[9]

$\tilde{X}\ ^2E_1''$ D_{5h}
B_0=0.240; C_0=0.120 LF[9]

[a]Alternatively, may be contributed by $2\nu_{12}$.

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cyc-$C_5H_6^+$

The gas-phase photoelectron spectrum[1] of *cyc*-C_5H_6 shows several overlapping bands with unresolved structure, corresponding to excited states of *cyc*-$C_5H_6^+$ between 25300 and 50300.

$\tilde{B}\ ^2B_1$ C_{2v}
T_0=27430 Ar AB[3] $\tilde{B}-\tilde{X}$ 300–370 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1062(15)	Ar	AB	3

$\tilde{A}\ ^2B_1$ C_{2v}
T_0=16570(20) gas PE[1–3]
16500T Ar AB[3] $\tilde{A}-\tilde{X}$ 450–650 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			807(15)	gas	PE	2,3
			835(15)	Ar	AB	3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3		2885	Ar	IR	3
	4		1452(15)	gas	PE	1–3
			1456	Ar	IR	3
	6		1325	Ar	IR	3
	7		1113(15)	gas	PE	1–3
	9		944	Ar	IR	3
	10		807(15)	gas	PE	1–3
b_1	15		2901	Ar	IR	3
	17		866	Ar	IR	3
	18		612	Ar	IR	3
b_2	22		1423	Ar	IR	3
	23		1313	Ar	IR	3
	24		1266	Ar	IR	3
	25		1071	Ar	IR	3
	26		920	Ar	IR	3

cyc-$C_5D_6^+$

$\tilde{B}\ ^2B_1$ C_{2v}
T_0=27600T Ar AB[3] $\tilde{B}-\tilde{X}$ 300–370 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			892(15)	Ar	AB	3

$\tilde{A}\ ^2B_1$ C_{2v}
T_0=16500T Ar AB[3] $\tilde{A}-\tilde{X}$ 450–650 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			760(15)	gas	PE	3
			775(15)	Ar	AB	3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4		1412(15)	gas	PE	3
			1418	Ar	IR	3
	5		1312	Ar	IR	3
	6		1035	Ar	IR	3
	7		954	Ar	IR	3
	8		823(15)	gas	PE	3
	9		760	Ar	IR	3
b_1	17		686	Ar	IR	3
	18		458	Ar	IR	3
b_2	22		1345	Ar	IR	3
	23		1204	Ar	IR	3
	27		707	Ar	IR	3

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n-C_5H_{11}

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		1-CH_2 a-stretch	3103	Ar	IR	1,2
		1-CH_2 s-stretch	3025	Ar	IR	1,2
		2-CH_2 a-stretch	2838	Ar	IR	1,2
		2-CH_2 s-stretch	2802	Ar	IR	1,2
		2-CH_2 deform.	1425	Ar	IR	1,2
		2-CH_2 deform.	1181	Ar	IR	1,2
			1096	Ar	IR	1
		$(C_4H_9)CCH_2$ OPLA	519s	Ar	IR	1,2

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m-C_6H_4

(m-Benzyne)

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CH stretch	3037w	Ar	IR	1
		Mixed	1402wm	Ar	IR	1
b_1		CH OPLA	824wm	Ar	IR	1
		CH OPLA	751ms	Ar	IR	1
b_2		Mixed	1486wm	Ar	IR	1
		HCC deform.	936m	Ar	IR	1
		Ring deform.	547vs	Ar	IR	1

Reference

[1] R. Marquardt, W. Sander, and E. Kraka, Angew. Chem. **108**, 825 (1996); Angew. Chem. Int. Ed. Engl. **35**, 746 (1996).

C_6H_5

A broad gas-phase absorption with maximum near 40820 (245 nm) has been attributed[7] to C_6H_5. In an argon matrix, a broad, very prominent absorption maximum at 41060, with a partially resolved shoulder at 38360, has also been attributed[12] to C_6H_5.

A prominent absorption near 34720 (288 nm) in argon-matrix studies has been assigned[4,9,12] to C_6H_5.

$\tilde{A}$ $^2B_1$ C_{2v}
T_0=18908 gas AB[1] $\tilde{A}-\tilde{X}$ 440–530 nm
18716 Ar AB[4] $\tilde{A}-\tilde{X}$ 530–535 nm

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

Gas-phase photoelectron spectra[10] suggest that there is an excited electronic state of C_6H_5 at or below 13700.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH s-stretch	3085w	Ar	IR	6,8,11
	2	CH s-stretch	3071vw	Ar	IR	11
	3	CH s-stretch	3052vw	Ar	IR	11
	4	Ring stretch	1499w	Ar	IR	11
	5	Ring stretch	1441wm	Ar	IR	8,11
	6	CH deform.	1080w	Ar	IR	11
	7	Ring deform.	1027wm	Ar	IR	6,8,11
	8	Ring breathing	1011vw	Ar	IR	11
	9	Ring deform.	968(15)	gas	PE	10
			976w	Ar	IR	8,11
	10	Ring deform.	600(10)	gas	PE	10
			605w	Ar	IR	8,11
b_1	14	CH deform.	971vw	Ar	IR	11
	15	CH deform.	878w	Ar	IR	11
	16	CH deform.	707s	Ar	IR	2–6,8,11
	17	CH deform.	656ms[a]	Ar	IR	8
	18	Deformation	416w	Ar	IR	11
b_2	19	CH a-stretch	3073wm	Ar	IR	8,11
	20	CH a-stretch	3060vw	Ar	IR	8,11
	21	Ring stretch	1593vw	Ar	IR	11
	22	Ring stretch	1433wm	Ar	IR	6,8,11
	23	CH deform.	1344vw	Ar	IR	11
	24	Ring deform.	1226wm	Ar	IR	6,11
	25	CH deform.	1086vw	Ar	IR	11
	26	Ring deform.	1067w	Ar	IR	8,11
	27	Ring stretch	586vw	Ar	IR	8,11

C_6D_5

A prominent absorption at 286 nm in argon-matrix studies of photolyzed benzene samples has been attributed[4] to C_6D_5.

$\tilde{A}$ $^2B_1$ C_{2v}
T_0=18840 Ar AB[4] $\tilde{A}-\tilde{X}$ 530–535 nm

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			960(20)	gas	PE	10
			588(10)	gas	PE	10
b_1		CD deform.	519s	Ar	IR	2,5

[a]This absorption is assigned to C_6H_5 formed by the photolysis of C_6H_5NO, but would be obscured by a very prominent CO_2 absorption when C_6H_5 is formed by the photolysis of a benzoyl peroxide. Its position and intensity agree more satisfactorily with the *ab initio* calculations of Ref. 11 than do those for the assignment proposed in that paper.

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$C_6H_6^+$

$\tilde{G}\ ^2A_{1g}$ D_{6h}
T^a=61290(100) gas PE[1,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1[b] (2)	CH stretch	2790(100)	gas	PE	1
	2 (1)	Ring stretch	930(100)	gas	PE	1

$\tilde{F}\ ^2B_{1u}$ D_{6h}
T^a=50160(100) gas PE[1,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1[b] (2)	CH stretch	2340(100)	gas	PE	1

$\tilde{E}\ ^2B_{2u}$ D_{6h}
T^a=45320(100) gas PE[5]

$\tilde{D}\ ^2E_{1u}$ D_{6h}
T^a=38220(100) gas PE[5]

$\tilde{C}\ ^2A_{2u}$ D_{6h}
T^a=25310(100) gas PE[5]

In the gas phase, the mass-selected ion-dip spectrum of $C_6H_6^+$ shows a broad, unstructured absorption with onset near 19000 and increasing in intensity up to the detection limit of 24000.[10]

A broad, unstructured absorption near 24000 may have been contributed by the $\tilde{C}$–$\tilde{X}$ transition of $C_6H_6^+$ produced by vacuum-ultraviolet photolysis of benzene isolated in a neon matrix.[2]

T_0≅19840 Ar LF[3]AB[4] $\tilde{C}$–$\tilde{X}$ 420–547 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e_{2g}	18[b] (6)	Ring deform.	600(30)T	Ar	AB	4

$\tilde{B}\ ^2E_{2g}$ D_{6h}
T_0=18113 gas PF[9]PRI[13] $\tilde{B}$–$\tilde{X}$ 510–550 nm

In an argon matrix, a weak, sharp absorption at 18100 has been attributed[3] to a vibronically allowed transition in the excitation of $C_6H_6^+$ to the $\tilde{B}$ state.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1[b] (2)	CH stretch	2850(100)	gas	PE	1
	2 (1)	Ring stretch	990[c]	gas	PF	9
e_{2g}	16 (8)	Ring stretch	1520(100)T	gas	PE	1
	17 (9)	CH bend	1140[c]	gas	PF	9
	18 (6)	Ring deform.	645(100)[d]	gas	PE	1
e_{2u}	19 (17)	CH bend	574	gas	PF	9
	20 (16)	Ring deform.	224	gas	PF	9

$\tilde{X}\ ^2E_{1g}$ D_{6h} Structure: TPE[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1[b] (2)	CH stretch	2960(100)T	gas	PE	1
	2 (1)	Ring stretch	975(15)	gas	PE, MPI	1,6,8
b_{2g}	8 (4)	Ring deform.	415(20)	gas	PE	6
e_{1g}	11 (10)	CH bend	835(15)	gas	MPI	8
e_{2g}	16 (8)	Ring stretch	1561(20)[d]	gas	PE	1,6
			1480(10)T	Ar	LF	3
	17 (9)	CH bend	1230(15)[d]	gas	PE, MPI	1,6,8
	18 (6)	Ring deform.	676.4[d]	gas	TPE, MPI	1,6,8,12
			630(10)T	Ar	LF	3
			365.4[e]	gas	TPE	12
			345.4[f]	gas	PE, TPE	6,12
e_{2u}	20 (16)	Ring deform.	295(5)	gas	PE, MPI	6,8

B_0=0.189; C_0=0.095 PE[7]TPE[11]TPI[14]

$C_6D_6^+$

$\tilde{G}\ ^2A_{1g}$ D_{6h}
T^a≅62000 gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1[b] (2)	CD stretch	2240(100)	gas	PE	1
	2 (1)	Ring stretch	920(100)	gas	PE	1

$\tilde{F}$ $^2B_{1u}$ D_{6h}
$T^a \cong 50000$ gas PE[1]

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

$\tilde{C}$ $^2A_{2u}$ D_{6h}
$T_0 \cong 19930$[c] Ar LF[3]AB[4] $\tilde{C}-\tilde{X}$ 470–545 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e_{2g}	18[b] (6)	Ring deform.	590(60)T	Ar	AB	4

$\tilde{B}$ $^2E_{2g}$ D_{6h}
$T^a \cong 18600$ gas PE[1]

In an argon matrix, a weak, sharp absorption at 18215 has been attributed[3] to a vibronically allowed transition in the excitation of $C_6D_6^+$ to the $\tilde{B}$ state.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1[b] (2)	CD stretch	2140(100)	gas	PE	1
e_{2g}	16 (8)	Ring stretch	1450(100)	gas	PE	1
	17 (9)	CD bend	870(100)	gas	PE	1
	18 (6)	Ring deform.	600(100)	gas	PE	1

$\tilde{X}$ $^2E_{1g}$ D_{6h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1[b] (2)	CD stretch	2330(100)	gas	PE	1
	2 (1)	Ring stretch	928(20)	gas	PE	1,6
b_{2g}	8 (4)	Ring deform.	351(20)	gas	PE	6
e_{2g}	16 (8)	Ring stretch	1565(100)	gas	PE	1
			1460(10)T	Ar	LF	3
	18 (6)	Ring deform.	637(20)[d]	gas	PE	1,6
			590(10)T	Ar	LF	3
			343(20)[g]	gas	PE	6
e_{2u}	20 (12)	Ring deform.	278(20)	gas	PE	6

$B=0.155$; $C=0.076$ TPI[14]

[a]From vertical ionization potentials. The first ionization potential of benzene is taken to equal 74555.0(4), or 9.2405 eV, from Ref. 7.
[b]In order to be consistent with other vibrational numberings in these tables, the vibrational numbering of Herzberg is used here. However, many authors use instead the vibrational numbering of Wilson (E. B. Wilson, Jr., Phys. Rev. **45**, 706 (1934)). This latter numbering is indicated in parentheses.
[c]From analysis of combination bands.
[d]$j=\pm 1/2$.
[e]$j=+3/2$.
[f]$j=-3/2$.
[g]$j=3/2$.

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$(CH_3)_3CCH{=}C$:

$\tilde{a}$ $^3A'$ C_s
$T_0=15930(120)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1230(50)	gas	PE	1
			800(50)	gas	PE	1
			520(50)	gas	PE	1
			340(50)	gas	PE	1

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

Reference

[1] R. F. Gunion and W. C. Lineberger, J. Phys. Chem. **100**, 4395 (1996).

$(CH_3)_3CCH{=}C^-$

Threshold for electron detachment from ground-state $(CH_3)_3CCH{=}C^-$
$=5200(120)$ gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			370(50)	gas	PE	1

Reference

[1] R. F. Gunion and W. C. Lineberger, J. Phys. Chem. **100**, 4395 (1996).

$C_7H_2^+$

$\tilde{A}\ ^2\Pi_u$ $D_{\infty h}$
T_0=16676(5)T Ne AB[1]

Reference

[1] P. Freivogel, J. Fulara, D. Lessen, D. Forney, and J. P. Maier, Chem. Phys. **189**, 335 (1994).

HC_7H

$^3\Sigma_u^-$ $D_{\infty h}$
T_0=19812(5) Ne AB[1] $^3\Sigma_u^- - \tilde{X}$ 410–506 nm
19770(5)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	2	C≡C s-stretch	1961(5)	Ne	AB	1
	4		647(5)	Ne	AB	1
Π		CH bend	286HT	Ne	AB	1

DC_7D

$^3\Sigma_u^-$ $D_{\infty h}$
T_0=19932(5) Ne AB[1] $^3\Sigma_u^- - \tilde{X}$ 410–503 nm
19891(5)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	2	C≡C s-stretch	1935(5)	Ne	AB	1
	4		551(5)	Ne	AB	1
Π		CD bend	202HT	Ne	AB	1

Reference

[1] J. Fulara, P. Freivogel, D. Forney, and J. P. Maier, J. Chem. Phys. **103**, 8805 (1995).

$C_6H_5CH_2^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	11		993(2)	gas	TPE	3
	12		820(2)	gas	TPE	3
	13	Ring deform.	525(2)	gas	PE,TPE	1–3
a_2	16		627T	gas	TPE	3
	17		316H	gas	TPE	3
b_1	23		400H	gas	TPE	3
	24		163H	gas	TPE	3
b_2	28		1547(2)	gas	TPE	3
	32		1183T	gas	TPE	3
	33		1115T	gas	TPE	3
	34		973(2)	gas	TPE	3
	35	Ring deform.	598(2)	gas	TPE	2,3
	36		353(2)	gas	TPE	3

$C_6H_5CD_2^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	11		951(2)	gas	TPE	3
	12		737(2)	gas	TPE	3
	13	Ring deform.	500T	gas	PE,TPE	1–3
a_2	17		278H	gas	TPE	3
b_1	23		349T	gas	TPE	3
	24		145T	gas	TPE	3
b_2	32		880T	gas	TPE	3
	33		862T	gas	TPE	3
	34		779T	gas	TPE	3
	35	Ring deform.	575(2)	gas	TPE	2,3
	36		302(2)	gas	TPE	3

[a]If, as in Refs. 2 and 3, the x axis is chosen in the molecular plane, interchange of the b_1 and b_2 representations results. However, the international convention established in 1955 is followed in the symmetry designations given here. This necessitates a renumbering of the vibrational fundamentals, so that modes 18–24 (numbered 30–36 in Refs. 2 and 3) are of b_1 symmetry and 25–36 (numbered 18–29 in Refs. 2 and 3) of b_2 symmetry.

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$C_6H_5CH_2$

$\tilde{E}$

A gas-phase absorption maximum near 230 nm has been attributed[9] to the first Rydberg transition of $C_6H_5CH_2$.

$\tilde{D}$

A gas-phase absorption between 260 and 245 nm, with maximum near 255 nm, has been attributed[9] to the $\tilde{D}-\tilde{X}$ transition of $C_6H_5CH_2$. This band may have been excited in the MPI studies of Ref. 16. In a neon matrix, the counterpart of this absorption maximum has been observed near 245 nm.[6]

$\tilde{C}\ ^2A_2$ C_{2v}
T_0=32760 gas AB[2,5,7] $\tilde{C}-\tilde{X}$ 291–309 nm
32730 Ne AB[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	7a	C-CH_2 stretch	1145	gas	AB	7
	18a	CH deform.	968	gas	AB	7
	1	Ring breathing	931	gas	AB	7
	12a	Ring deform.	804	gas	AB	7
	6a	Ring deform.	432	gas	AB	7
b_2	6b	Ring deform.	525	gas	AB	7
	18b	CH deform.	276	gas	AB	7

$\tilde{B}\ ^2B_1$[a] C_{2v}
T_0=22850T gas AB[11]EM[11]LF[22,24]
Vibronically coupled to modes of b_2 symmetry in the $\tilde{A}$ state.[11,22,24,27]
A^b=0.179; B^b=0.088; C^b=0.059 gas LF[24]

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

T_0=22001.5 gas EM[1,3,5,10]AB[4]LF[12,20–22,26] $\tilde{A}-\tilde{X}$ 429–455 nm

22003 Ne AB[6] $\tilde{A}-\tilde{X}$ 429–455 nm

21862 Ar LF[13] $\tilde{A}-\tilde{X}$ 430–510 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			910	Ar	LF	13
			770T	gas	LF	20
			798	Ar	LF	13
	6a	Ring deform.	437	gas	AB,LF	11,18,20,22
			433	Ne	AB	6
			456	Ar	LF	13
	6b	Ring deform.	388[c]	gas	AB,LF	11,17,18,22
			402	Ne	AB	6
	6b	Ring deform.	328[c]	gas	AB,LF	11,17,18,22
			344	Ne	AB	6

$\tau_{0(1)}$=0.4 μs; $\tau_{0(2)}$=1.85 μs gas LF[15,20,21]

A^d=0.180; B^d=0.088; C^d=0.059 EM[10,17,19]LF[22,24]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CH stretch	3069w	Ar	IR	25
	8a	Ring stretch	1603	gas	EM	5,8,18
		C-CH$_2$ stretch	1510(25)T	gas	PE	23
			1469m	Ar	IR	25
	19a	Ring stretch	1431	gas	EM	5,8,18
			1423	Ar	LF	13
		CH$_2$ deform.	1409m	Ar	IR	25
	7a		1258	gas	EM,LF	5,7,18,20
			1264m	Ar	IR	25
	9a	CH deform.	1181	gas	EM	5,8
	18a	CH deform.	1046	gas	EM	18
	1	Ring breathing	987.4	gas	EM,LF	5,8,10,18,20
			982	Ar	LF	13
	12a	Ring deform.	830	gas	EM,LF	5,8,18,20
	6a	Ring deform.	524	gas	EM,LF,PE	5,8,10,20,23
			520	Ar	LF	13
a_2	17a	CH deform.	963	gas	EM	18
	10a	CH deform.	860	gas	EM	8,18
	16a	Ring deform.	393	gas	EM	8
b_1			882.0w	Ar	IR	25
			762.0vs	Ar	IR	25
		CH$_2$ wag	710.9w	Ar	IR	25
			667.0s	Ar	IR	25
			465.0s	Ar	IR	25
	16b	Ring deform.	430	gas	EM	8
b_2		CH$_2$ a-stretch	3111w	Ar	IR	25
	8b	Ring stretch	1549	gas	EM	5,8,18
			1530	Ar	LF	13
			1446m	Ar	IR	25
			1305w	Ar	IR	25
	9b	CH deform.	1152	gas	EM	5,8,18
	15	CH deform.	1089	gas	EM	5,8
			1015w	Ar	IR	25
			948.1vw	Ar	IR	25
	6b	Ring deform.	615	gas	EM,LF	5,8,10,18,20
			612	Ar	LF	13
	18b	CH deform.	356	gas	EM,LF	5,8,18,20
			357	Ar	LF	13

A_0=0.184; B_0=0.090; C_0=0.060 EM[10,17,19]LF[24]

$C_6D_5CD_2$

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

T_0=22455(10) gas AB[11]EM[11]

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

T_0=22093.7 gas EM[5,10]

21962 Ar LF[13] $\tilde{A}-\tilde{X}$ 434–502 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			844	Ar	LF	13
			731	Ar	LF	13
	6a	Ring deform.	404	Ar	LF	13

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

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	8a	Ring stretch	1593	gas	EM	5,8
	19a	Ring stretch	1327	gas	EM	5,8
			1323	Ar	LF	13
	7a	C-CD$_2$ stretch	1204	gas	EM	5,8
	1	Ring breathing	945.7	gas	EM	5,8,10
			945	Ar	LF	13
	9a	CD deform.	895	gas	EM	5,8
	18a	CD deform.	848	gas	EM	8
	12a	Ring stretch	791	gas	EM	5,8
	6a	Ring deform.	497.5	gas	EM	5,8,10
			495	Ar	LF	13
a_2	10a	CD deform.	750	gas	EM	8
	16a	Ring deform.	305	gas	EM	8
b_1	16b	Ring deform.	376	gas	EM	8
b_2	8b	Ring stretch	1495	gas	EM	5,8
			1490	Ar	LF	13
	15	CD deform.	848	gas	EM	5,8
	6b	Ring deform.	589.1	gas	EM	5,8,10
			588	Ar	LF	13
	18b	CD deform.	305	gas	EM	5,8
			303	Ar	LF	13

[a]In many of the references concerned with this molecule, the x axis is chosen in the molecular plane, resulting in an interchange of the B_1 and B_2 representations. However, the international convention established in 1955 is followed in the symmetry designations given here. In all of the references, the vibrational numbering follows that introduced by Wilson (E. B. Wilson, Jr., Phys. Rev. **45**, 706 (1934)). In view of this unanimity, the common vibrational numbering is retained.

[b]From analysis of band at 22326.368(2).

[c]Data presented in Ref. 22 suggest that this level is mixed with a nearby a_1 level of the $\tilde{B}\ ^2B_1$ state.

[d]From analysis of band at 22432.395(2).

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C_8H

$^2\Pi$ $C_{\infty v}$
T_0=15848(5) Ne AB^1 $^2\Pi-\tilde{X}$ 515–631 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3		2080(5)	Ne	AB	1
	5		1607(5)	Ne	AB	1
	6		783(5)	Ne	AB	1

$\tilde{X}$ $^2\Pi$ $C_{\infty v}$
A_{eff}=−19.33 MW^2
B=0.0196 MW^2

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$C_8H_2^+$

$\tilde{C}$ $^2\Pi_u$ $D_{\infty h}$
T_0=31300(200) gas PE^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			400T	gas	PE	1

$\tilde{B}$ $^2\Pi_g$ $D_{\infty h}$
T_0=24600(200) gas PE^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+			1960(80)	gas	PE	1
			1380(80)	gas	PE	1

$\tilde{A}$ $^2\Pi_u$ $D_{\infty h}$
T_0=14160(10) gas PE^1EF^2
13975 Ne LF^3AB^4 $\tilde{A}-\tilde{X}$ 625–845 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	3	C≡C stretch	1950(80)	gas	PE	1
			2029.5	Ne	LF,AB	3,4
	5	C-C stretch	463	Ne	LF,AB	3,4

$\tau_0 \leq 6$ ns gas EF^2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	2	C≡C stretch	2100(80)	gas	PE	1
			2141.0	Ne	LF	3
	3	C≡C stretch	2040.5	Ne	LF	3
	5	C-C stretch	472.2	Ne	LF	3
Π	17	Deform.	88.5HT	Ne	LF	3

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m-$(CH_2)_2C_6H_4$

$\tilde{b}$ $^1B_2$ C_{2v}
T_0=7520U gas PE^1

$\tilde{a}$ $^1A_1$ C_{2v}
T_0=3350(65) gas PE^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1260(40)	gas	PE	1
			1000(40)	gas	PE	1
			265(20)	gas	PE	1

$\tilde{X}$ $^3B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CH_2 scissors	1500(40)	gas	PE	1
		Ring deform.	540(20)	gas	PE	1
		Ring=C bend	290(20)	gas	PE	1

Reference

[1] P. G. Wenthold, J. B. Kim, and W. C. Lineberger, J. Am. Chem. Soc. **119**, 1354 (1997).

p-$(CH_2)_2C_6H_4$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			3102m	Ar	IR	1,2
			3059m	Ar	IR	1,2
			3047m	Ar	IR	1
			3038m	Ar	IR	1
			3010w	Ar	IR	1
			1603m	Ar	IR	1,2
			1449m	Ar	IR	1,2
			1342m	Ar	IR	1,2
			1136w	Ar	IR	1,2
			966w	Ar	IR	1
			940w	Ar	IR	1,2
			868s	Ar	IR	1,2
			821m	Ar	IR	1
			780m	Ar	IR	1,2
			468s	Ar	IR	1,2

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m-$(CH_2)_2C_6H_4^-$

Threshold for electron detachment from ground-state *m*-$(CH_2)_2C_6H_4^-$ =7410(65) gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			275(20)	gas	PE	1

Reference

[1] P. G. Wenthold, J. B. Kim, and W. C. Lineberger, J. Am. Chem. Soc. **119**, 1354 (1997).

C_9

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

T_0=33895(25) Ne AB[9] $^1\Sigma_u^+-\tilde{X}$ 292–295 nm

32480[a] Ar AB[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			306(30)	Ne	AB	9

T_0=26777(15)T Ne AB[9] 324–374 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		2535(20)	Ne	AB	9
	3		1041(20)	Ne	AB	9
	4		443(20)	Ne	AB	9

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	3	Sym. stretch	1258(50)	gas	PE	6
	4	Sym. stretch	484(48)	gas	PE	6
			448T	Ar	IR	12
Σ_u^+	5	Asym. stretch	2079.67	gas	DL	11
			2081.1	Ne	IR	12,13
			2078.1	Ar	IR	12
			2079.0T	Kr	IR	12
	6	Asym. stretch	2014.28	gas	DL	3,7
			2010.0	Ne	IR	12,13
			1998.0[a]	Ar	IR	1,2,5,12
			1994.2	Kr	IR	12
			2007.3	H_2	IR	10
	7	Asym. stretch	1602.8	Ne	IR	12
			1601.0	Ar	IR	8,12
			1600.8	Kr	IR	12

B_0=0.0143 DL[3,7,11]

[a]Previously assigned to C_8. Reassignment to C_9 dictated by arguments presented in Ref. 4.

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C_9^-

Threshold for electron detachment from ground-state C_9^- =29720(80) gas PE[1,2]

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

T_0=34536(24) Ne AB[6] $\tilde{D}-\tilde{X}$ 281–290 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	3		983(25)	Ne	AB	6
	4		474(24)	Ne	AB	6

$\tilde{C}\ ^2\Pi_g$ $D_{\infty h}$
T_0=29446(17) Ne AB[6] $\tilde{C}-\tilde{X}$ 295–340 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		2177(19)	Ne	AB	6
	2		1666(19)	Ne	AB	6
	4		435(17)	Ne	AB	6

$\tilde{B}\ ^2\Pi_g$ $D_{\infty h}$
T_0=16470(10) gas MPD[5] $\tilde{B}-\tilde{X}$ 530–608 nm
16468(5) Ne AB[6] $\tilde{B}-\tilde{X}$ 528–608 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		2001(6)	Ne	AB	6

$\tilde{A}\ ^2\Pi_g$ $D_{\infty h}$
T_0=13020(10) gas MPD[5]
13082(3) Ne AB[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+			1200(40)	gas	MPD	5

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	6	Asym. stretch	1692.6	Ne	IR	4
			1686.7	Ar	IR	3
	7	Asym. stretch	1583.3T	Ar	IR	3

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C_9H

$\tilde{X}\ ^2\Pi_{1/2}$ $C_{\infty v}$
B_0=0.0138 MW[1]

Reference

[1] M. C. McCarthy, M. J. Travers, P. Kalmus, C. A. Gottlieb, and P. Thaddeus, Astrophys. J. **467**, L125 (1996).

$C_9H_2^+$

$\tilde{A}\ ^2\Pi_g$ $D_{\infty h}$
T_0=14387(5)T Ne AB[1] $\tilde{A}-\tilde{X}$ 609–695 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+		CC stretch	2005(5)T	Ne	AB	1

Reference

[1] P. Freivogel, J. Fulara, D. Lessen, D. Forney, and J. P. Maier, Chem. Phys. **189**, 335 (1994).

HC_9H

$^3\Sigma_u^-$ $D_{\infty h}$
T_0=17218(5) Ne AB[1] $^3\Sigma_u^- - \tilde{X}$ 433–583 nm
17160(5)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	3	C≡C s-stretch	1969(5)	Ne	AB	1
			770(5)	Ne	AB	1

DC_9D

$^3\Sigma_u^-$ $D_{\infty h}$
T_0=17292(5) Ne AB[1] $^3\Sigma_u^- - \tilde{X}$ 432–581 nm
17236(5)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	3	C≡C s-stretch	1966(5)	Ne	AB	1

Reference

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C_{10}

$\tilde{X}\ ^3\Sigma_g^-$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+			2074.5	Ne	IR	1
			1915.4	Ne	IR	1

Reference

[1] P. Freivogel, M. Grutter, D. Forney, and J. P. Maier, Chem. Phys. **216**, 401 (1997).

C_{10}^-

(2) $^2\Pi_g$ $D_{\infty h}$
T_0=13596(5) Ne AB[1,3] 447–736 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		2022(7)	Ne	AB	1,3
	2		1913(7)	Ne	AB	3
	5		400(6)	Ne	AB	1,3

$\tilde{C}$ $^2\Pi_g$ $D_{\infty h}$
T_0=10338(5) Ne AB[1] $\tilde{C}$–$\tilde{X}$ 804–968 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	2		2092(5)	Ne	AB	1
	3		1992(5)	Ne	AB	1
	4		488(5)	Ne	AB	1
	5		372(5)	Ne	AB	1

$\tilde{B}$ $^2\Sigma_g^+$ $D_{\infty h}$
T_0=8964(2) Ne AB[3]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+			2094.5	Ne	IR	2

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$C_{10}H$

$^2\Pi$ $C_{\infty v}$
T_0=13852(5) Ne AB[1] $^2\Pi$–$\tilde{X}$ 627–722 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3		2097(5)	Ne	AB	1
	5		1520(5)T	Ne	AB	1

Reference

[1] P. Freivogel, J. Fulara, M. Jakobi, D. Forney, and J. P. Maier, J. Chem. Phys. **103**, 54 (1995).

$C_{10}H_2^+$

$\tilde{A}$ $^2\Pi_g$ $D_{\infty h}$
T_0=12143(5) Ne AB[1] $\tilde{A}$–$\tilde{X}$ 703–824 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+		C≡C stretch	2072(5)	Ne	AB	1
		C-C stretch	396(5)	Ne	AB	1

Reference

[1] P. Freivogel, J. Fulara, D. Lessen, D. Forney, and J. P. Maier, Chem. Phys. **189**, 335 (1994).

C_{11}

$^1\Sigma_u^+$ $D_{\infty h}$
T_0=29732(20) Ne AB[2] $^1\Sigma_u^+$–$\tilde{X}$ 323–337 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+			1166(30)	Ne	AB	2
			872(30)	Ne	AB	2
			528(30)	Ne	AB	2
			240(30)	Ne	AB	2

T_0=22245(10)T Ne AB[2] 399–450 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		2440(15)	Ne	AB	2
	2		2298(15)	Ne	AB	2
	5		357(15)	Ne	AB	2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+		Sym. stretch	440T	gas	PE	1
Σ_u^+	7	Asym. stretch	1938.6	Ne	IR	3
	8	Asym. stretch	1853.4	Ne	IR	3

References

[1] D. W. Arnold, S. E. Bradforth, T. N. Kitsopoulos, and D. M. Neumark, J. Chem. Phys. **95**, 8753 (1991).
[2] D. Forney, P. Freivogel, M. Grutter, and J. P. Maier, J. Chem. Phys. **104**, 4954 (1996).
[3] P. Freivogel, M. Grutter, D. Forney, and J. P. Maier, Chem. Phys. **216**, 401 (1997).

$C_{11}H$

$\tilde{X}$ $^2\Pi$ $D_{\infty h}$
A_0=25T; B_0=0.0076 MW[1]

Reference

[1] M. C. McCarthy, M. J. Travers, P. Kalmus, C. A. Gottlieb, and P. Thaddeus, Chem. Phys. Lett. **264**, 252 (1997).

$C_{11}H_2^+$

$\tilde{A}\ ^2\Pi_u$ $D_{\infty h}$
T_0=12674(5)T Ne AB[1] $\tilde{A}-\tilde{X}$ 681–789 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+		CC stretch	1993(5)T	Ne	AB	1

Reference

[1] P. Freivogel, J. Fulara, D. Lessen, D. Forney, and J. P. Maier, Chem. Phys. **189**, 335 (1994).

$HC_{11}H$

$^3\Sigma_u^-$ $D_{\infty h}$
T_0=15302(5) Ne AB[1] $^3\Sigma_u^- - \tilde{X}$ 519–656 nm
15268(5)
15251(5)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+		C≡C s-stretch	1973(5)	Ne	AB	1
		C≡C s-stretch	1885(5)	Ne	AB	1

$DC_{11}D$

$^3\Sigma_u^-$ $D_{\infty h}$
T_0=15294(5) Ne AB[1]

Reference

[1] J. Fulara, P. Freivogel, D. Forney, and J. P. Maier, J. Chem. Phys. **103**, 8805 (1995).

C_{12}

$\tilde{X}\ ^3\Sigma_g^-$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+			2003.9T	Ne	IR	1

Reference

[1] P. Freivogel, M. Grutter, D. Forney, and J. P. Maier, Chem. Phys. **216**, 401 (1997).

C_{12}^-

(2) $^2\Pi_u$ $D_{\infty h}$
T_0=11636(5) Ne AB[1,3] 642–860 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		2014(6)	Ne	AB	3
	2		1923(6)	Ne	AB	1,3
	4		1463(5)	Ne	AB	3
	6		320(4)	Ne	AB	1,3

$\tilde{C}\ ^2\Pi_u$ $D_{\infty h}$
T_0=8006(5) Ne AB[1] $\tilde{C}-\tilde{X}$ 1200–1250 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	6		323(5)	Ne	AB	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+			2012.6	Ne	IR	2
			1819.3	Ne	IR	2

References

[1] P. Freivogel, J. Fulara, M. Jakobi, D. Forney, and J. P. Maier, J. Chem. Phys. **103**, 54 (1995).
[2] P. Freivogel, M. Grutter, D. Forney, and J. P. Maier, Chem. Phys. **216**, 401 (1997).
[3] P. Freivogel, M. Grutter, D. Forney, and J. P. Maier, J. Chem. Phys. **107**, 4468 (1997).

$C_{12}H$

$^2\Pi$ $C_{\infty v}$
T_0=12492(5) Ne AB[1] $^2\Pi-\tilde{X}$ 685–801 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3		2089(5)	Ne	AB	1
	5		1395(5)T	Ne	AB	1

Reference

[1] P. Freivogel, J. Fulara, M. Jakobi, D. Forney, and J. P. Maier, J. Chem. Phys. **103**, 54 (1995).

$C_{12}H_2^+$

$\tilde{A}\ ^2\Pi_u$ $D_{\infty h}$
T_0=10703(5) Ne AB[1] $\tilde{A}-\tilde{X}$ 777–935 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+		C≡C stretch	2154(5)	Ne	AB	1
		C-C stretch	322(5)	Ne	AB	1

Reference

[1] P. Freivogel, J. Fulara, D. Lessen, D. Forney, and J. P. Maier, Chem. Phys. **189**, 335 (1994).

C_{13}

$^1\Sigma_u^+$ $D_{\infty h}$
T_0=26341(15) Ne AB[2] $^1\Sigma_u^+-\tilde{X}$ 370–380 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			669(20)	Ne	AB	2
			424(20)	Ne	AB	2
			207(20)	Ne	AB	2

T_0=18761(7)T Ne AB[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		2409(10)	Ne	AB	2
	2		2258(10)	Ne	AB	2
	6		307(10)	Ne	AB	2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+			1808.96	gas	DL	1

B_0=0.0047 DL[1]

References

[1] T. F. Giesen, A. Van Orden, H. J. Hwang, R. S. Fellers, R. A. Provençal, and R. J. Saykally, Science **265**, 756 (1994).
[2] D. Forney, P. Freivogel, M. Grutter, and J. P. Maier, J. Chem. Phys. **104**, 4954 (1996).

$C_{13}H_2^+$

$\tilde{A}$ $^2\Pi_g$ $D_{\infty h}$
T_0=11418(5)T Ne AB[1] $\tilde{A}-\tilde{X}$ 746–874 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+		CC stretch	1924(5)T	Ne	AB	1

Reference

[1] P. Freivogel, J. Fulara, D. Lessen, D. Forney, and J. P. Maier, Chem. Phys. **189**, 335 (1994).

$HC_{13}H$

$^3\Sigma_u^-$ $D_{\infty h}$
T_0=13901(5) Ne AB[1] $^3\Sigma_u^--\tilde{X}$ 562–722 nm
13866(5)
13852(5)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+		C≡C s-stretch	1967(5)	Ne	AB	1
		C≡C s-stretch	1904(5)	Ne	AB	1
			619(5)	Ne	AB	1

Reference

[1] J. Fulara, P. Freivogel, D. Forney, and J. P. Maier, J. Chem. Phys. **103**, 8805 (1995).

C_{14}^-

(2) $^2\Pi_g$ $D_{\infty h}$
T_0=10202(2) Ne AB[1,2] 723–981 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		1810(4)	Ne	AB	2

$\tilde{C}$ $^2\Pi_g$ $D_{\infty h}$
T_0=6849(5) Ne AB[1] $\tilde{C}-\tilde{X}$ 1402–1460 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	7		283(2)	Ne	AB	1

References

[1] P. Freivogel, J. Fulara, M. Jakobi, D. Forney, and J. P. Maier, J. Chem. Phys. **103**, 54 (1995).
[2] P. Freivogel, M. Grutter, D. Forney, and J. P. Maier, J. Chem. Phys. **107**, 4468 (1997).

$C_{14}H$

$^2\Pi$ $C_{\infty v}$
T_0=11554(5)T Ne AB[1]

Reference

[1] P. Freivogel, J. Fulara, M. Jakobi, D. Forney, and J. P. Maier, J. Chem. Phys. **103**, 54 (1995).

$C_{14}H_2^+$

$\tilde{A}$ $^2\Pi_g$ $D_{\infty h}$
T_0=9548(5) Ne AB[1] $\tilde{A}-\tilde{X}$ 858–1048 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+		C≡C stretch	2097(5)	Ne	AB	1
		C-C stretch	258(5)	Ne	AB	1

Reference

[1] P. Freivogel, J. Fulara, D. Lessen, D. Forney, and J. P. Maier, Chem. Phys. **189**, 335 (1994).

C_{15}

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

T_0=23832(12) Ne AB[1] $^1\Sigma_u^+-\tilde{X}$ 410–420 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			277(20)	Ne	AB	1

T_0=16090(5)T Ne AB[1] 611–622 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	7		266(7)	Ne	AB	1

Reference

[1] D. Forney, P. Freivogel, M. Grutter, and J. P. Maier, J. Chem. Phys. **104**, 4954 (1996).

C_{16}^-

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

T_0=5784(5) Ne AB[1] $^2\Pi_g-\tilde{X}$ 1658–1730 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	8		245(5)	Ne	AB	1

Reference

[1] P. Freivogel, J. Fulara, M. Jakobi, D. Forney, and J. P. Maier, J. Chem. Phys. **103**, 54 (1995).

8.16. Non-Hydrocarbons with More Than Eight Atoms

$(CH_3)_2Zn^+$

T_0=32220T gas EF[2] 633–635 nm

$\tilde{A}$

T_0=16440 gas PE[1]EF[2] $\tilde{A}-\tilde{X}$ 594–669 nm

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_3 s-deform.	1086	gas	EF	2

References

[1] G. M. Bancroft, D. K. Creber, M. A. Ratner, J. W. Moskowitz, and S. Topiol, Chem. Phys. Lett. **50**, 233 (1977).
[2] F. J. Grieman, E. S. Fujikawa, and J. C. Phillips, J. Phys. Chem. **100**, 9276 (1996).

C_2H_5HgH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		HgH stretch	1954.8	Ar	IR	1
			1946.8			
			1926.8			
		CH_2 rock	698.4	Ar	IR	1

Reference

[1] T. M. Greene, L. Andrews, and A. J. Downs, J. Am. Chem. Soc. **117**, 8180 (1995).

cyc-C_5Cl_4

In a nitrogen matrix, structured absorption between 304 and 345 nm has been assigned[1] to *cyc*-C_5Cl_4.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1512w	N_2	IR	1
			1508w	N_2	IR	1
			1356w	N_2	IR	1
			1138w	N_2	IR	1
			1127m	N_2	IR	1
			892w	N_2	IR	1
			882w	N_2	IR	1
			703w	N_2	IR	1
			550w	N_2	IR	1
			530w	N_2	IR	1

Reference

[1] G. A. Bell and I. R. Dunkin, J. Chem. Soc. Faraday Trans. 2 **81**, 725 (1985).

cyc-C_5Br_4

In an argon matrix, absorption maxima at 21790 (459 nm), 24330 (411 nm), and 25710 (389 nm) have been attributed[1] to *cyc*-C_5Br_4.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1182	Ar	IR	1
			1170	Ar	IR	1

Reference

[1] I. R. Dunkin and A. McCluskey, Spectrochim. Acta A **49**, 1179 (1993).

cyc-$C_2H_2Si(CH_3)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3023.1wm	Ar	IR	1
		CH stretch	2992.5wm	Ar	IR	1
		CH stretch	2959.1wm	Ar	IR	1
		C=C stretch	1447.1wm	Ar	IR	1
		CH_3 deform.	1444.2wm	Ar	IR	1
		CH_3 deform.	1438.1wm	Ar	IR	1
		CH_3 deform.	1400.2w	Ar	IR	1
			1250.2m	Ar	IR	1
			1216.1w	Ar	IR	1
			1132.0wm	Ar	IR	1
			1129.8wm	Ar	IR	1
			1127.7wm	Ar	IR	1
			991.6wm	Ar	IR	1
			922.1wm	Ar	IR	1
			884.1s	Ar	IR	1
			788.4vs	Ar	IR	1
			784.9m	Ar	IR	1
		SiC s-stretch	694.1wm	Ar	IR	1
		SiC a-stretch	691.1wm	Ar	IR	1
			616.1m	Ar	IR	1
			613.7m	Ar	IR	1

Reference

[1] M. Trommer, W. Sander, and C. Marquard, Angew. Chem. **106**, 816 (1994); Angew. Chem. Int. Ed. Engl. **33**, 766 (1994).

cyc-$C_4H_4SiH_2$

In an argon matrix, an absorption maximum has been observed[1] at 36000 (278 nm).

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		SiH_2 s-stretch	2144m	Ar	IR	1
		C=C s-stretch	1478w	Ar	IR	1
		CH deform.	1346m	Ar	IR	1
		CH deform.	1088w	Ar	IR	1
		SiH_2 scissors	955s	Ar	IR	1
		Ring deform.	490m	Ar	IR	1
b_1		OPLA CH bend	713vs	Ar	IR	1
b_2		CH stretch	3038w	Ar	IR	1
		CH stretch	3001vw	Ar	IR	1
		SiH_2 a-stretch	2174s	Ar	IR	1
		C=C a-stretch	1608m	Ar	IR	1
		CH deform.	1285w	Ar	IR	1
		SiH_2 wag	880vs	Ar	IR	1
		SiC_2 a-stretch	677w	Ar	IR	1

Reference

[1] V. N. Khabashesku, V. Balaji, S. E. Boganov, O. M. Nefedov, and J. Michl, J. Am. Chem. Soc. **116**, 7863 (1994).

cyc-C_4H_6Si:

In an argon matrix, absorption maxima have been observed[1] at 20800 (480 nm) and at 40000 (250 nm).

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		=CH stretch	3028vw	Ar	IR	1
		CH_2 stretch	2876vw	Ar	IR	1
		C=C stretch	1624s	Ar	IR	1
		CH_2 scissors	1406m	Ar	IR	1
		=CH s-rock	1208w	Ar	IR	1
		CH_2 rock	1108s	Ar	IR	1
		Ring deform.	881m	Ar	IR	1
		SiC_2 s-stretch	616m	Ar	IR	1
		Ring deform.	463w	Ar	IR	1
b_1		CH_2 stretch	2962vw	Ar	IR	1
		=CH wag	770m	Ar	IR	1
b_2		=CH stretch	3002vw	Ar	IR	1
		CH_2 stretch	2854vw	Ar	IR	1
		=CH a-rock	1397s	Ar	IR	1
		CH_2 wag	1307w	Ar	IR	1
		CH_2 twist	1174w	Ar	IR	1
		Ring deform.	944w	Ar	IR	1
		SiC_2 a-stretch	741s	Ar	IR	1
		Ring deform.	528w	Ar	IR	1

Reference

[1] V. N. Khabashesku, V. Balaji, S. E. Boganov, O. M. Nefedov, and J. Michl, J. Am. Chem. Soc. **116**, 7863 (1994).

cyc-C_4H_5SiH

(1-Silacyclopenta-1,3-diene)

In an argon matrix, an absorption maximum has been observed[1] at 33800 (296 nm).

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		=CH stretch	3066m	Ar	IR	1
		=CH stretch	3038s	Ar	IR	1
		=CH stretch	2994w	Ar	IR	1
		CH_2 stretch	2939m	Ar	IR	1
		CH_2 stretch	2865m	Ar	IR	1
		SiH stretch	2210m	Ar	IR	1
		C=C stretch	1551m	Ar	IR	1
		CH_2 scissors	1406m	Ar	IR	1
		=CH bend	1354m	Ar	IR	1
		Mixed	1282w	Ar	IR	1
		=CH bend	1181w	Ar	IR	1
		CH_2 wag	1092s	Ar	IR	1
		=CH bend	961m	Ar	IR	1
		Si=C stretch	929m	Ar	IR	1
		C-C ring	852w	Ar	IR	1
		C-C ring	819w	Ar	IR	1
		SiH deform.	680w	Ar	IR	1
		Ring deform.	488m	Ar	IR	1
a''		=CH bend	974m	Ar	IR	1
		=CH bend	790w	Ar	IR	1
		CH_2 rock	736m	Ar	IR	1
		=SiH OPLA	637m	Ar	IR	1
		Ring deform.	466w	Ar	IR	1

Reference

[1] V. N. Khabashesku, V. Balaji, S. E. Boganov, O. M. Nefedov, and J. Michl, J. Am. Chem. Soc. **116**, 7863 (1994).

cyc-C_4H_5SiH

(1-Silacyclopenta-1,4-diene)

In an argon matrix, an absorption maximum has been observed[1] at 37000 (270 nm).

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		=CH stretch	3095w	Ar	IR	1
		=CH stretch	3061w	Ar	IR	1
		=CH stretch	3025w	Ar	IR	1
		SiH stretch	2216m	Ar	IR	1
		C=C stretch	1543m	Ar	IR	1
		CH_2 scissors	1426w	Ar	IR	1
		=CH bend	1278w	Ar	IR	1
		=CH bend	1149w	Ar	IR	1
		=CH bend	1103m	Ar	IR	1
		=CH bend	985w	Ar	IR	1
		Si=C stretch	936s	Ar	IR	1
		CH_2 rock	859s	Ar	IR	1
		Ring deform.	470w	Ar	IR	1
a''		CH_2 stretch	2904w	Ar	IR	1
		CH_2 wag	1135w	Ar	IR	1
		=CH bend	913m	Ar	IR	1
		=CH OPLA	742s	Ar	IR	1
		=SiH OPLA	597m	Ar	IR	1

Reference

[1] V. N. Khabashesku, V. Balaji, S. E. Boganov, O. M. Nefedov, and J. Michl, J. Am. Chem. Soc. **116**, 7863 (1994).

cyc-$C_4H_4GeH_2$

In an argon matrix, unstructured absorption has been observed[1] between 260 and 320 nm, with maximum near 36760 (272 nm).

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	=CH s-stretch	3015	Ar	IR	1
	3	GeH_2 s-stretch	2099	Ar	IR	1
	4	C=C s-stretch	1532	Ar	IR	1
	5	CH bend	1321	Ar	IR	1
	6	CH scissor	1064	Ar	IR	1
	8	GeH_2 scissor	906	Ar	IR	1
b_1	15	GeH_2 a-stretch	2096	Ar	IR	1
	16	=CH twist	1031	Ar	IR	1
	17	=CH wag	722	Ar	IR	1
	18	Mixed	505	Ar	IR	1
b_2	22	C=C a-stretch	1593	Ar	IR	1
	23	=CH bend	1285	Ar	IR	1
	24	=CH scissor	1168	Ar	IR	1
	25	GeCH rock	783	Ar	IR	1
	26	GeH_2 wag	682	Ar	IR	1

cyc-$C_4D_4GeD_2$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	=CD s-stretch	2262	Ar	IR	1
	2	=CD a-stretch	2229	Ar	IR	1
	4	GeD_2 s-stretch	1522	Ar	IR	1
	5	Mixed	1168	Ar	IR	1
	9	GeD_2 scissor	641	Ar	IR	1
b_1	15	GeD_2 a-stretch	1507	Ar	IR	1
	17	=CD wag	594	Ar	IR	1
b_2	24	DC-CD rock	878	Ar	IR	1
	25	DCGeCD scissor	707	Ar	IR	1
	27	GeD_2 wag	486	Ar	IR	1

Reference

[1] V. N. Khabashesku, S. E. Boganov, D. Antic, O. M. Nefedov, and J. Michl, Organometallics **15**, 4714 (1996).

cyc-C_4H_6Ge:

In an argon matrix, an absorption maximum at 40320 (248 nm) and absorption between 370 and 460 nm have been assigned[1] to this species.

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	=CH s-stretch	3017	Ar	IR	1
	3	C=C stretch	1615	Ar	IR	1
	5	=CH s-rock	1186	Ar	IR	1
	6	CH_2 rock	1078	Ar	IR	1
	8	CGeC s-stretch	508	Ar	IR	1
b_1	15	CH_2 a-stretch	2908	Ar	IR	1
	17	=CH wag	732	Ar	IR	1
b_2	21	CH_2 s-stretch	2865	Ar	IR	1
	22	CH_2 bend	1389	Ar	IR	1
	23	=CH rock	1346	Ar	IR	1
	25	C—C a-stretch	949	Ar	IR	1
	27	CGeC a-stretch	478	Ar	IR	1

cyc-C_4D_6Ge:

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	=CD s-stretch	2256	Ar	IR	1
	3	C=C stretch	1579	Ar	IR	1
	4	C-C s-stretch	1072	Ar	IR	1
	6	=CD rock	804	Ar	IR	1
	7	CD_2 wag	748	Ar	IR	1
b_1	15	CD_2 a-stretch	2171	Ar	IR	1
	16	CD_2 twist	837	Ar	IR	1
	17	DC=CD wag	551	Ar	IR	1
b_2	21	CD_2 s-stretch	2077	Ar	IR	1
	22	C—C a-stretch	1164	Ar	IR	1
	23	CD_2 bend	1024	Ar	IR	1
	24	Mixed	976	Ar	IR	1
	25	=CD a-rock	772	Ar	IR	1
	27	CGeC a-stretch	438	Ar	IR	1

Reference

[1] V. N. Khabashesku, S. E. Boganov, D. Antic, O. M. Nefedov, and J. Michl, Organometallics **15**, 4714 (1996).

cyc-C_4H_5GeH

(1-Germacyclopenta-1,3-diene)

In an argon matrix, an absorption maximum at 33220 (301 nm) has been tentatively assigned[1] to this product.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	=CH s-stretch	3048	Ar	IR	1
	4	CH_2 s-stretch	2894	Ar	IR	1
	5	GeH stretch	2115	Ar	IR	1
	6	C=C stretch	1574	Ar	IR	1
	8	=CH rock	1352	Ar	IR	1
	9	Mixed	1262	Ar	IR	1
	12	Mixed	959	Ar	IR	1
	13	Mixed	922	Ar	IR	1
	14	Ge=CC s-stretch	838	Ar	IR	1
	16	GeH rock	631	Ar	IR	1
a''	19	CH_2 a-stretch	2972	Ar	IR	1
	22	GeCH rock	778	Ar	IR	1
	24	Mixed	698	Ar	IR	1

cyc-C_4D_5GeD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	=CD a-stretch	2232	Ar	IR	1
	4	CD_2 s-stretch	2090	Ar	IR	1
	6	GeD stretch	1536	Ar	IR	1
	12	DC=CD rock	820	Ar	IR	1
	14	Ge=CC s-stretch	691	Ar	IR	1
	15	C—C=C bend	663	Ar	IR	1
	16	Ge—C stretch	529	Ar	IR	1
	17	GeD rock	454	Ar	IR	1
a''	22	C—Ge=C twist	621	Ar	IR	1
	24	DC=C—CD wag	465	Ar	IR	1
	25	DC=CD wag	416	Ar	IR	1

Reference

[1] V. N. Khabashesku, S. E. Boganov, D. Antic, O. M. Nefedov, and J. Michl, Organometallics **15**, 4714 (1996).

cyc-C_4H_5GeH

(1-Germacyclopenta-1,4-diene)

In an argon matrix, an absorption maximum at 38170 (262 nm) has been tentatively assigned[1] to this product.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	5	GeH stretch	2127	Ar	IR	1
	6	C=C stretch	1553	Ar	IR	1
	13	Ge=C s-stretch	834	Ar	IR	1
	14	Mixed	787	Ar	IR	1
a''	23	Ge=CH wag	682	Ar	IR	1
	24	CH_2 rock	635	Ar	IR	1

cyc-C_4D_5GeD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	4	CD_2 s-stretch	2068	Ar	IR	1
	6	GeD stretch	1547	Ar	IR	1
	10	CD_2 bend	1072	Ar	IR	1
	14	Skel. stretch	686	Ar	IR	1
a''	24	Wag	509	Ar	IR	1

Reference

[1] V. N. Khabashesku, S. E. Boganov, D. Antic, O. M. Nefedov, and J. Michl, Organometallics **15**, 4714 (1996).

CaC_5H_5

$\tilde{B}$ $^2A_1$ C_{5v}

T_0=16772(5)T gas LF[1,3] $\tilde{B}-\tilde{X}$ 585–607 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		Ca··C_5 stretch	300(5)T	gas	LF	1

$\tilde{A}$ $^2E_1$ C_{5v} Structure: LF[4]

T_0=14535.44 gas LF[1–3] $\tilde{A}-\tilde{X}$ 645–745 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CH wag	738	gas	LF	3
	4	Ca··C_5 stretch	330.19	gas	LF	1–4
e_1	10	Ca··C_5 bend	222H	gas	LF	3
e_2	13	CH deform.	1039T	gas	LF	3
	15	CH wag	869T	gas	LF	3

A=57.66 gas LF[1–4]
B_0=0.091 LF[4]

$\tilde{X}$ $^2A_1$ C_{5v} Structure: LF[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4	Ca··C_5 stretch	311	gas	LF	1,3

B_0=0.088 LF[4]

CaC_5D_5

$\tilde{A}\ ^2E_1$ C_{5v}
T_0=14536 gas LF[3] $\tilde{A}-\tilde{X}$ 645–690 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CD wag	512	gas	LF	3
	4	Ca··C_5 stretch	316	gas	LF	3
e_1	10	Ca··C_5 bend	221H	gas	LF	3
e_2	13	CD deform.	727T	gas	LF	3
	15	CD wag	614T	gas	LF	3

A=56 gas LF[3]

References

[1] L. C. O'Brien and P. F. Bernath, J. Am. Chem. Soc. **108**, 5017 (1986).
[2] A. M. Ellis, E. S. J. Robles, and T. A. Miller, J. Chem. Phys. **94**, 1752 (1991).
[3] E. S. J. Robles, A. M. Ellis, and T. A. Miller, J. Am. Chem. Soc. **114**, 7171 (1992).
[4] T. M. Cerny, J. M. Williamson, and T. A. Miller, J. Chem. Phys. **102**, 2372 (1995).

$H_2BSC_2H_5$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	2984	Ar	IR	1
		CH stretch	2980	Ar	IR	1
		CH stretch	2951	Ar	IR	1
		CH stretch	2941	Ar	IR	1
		CH stretch	2892	Ar	IR	1
		BH_2 a-stretch	2599	Ar	IR	1
		BH_2 s-stretch	2522	Ar	IR	1
			1456	Ar	IR	1
			1444	Ar	IR	1
		BH_2 scissors	1184	Ar	IR	1
			1167	Ar	IR	1
			1145	Ar	IR	1
			1085	Ar	IR	1
			1040	Ar	IR	1
			971	Ar	IR	1
		BH_2 OPLA	923	Ar	IR	1
		B-S stretch	829	Ar	IR	1
		BH_2 rock	798	Ar	IR	1

Reference

[1] J. D. Carpenter and B. S. Ault, J. Phys. Chem. **97**, 3697 (1993).

$H_2C{=}(cyc\text{-}CN{=}CCH_3)$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1865	Kr	IR	1
			1554	Kr	IR	1
			1228	Kr	IR	1
			696	Kr	IR	1

Reference

[1] K. Banert, M. Hagedorn, E. Knözinger, A. Becker, and E.-U. Würthwein, J. Am. Chem. Soc. **116**, 60 (1994).

bicyc-$C_6H_3F_2N$

(7-Aza-1,5-difluoro-2,4,6-bicyclo[4.1.0.]heptatriene)

In an argon matrix, an absorption maximum at 39700 (252 nm) has been assigned[1] to *bicyc*-$C_6H_3F_2N$.

In an argon matrix,[1] irradiation at 27300 (366 nm) results in partial rearrangement to the phenylnitrene, 2,6-$C_6H_3F_2N$:.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C=N stretch	1679.3m	Ar	IR	1
		C=C stretch	1609.8vs	Ar	IR	1
		C=C stretch	1519.7m	Ar	IR	1
			1412.2ms	Ar	IR	1
		C-C stretch	1318.0m	Ar	IR	1
		CF stretch	1258.9s	Ar	IR	1
		CF stretch	1179.7s	Ar	IR	1
		6-ring deform.	1138.3m	Ar	IR	1
		6-ring deform.	1006.7wm	Ar	IR	1
		6-ring OPLA	939.2m	Ar	IR	1
		CH OPLA	896.1w	Ar	IR	1
		3-ring deform.	856.9wm	Ar	IR	1
			796.0m	Ar	IR	1
			737.4wm	Ar	IR	1
			688.2wm	Ar	IR	1
			608.5vw	Ar	IR	1
			557.1vw	Ar	IR	1
			535.7vw	Ar	IR	1
			500.3w	Ar	IR	1
			430.0w	Ar	IR	1

Reference

[1] J. Morawietz and W. Sander, J. Org. Chem. **61**, 4351 (1996).

bicyc-C_6F_5N

(Perfluoro-7-aza-2,4,6-bicyclo[4.1.0]heptatriene)

In an argon matrix,[1] irradiation at 27300 (366 nm) results in reversible isomerization to C_6F_5N:.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1664.2wm	Ar	IR	1
			1589.3wm	Ar	IR	1
			1395.3m	Ar	IR	1
			1374.5m	Ar	IR	1
			1308.7wm	Ar	IR	1
			1222.6wm	Ar	IR	1
			1187.8wm	Ar	IR	1
			1095.3wm	Ar	IR	1
			1007.6vs	Ar	IR	1
			947.5wm	Ar	IR	1
			937.3wm	Ar	IR	1
			816.0w	Ar	IR	1
			660.6w	Ar	IR	1
			524.8vw	Ar	IR	1

Reference

[1] J. Morawietz and W. Sander, J. Org. Chem. **61**, 4351 (1996).

$H(C{\equiv}C)_3CN^+$

$\tilde{A}\ ^2\Pi$ $C_{\infty v}$

T_0=14836 Ne AB^1LF^2 $\tilde{A}$–$\tilde{X}$ 594–820 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	5	CN stretch	1969(5)	Ne	AB	1
	6	C-C stretch	1578(5)	Ne	AB	1
	7	C-C stretch	1017(5)	Ne	AB	1
	8	C-C stretch	459(5)	Ne	AB	1

A=19T Ne LF^2

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$

Vib sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	C≡N stretch	2180.2	Ne	LF	2
	3	C≡C stretch	2159.6	Ne	LF	2
	4	C≡C stretch	2128.5	Ne	LF	2
	5	C≡C stretch	1938.3	Ne	LF	2
	6	C-C stretch	957.2	Ne	LF	2
	7	C-C stretch	881.0	Ne	LF	2
	8	C-C stretch	464.5	Ne	LF	2

A=92T Ne LF^2

References

[1] D. Forney, P. Freivogel, J. Fulara, and J. P. Maier, J. Chem. Phys. **102**, 1510 (1995).
[2] A. M. Smith, J. Agreiter, and V. E. Bondybey, Chem. Phys. Lett. **244**, 379 (1995).

HC_7CN^+

$\tilde{A}$

T_0=15217(5) Ne AB^1

Reference

[1] D. Forney, P. Freivogel, J. Fulara, and J. P. Maier, J. Chem. Phys. **102**, 1510 (1995).

NCC_5CN^+

$\tilde{A}$ $C_{\infty v}$

T_0=15897(5) Ne AB^1 $\tilde{A}$–$\tilde{X}$ 558–630 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		C≡C stretch	2012(5)	Ne	AB	1

Reference

[1] D. Forney, P. Freivogel, J. Fulara, and J. P. Maier, J. Chem. Phys. **102**, 1510 (1995).

$H(C{\equiv}C)_4CN^+$

$\tilde{A}\ ^2\Pi$ $C_{\infty v}$

T_0=12978(5) Ne AB^1 $\tilde{A}$–$\tilde{X}$ 663–771 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	6	C≡C stretch	2106(5)	Ne	AB	1
	8	C-C stretch	1223(5)	Ne	AB	1
	10	C-C stretch	363(5)	Ne	AB	1

Reference

[1] D. Forney, P. Freivogel, J. Fulara, and J. P. Maier, J. Chem. Phys. **102**, 1510 (1995).

$NC(C{\equiv}C)_3CN^+$

$\tilde{A}\ ^2\Pi_g$ $D_{\infty h}$

T_0=13480 Ne AB^1LF^2 $\tilde{A}$–$\tilde{X}$ 638–1090 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	2	C≡C s-stretch	2163(5)	Ne	AB	1
	3	C≡C s-stretch	1952(5)	Ne	AB	1
	4	C-C s-stretch	1105(5)	Ne	AB	1
	5	C-C s-stretch	395(5)	Ne	AB	1
Π		Bend	423(5)H	Ne	AB	1

$\tilde{X}\ ^2\Pi_u$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	CN s-stretch	2136.8(5)	Ne	LF	2
	2	C≡C s-stretch	2127.9(5)	Ne	LF	2
	3	C≡C s-stretch	1974.4(5)	Ne	LF	2
	5	C-C s-stretch	362T	Ne	LF	2

References

[1] D. Forney, P. Freivogel, J. Fulara, and J. P. Maier, J. Chem. Phys. **102**, 1510 (1995).

[2] J. Agreiter, A. M. Smith, and V. E. Bondybey, Chem. Phys. Lett. **241**, 317 (1995).

HC_9CN^+

$\tilde{A}$

T_0=13395(5) Ne AB[1]

Reference

[1] D. Forney, P. Freivogel, J. Fulara, and J. P. Maier, J. Chem. Phys. **102**, 1510 (1995).

NCC_7CN^+

$\tilde{A}$ $C_{\infty v}$

T_0=14024(5) Ne AB[1] $\tilde{A}-\tilde{X}$ 623–714 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		C≡C stretch	2022(5)T	Ne	AB	1

Reference

[1] D. Forney, P. Freivogel, J. Fulara, and J. P. Maier, J. Chem. Phys. **102**, 1510 (1995).

$H(C{\equiv}C)_5CN^+$

$\tilde{A}$ $^2\Pi$ $C_{\infty v}$

T_0=11468(5) Ne AB[1] $\tilde{A}-\tilde{X}$ 734–872 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	5	C≡N stretch	2154(5)T	Ne	AB	1
	6	C≡C stretch	2007(5)T	Ne	AB	1
	7	C≡C stretch	1849(5)T	Ne	AB	1
	8	C-C stretch	1611(5)T	Ne	AB	1
	12	C-C stretch	323(5)	Ne	AB	1

Reference

[1] D. Forney, P. Freivogel, J. Fulara, and J. P. Maier, J. Chem. Phys. **102**, 1510 (1995).

$NC(C{\equiv}C)_4CN^+$

$\tilde{A}$ $^2\Pi_u$ $D_{\infty h}$

T_0=12029(5) Ne AB[1] $\tilde{A}-\tilde{X}$ 704–832 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	3	CN sym. stretch	2168(5)T	Ne	AB	1
	4	C-C sym. stretch	1852(5)T	Ne	AB	1
	6	C-C sym. stretch	310(5)	Ne	AB	1
Π		Bend	350(5)H	Ne	AB	1

Reference

[1] D. Forney, P. Freivogel, J. Fulara, and J. P. Maier, J. Chem. Phys. **102**, 1510 (1995).

$HC_{11}CN^+$

$\tilde{A}$

T_0=12026(5) Ne AB[1]

Reference

[1] D. Forney, P. Freivogel, J. Fulara, and J. P. Maier, J. Chem. Phys. **102**, 1510 (1995).

NCC_9CN^+

$\tilde{A}$

T_0=12587(5) Ne AB[1] $\tilde{A}-\tilde{X}$ 682–795 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C≡C stretch	2058(5)T	Ne	AB	1

Reference

[1] D. Forney, P. Freivogel, J. Fulara, and J. P. Maier, J. Chem. Phys. **102**, 1510 (1995).

$H(C{\equiv}C)_6CN^+$

$\tilde{A}$ $^2\Pi$ $C_{\infty v}$

T_0=10276(5) Ne AB[1] $\tilde{A}-\tilde{X}$ 929–974 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	9	C-C stretch	1795(5)T	Ne	AB	1
	10	C-C stretch	1353(5)T	Ne	AB	1
	14	C-C stretch	276(5)	Ne	AB	1

Reference

[1] D. Forney, P. Freivogel, J. Fulara, and J. P. Maier, J. Chem. Phys. **102**, 1510 (1995).

$NC(C{\equiv}C)_5CN^+$

$\tilde{A}$ $^2\Pi_g$ $D_{\infty h}$

T_0=10831(5) Ne AB[1] $\tilde{A}-\tilde{X}$ 806–924 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	5	C-C sym. stretch	1572(5)T	Ne	AB	1
	7	C-C sym. stretch	272(5)	Ne	AB	1

Reference

[1] D. Forney, P. Freivogel, J. Fulara, and J. P. Maier, J. Chem. Phys. **102**, 1510 (1995).

$H_9O_4^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		H_2O in-phase a-stretch	3730.4	gas	PF	1,2
		H_2O out-of-phase s-stretch	3644.9	gas	PF	1

References

[1] L. I. Yeh, M. Okumura, J. D. Myers, J. M. Price, and Y. T. Lee, J. Chem. Phys. **91**, 7319 (1989).
[2] L. I. Yeh, Y. T. Lee, and J. T. Hougen, J. Mol. Spectrosc. **164**, 473 (1994).

C_2H_5IO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1195.4wm	Ar	IR	1
		IO stretch	717.0ms	Ar	IR	1

C_2D_5IO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			958.1wm	Ar	IR	1
		IO stretch	717.0ms	Ar	IR	1

Reference

[1] R. J. H. Clark and J. R. Dann, J. Phys. Chem. **100**, 532 (1996).

C_2H_5OI

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1106.0wm	Ar	IR	1
		C-O stretch	1076.7w	Ar	IR	1
			1071.9w			
		CH_2 deform.	961.9m	Ar	IR	1
		OI stretch	570.5wm	Ar	IR	1

C_2D_5OI

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1112.9w	Ar	IR	1
		C-O stretch	1075.3w	Ar	IR	1
		CD_2 deform.	735.8m	Ar	IR	1
		OI stretch	565.6wm	Ar	IR	1

Reference

[1] R. J. H. Clark and J. R. Dann, J. Phys. Chem. **100**, 532 (1996).

C_8O

$\tilde{X}\ ^3\Sigma^-$ $C_{\infty v}$
B_0=0.013 MW[1]

Reference

[1] Y. Ohshima, Y. Endo, and T. Ogata, J. Chem. Phys. **102**, 1493 (1995).

C_9O

$\tilde{X}$ $C_{\infty v}$
B_0=0.010 MW[1]

Reference

[1] T. Ogata, Y. Ohshima, and Y. Endo, J. Am. Chem. Soc. **117**, 3593 (1995).

$C_2H_5IO_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		IO_2 a-stretch	837.2wm	Ar	IR	1
			829.3m			
		IO_2 s-stretch	803.1wm	Ar	IR	1
			795.4m			

$C_2D_5IO_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		IO_2 a-stretch	837.1wm	Ar	IR	1
			829.3m			
		IO_2 s-stretch	802.8wm	Ar	IR	1
			794.1m			

Reference

[1] R. J. H. Clark and J. R. Dann, J. Phys. Chem. **100**, 532 (1996).

$CH_3SiHOHCHO$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3656.4m	Ar	IR	1
			3645.7wm	Ar	IR	1
			2768.4w	Ar	IR	1
			2760.7w	Ar	IR	1
			2664.1wm	Ar	IR	1
			2654.3w	Ar	IR	1
		SiH stretch	2133.4ms	Ar	IR	1
		C=O stretch	1656.9m	Ar	IR	1
			1258.2ms	Ar	IR	1
			940.3ms	Ar	IR	1
			909.4vs	Ar	IR	1
			867.8s	Ar	IR	1
			748.2m	Ar	IR	1

Reference

[1] M. Trommer, W. Sander, and A. Patyk, J. Am. Chem. Soc. **115**, 11775 (1993).

$(CH_3)_2SiOHCHO$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3660.2ms	Ar	IR	1
			3651.2m	Ar	IR	1
			3645.9m	Ar	IR	1
			2764.2wm	Ar	IR	1
			2658.9wm	Ar	IR	1
			2653.7m	Ar	IR	1
		C=O stretch	1655.0m	Ar	IR	1
			1258.8vs	Ar	IR	1
			1051.3s	Ar	IR	1
			952.2vs	Ar	IR	1
			941.6vs	Ar	IR	1
			868.8s	Ar	IR	1
			805.7s	Ar	IR	1
			547.8wm	Ar	IR	1

Reference

[1] M. Trommer, W. Sander, and A. Patyk, J. Am. Chem. Soc. **115**, 11775 (1993).

cyc-C_5H_4O-1-O

(Cyclopentadienone O-Oxide)

In a nitrogen matrix,[2] an absorption maximum at 23800 (420 nm) can be assigned to cyclopentadienone O-oxide.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			3158w	N_2	IR	1
			1478w	Ar	IR	3
			1481w	N_2	IR	1
			1397w	Ar	IR	3
			1398	N_2	IR	1
			1320m	Ar	IR	3
			1321	N_2	IR	1
			1303w	N_2	IR	1
			1221w	Ar	IR	3
			1075w	Ar	IR	3
			1063w	Ar	IR	3
			1066w	N_2	IR	1
		OO stretch	1018m	Ar	IR	3
			1014	N_2	IR	1
			1007w	Ar	IR	3
			949m	Ar	IR	3
			947	N_2	IR	1
			940	N_2	IR	1
			888m	Ar	IR	3
			888	N_2	IR	1
			754m	Ar	IR	3
			758	N_2	IR	1
			693w	Ar	IR	3
			694w	N_2	IR	1
			603w	Ar	IR	3
			606w	N_2	IR	1
			498w	N_2	IR	1

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[1] G. A. Bell and I. R. Dunkin, J. Chem. Soc., Chem. Commun. 1213 (1983).
[2] G. A. Bell, I. R. Dunkin, and C. J. Shields, Spectrochim. Acta A **41**, 1221 (1985).
[3] I. R. Dunkin and C. J. Shields, J. Chem. Soc., Chem. Commun. 154 (1986).

cyc-C_5Cl_4O-1-O

In argon and nitrogen matrices,[1,2] an absorption maximum near 25300 (395 nm) is associated with photoisomerization of and O-atom photoelimination from *cyc*-C_5Cl_4O-1-O.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1555w	Ar	IR	2
			1558w	N_2	IR	2
		CO stretch	1371w	Ar	IR	2
			1380w	N_2	IR	2
			1231m	Ar	IR	2
			1230m	N_2	IR	2
			1135w	Ar	IR	2
			1137w	N_2	IR	2
		OO stretch	1016w	Ar	IR	2
			1007w			
			1017w	N_2	IR	2
			1005w			
			974vw	Ar	IR	2
			976w	N_2	IR	2
			835w	Ar	IR	2
			833w	N_2	IR	2
			748w	Ar	IR	2
			750w	N_2	IR	2
			668w	Ar	IR	2
			669w	N_2	IR	2
			506w	Ar	IR	2
			508w	N_2	IR	2

References

[1] G. A. Bell, I. R. Dunkin, and C. J. Shields, Spectrochim. Acta A **41**, 1221 (1985).
[2] I. R. Dunkin, G. A. Bell, F. G. McCleod, and A. McCluskey, Spectrochim. Acta A **42**, 567 (1986).

cyc-C_5Br_4O-1-O

In argon and nitrogen matrices,[1] an absorption between 380 and 520 nm is associated with photoisomerization of and O-atom photoelimination from *cyc*-C_5Br_4O-1-O.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1522w	Ar	IR	1
			1525w	N_2	IR	1
		CO stretch	1363w	Ar	IR	1
			1355w			
			1371w	N_2	IR	1
			1187m	Ar	IR	1
			1185m	N_2	IR	1
			1107w	Ar	IR	1
			1107w	N_2	IR	1
		OO stretch	1000w	Ar	IR	1
			1001w	N_2	IR	1
			997w			
			987w	N_2	IR	1

Reference

[1] I. R. Dunkin and A. McCluskey, Spectrochim. Acta A **50**, 151 (1994).

1,2,3-*cyc*-$C_2H_4O_3$

$\tilde{X}$ C_s Structure: MW[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_2 deform.	1214m	Xe	IR	2
		CO stretch + CH_2 deform.	983s	Xe	IR	2
			982	CO_2	IR	1,2
		CO stretch	927s	Xe	IR	2
			926	CO_2	IR	1,2
		O_3 s-stretch	846wm	Xe	IR	2
		COO bend + CO stretch	727vs	Xe	IR	2
			726	CO_2	IR	1,2
		O_3 a-stretch	647vs	Xe	IR	2
			648	CO_2	IR	1,2
		O_3 bend	409m	Xe	IR	2
			406	CO_2	IR	1,2

$A_0 = 0.273$; $B_0 = 0.252$; $C_0 = 0.147$ MW[3]

1,2,3-$C_2D_4O_3$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD_2 deform.	1089wm	Xe	IR	2
		CO stretch	892s	Xe	IR	2
		O_3 a-stretch	636vs	Xe	IR	2
		O_3 bend	387m	Xe	IR	2

$A_0 = 0.231$; $B_0 = 0.222$; $C_0 = 0.131$ MW[4]

References

[1] B. Nelander and L. Nord, Tetrahedron Lett. 2821 (1977).
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1,2,4-*cyc*-$C_2H_4O_3$

$\tilde{X}$ C_2 Structure: MW[1,2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	CH stretch	2973m	Ar	IR	3,7
	2	CH stretch	2894vs	Ar	IR	3,7
	4	CH_2 wag	1387m	Ar	IR	3,7
	5	CH_2 twist	1196m	Ar	IR	3,7
	6	CH_2 rock	1129s	Ar	IR	3,6,7
			1130	Xe	IR	6
	7	C-O_e stretch	955wm	gas	IR	5
			952vs	Ar	IR	3,6,7
			945	Xe	IR	6
	8	C-O_p stretch	926w	Ar	IR	3,7
	9	O-O stretch	810w	gas	IR	5
			808s	Ar	IR	3,6,7
			802	Xe	IR	6
	10	Skeletal	737vw	Ar	IR	3,7
	11	Ring pucker	352vw	Ar	IR	3
b	12	CH stretch	2967s	Ar	IR	3,7
	13	CH stretch	2900m	Ar	IR	3,7
	14	CH_2 bend	1483vw	Ar	IR	3
	15	CH_2 wag	1346m	Ar	IR	3,7
	16	CH_2 twist	1202m	Ar	IR	3,7
	17	CH_2 rock	1143vw	Ar	IR	3
	18	C-O_e stretch	1081.8s	gas	IR	5
			1078vs	Ar	IR	3,6,7
			1072	Xe	IR	6
	19	C-O_p stretch	1029s	Ar	IR	3,6,7
			1021	Xe	IR	6
	20	Skeletal	698m	Ar	IR	3,7
	21	Ring bend	193m	Ar	IR	3

$A_0=0.275$; $B_0=0.270$; $C_0=0.153$ MW[1]

1,2,4-*cyc*-$C_2D_4O_3$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	CD stretch	2249m	Ar	IR	3,7
	2	CD stretch	2118w	Ar	IR	3,7
	3	CD_2 wag+skel.	1160s	Ar	IR	3,7
	4	CD_2 def.+skel.	1135s	Ar	IR	3,7
	5	Skeletal	1021s	Ar	IR	3,7
	6	Skeletal	972m	Ar	IR	3,7
	7	CD_2 rock+skel.	911w	Ar	IR	3,7
	8	CD_2 twist	851m	Ar	IR	3,7
	9	OO stretch	759s	Ar	IR	3,7
	10	Skeletal	672m	Ar	IR	3,7
	11	Ring pucker	338vw	Ar	IR	3
b	12	CD stretch	2246w	Ar	IR	3,7
	13	CD stretch	2092w	Ar	IR	3,7
	14	CD_2 wag	1143s	Ar	IR	3,7
	15	CD_2 bend	1059vs	Ar	IR	3,7
	16	Skeletal	980w	Ar	IR	3,7
	17	CD_2 twist	930m	Ar	IR	3,7
	18	CD_2 rock	904m	Ar	IR	3,7
	19	CD_2 rock	830w	Ar	IR	3,7
	20	Skeletal	707w	Ar	IR	3,7

[a]Assignments of Ref. 3 adopted, except for C-O and O-O stretching modes of sec-$C_2H_4O_3$, for which assignments of Ref. 7, suggested by data for ^{18}O-substituted species, are used.
O_p—peroxy O-atom; O_e—ether O-atom.

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$CH_3C(=NO)CHO$

$\tilde{X}$[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C=O stretch	1717.0	Ar	IR	1
			1710.3			
		C=N stretch	1587.8	Ar	IR	1
		CH_3 deform.	1394.5	Ar	IR	1
		CH_3 deform.	1374.0	Ar	IR	1
			1241.1	Ar	IR	1
			1020.5	Ar	IR	1
			994.3	Ar	IR	1
			807.9	Ar	IR	1
			546.1	Ar	IR	1

$CD_3C(=NO)CDO$

$\tilde{X}$[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C=N stretch	1586.6	Ar	IR	1

[a]Four different conformers of this species were stabilized upon photoinduced reaction of NO_2 with CH_3CCH in an argon matrix.[1] Their relative energies could not be determined. The vibrational frequencies for conformer B1, which grew in on 514 nm irradiation of the initial sample deposit, are chosen as typical.

Reference

[1] J. A. Harrison and H. Frei, J. Phys. Chem. **98**, 12142 (1994).

CF_3OONO_2

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO_2 a-stretch	1764s	gas	IR	1,2
	3	CF_3 s-stretch	1296s	gas	IR	1,2
	4	CF_3 a-stretch	1243vs	gas	IR	1,2
	5	CO stretch	956ms	gas	IR	1,2
	7	NO stretch	787s	gas	IR	1,2
	8	CF_3 s-deform.	669wm	gas	IR	1
	9	NO_2 scissors	600wm	gas	IR	1
	10	CF_3 a-deform.	485wm	gas	IR	1
	11	NO_2 rock	436vw	gas	IR	1
	12	CF_3 rock	371wm	gas	IR	1
	13	COO deform.	284vw	gas	IR	1
	14	OON deform.	253wm	gas	IR	1
a''	15	CF_3 a-stretch	1190vs	gas	IR	1,2
	16	ONO_2 OPLA	702wm	gas	IR	1
	17	CF_3 a-deform.	562wm	gas	IR	1

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[2] J. Chen, V. Young, T. Zhu, and H. Niki, J. Phys. Chem. **97**, 11696 (1993).

8.17. Molecules Related to Benzene

$C_6H_5Cl^+$

$\tilde{F}$ $^2B_1$ C_{2v}
T^a=33430(160) gas PE[3]
T_0=33410(10) Ar AB[6] $\tilde{F}-\tilde{X}$ 287–300 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			710(10)	Ar	AB	6

$\tilde{E}$ $^2B_2$ C_{2v}
T^a=31570(160) gas PE[3]

$\tilde{D}$ $^2A_1$ C_{2v}
T^a=25920(160) gas PE[1,3]

$\tilde{C}$ $^2B_1$ C_{2v}
T_0=21250(80) gas PE[1,3]
20750(10) Ar AB[4,6] $\tilde{C}-\tilde{X}$ 434–482 nm
Photodissociation into $C_6H_5^+$ + Cl occurs.[2,7–9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1370(10)	Ar	AB	6
			900(80)	gas	PE	3
			900(10)	Ar	AB	6
			370(10)	Ar	AB	6

$\tilde{B}$ $^2B_2$ C_{2v}
T_0=18300(80) gas PE[1,3]PF[7–9] $\tilde{B}-\tilde{X}$ 485–580 nm
Ar AB[6] $\tilde{B}-\tilde{X}$ 498–534 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			940T	gas	PE,PF	3,7
			930(10)	Ar	AB	6
			385T	gas	PE,PF	3,7
a_2			627T	gas	PF	7
			179T	gas	PF	7
b_2			430T	Ar	AB	6

$\tilde{A}$ $^2A_2$ C_{2v}
T^a=5160(160) gas PE[1,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1020(80)	gas	PE	3

$\tilde{X}$ $^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	5		1429(2)	gas	PE,TPE	3,12
	6		1200(2)	gas	TPE	11,12
	7		1116(2)	gas	TPE	11,12
	8		995(2)	gas	TPE	11,12
	9		975(2)	gas	TPE	11,12
	10		716(2)	gas	TPE	11,12
	11		422(2)	gas	TPE, PF,MPI	3,5,7 10–12
a_2	14		348(2)	gas	MPI,PE	10–12
b_1	15		909(20)	gas	TPE	11
	16		812(20)	gas	TPE	11
	17		603(20)	gas	TPE	11
	18		558(20)	gas	TPE	11
	19		394(2)	gas	TPE	11,12
	20		154(10)	gas	MPI,PE	10,11
b_2	29		531(2)	gas	MPI,PE	10–12
	30		311(2)	gas	MPI,PE	10–12

$C_6D_5Cl^+$

$\tilde{X}$ $^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	11		413(20)	gas	TPE	11

[a]From vertical ionization potential.

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1,4-$C_6H_4F_2^+$

$\tilde{E}$ ^2A_g D_{2h}
T^a=41600(1000) gas PE[2]

$\tilde{D}$ $^2B_{2u}$ D_{2h}
T^a=36800(1000) gas PE[2]

$\tilde{C}$ $^2B_{3g}$ D_{2h}
T^a=27100(1000) gas PE[2]

$\tilde{B}$ $^2B_{3u}$ D_{2h}
T_0=23754 gas PE[2]ID[5,6] $\tilde{B}-\tilde{X}$ 390–425 nm
23200 Ne AB[1]
Ar AB[3] $\tilde{B}-\tilde{X}$ 395–425 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g			1450(40)	gas	PE	2
			404(10)	gas	ID	6
			400T	Ne	AB	1
			400	Ar	AB	3
a_u	8		200H	gas	ID	6
b_{3u}	30		144H	gas	ID	5,6

$\tilde{A}$ $^2B_{1g}$ D_{2h}
T_0=7180(160) gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g			1355(40)	gas	PE	2

$\tilde{X}$ $^2B_{2g}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1		3098	gas	TPE	8
	2		1640	gas	TPE	7,8
	3		1375	gas	TPE	7,8
	4		1149	gas	TPE	7,8
	5		836	gas	TPE	7,8
	6		440	gas	ID,TPE	6–8
a_u	8		358	gas	ID,TPE	6–8
b_{1g}	9		726	gas	TPE	8
b_{2g}	17		302	gas	TPE	7,8
b_{3g}	27		430	gas	TPE	8
b_{3u}	28		859T	gas	TPE	8
	29		508(10)H	gas	PE	4
	30		126	gas	ID,TPE	5,7,8

1,4-$C_6D_4F_2^+$

$\tilde{B}$ $^2B_{3g}$ D_{2h}
T_0=23340 Ne AB[1]

[a]From vertical ionization potential.

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(2-FC_6H_4)CH_2

$\tilde{A}$
T_0=21924 gas EM[1]LF[2] $\tilde{A}-\tilde{X}$ 435–475 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1022	gas	LF	2
			704	gas	LF	2
			501	gas	LF	2
			386	gas	LF	2

τ_0=1220(40) ns gas LF[2]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			882	gas	LF	2

References

[1] T. F. Bindley, A. T. Watts, and S. Walker, Trans. Faraday Soc. **60**, 1 (1964).
[2] T. R. Charlton and B. A. Thrush, Chem. Phys. Lett. **125**, 547 (1986).

(3-FC_6H_4)CH_2

$\tilde{A}$
T_0=21691 gas EM[1]LF[2] $\tilde{A}-\tilde{X}$ 445–477 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			734	gas	LF	2
			466	gas	LF	2

τ_0=597(15) ns gas LF[2]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			741	gas	LF	2
			506	gas	EM,LF	1,2

References

[1] T. F. Bindley, A. T. Watts, and S. Walker, Trans. Faraday Soc. **60**, 1 (1964).
[2] T. R. Charlton and B. A. Thrush, Chem. Phys. Lett. **125**, 547 (1986).

$(4\text{-}FC_6H_4)CH_2$

$\tilde{A}\ ^2A_2$ C_{2v}
T_0=21524.0(2) gas EM[1,3]LF[2] $\tilde{A}-\tilde{X}$ 429–475 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1760	gas	LF	2
	7a		1228	gas	LF	4
	13		1194	gas	LF	2,4
	18a		846	gas	LF	4
	1		813	gas	LF	2,4
	6b		524	gas	LF	4
	6a		411	gas	LF	4
	9b		398	gas	LF	4
	15		222	gas	LF	4

τ_0=532(5) ns gas LF[2,4]

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1		835	gas	EM,LF	3,4
	6a		453	gas	EM,LF	1–4

References

[1] T. F. Bindley, A. T. Watts, and S. Walker, Trans. Faraday Soc. **60**, 1 (1964).
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[3] C. Cossart-Magos and D. Cossart, Mol. Phys. **65**, 627 (1988).
[4] M. Fukushima and K. Obi, J. Chem. Phys. **93**, 8488 (1990).

$(4\text{-}ClC_6H_4)CH_2$

$\tilde{B}\ ^2B_1$ C_{2v}
T_0=21732 gas LF[1] $\tilde{A},\tilde{B}-\tilde{X}$ 436–462 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1194	gas	LF	1
			1076	gas	LF	1
			960	gas	LF	1
			779	gas	LF	1
			340	gas	LF	1
			242	gas	LF	1
b_2	6b		623	gas	LF	1
			122	gas	LF	1

$\tilde{A}\ ^2A_2$ C_{2v}
T_0=21638 gas LF[1] $\tilde{A},\tilde{B}-\tilde{X}$ 436–462 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	12		726	gas	LF	1

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	8a		1544	gas	LF	2
	9a		1079	gas	LF	2
	1		811	gas	LF	2
	12		726	gas	LF	1
	6a		559	gas	LF	2
b_2	6b		634	gas	LF	1
			209	gas	LF	1

References

[1] M. Fukushima and K. Obi, Chem. Phys. Lett. **248**, 269 (1996).
[2] M. Fukushima, K. Saito, and K. Obi, J. Mol. Spectrosc. **180**, 389 (1996).

$(4\text{-}NC\text{-}C_6H_4)CH_2$

$\tilde{A}\ ^2B_1$ C_{2v}
T_0=20738T gas LF[1] $\tilde{A}-\tilde{X}$ 445–580 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	6b		516	gas	LF	1

τ_0=400T ns gas LF[1]
A_0=0.172; B_0=0.032; C_0=0.028 LF[1]

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CN stretch	2216	gas	LF	1
	8a		1558	gas	LF	1
	9a		1143	gas	LF	1
	1		818	gas	LF	1
	6a		513	gas	LF	1
b_2	6b		637	gas	LF	1

A_0 = 0.182; B_0 = 0.032; C_0 = 0.028 LF[1]

Reference

[1] M. Fukushima, K. Saito, and K. Obi, J. Mol. Spectrosc. **180**, 389 (1996).

C_6H_5N

In an argon or a nitrogen matrix, irradiation at wavelengths longer than 450 nm leads to isomerization to *cyc*-C_6H_5N.[1]

$\tilde{a}\ ^1A_2$ C_{2v}
T_0=6300(700) gas PE[2]PD[3]

$\tilde{X}\ ^3A_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1552s	Ar	IR	1
			1524m	Ar	IR	1
			1497w	Ar	IR	1
			1426wm	Ar	IR	1
			1408w	Ar	IR	1
			1309w	Ar	IR	1
			1300T	gas	PE	2
			1299w	Ar	IR	1
			1286ms	Ar	IR	1
			1250w	Ar	IR	1
			1148m	Ar	IR	1
			1079wm	Ar	IR	1
			1008wm	Ar	IR	1
			964w	Ar	IR	1
			885w	Ar	IR	1
			820wm	Ar	IR	1
		OPLA CH-bend	746vs	Ar	IR	1
		Ring torsion	654s	Ar	IR	1
		Ring breathing	515T	gas	PE,PD	2,3

References

[1] J. C. Hayes and R. S. Sheridan, J. Am. Chem. Soc. **112**, 5879 (1990).
[2] M. J. Travers, D. C. Cowles, E. P. Clifford, and G. B. Ellison, J. Am. Chem. Soc. **114**, 8699 (1992).
[3] R. N. McDonald and S. J. Davidson, J. Am. Chem. Soc. **115**, 10857 (1993).

2,6-$C_6H_3F_2N$:

In an argon matrix, a prominent absorption at 42400 (236 nm) and weaker absorptions at 35200 (284 nm) and 32000 (312 nm) have been assigned[1] to 2,6-$C_6H_3F_2N$:.

In an argon matrix, prolonged irradiation at 22500 (444 nm) results in reversible rearrangement to the azirine (cf. *bicyc*-$C_6H_3F_2N$).[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1585.1m	Ar	IR	1
			1577.7s	Ar	IR	1
			1459.4m	Ar	IR	1
			1452.2vs	Ar	IR	1
			1411.2wm	Ar	IR	1
			1312.4m	Ar	IR	1
			1281.1wm	Ar	IR	1
			1242.0m	Ar	IR	1
			1229.3m	Ar	IR	1
			1002.8w	Ar	IR	1
			991.6s	Ar	IR	1
			850.4wm	Ar	IR	1
			836.6w	Ar	IR	1
			772.4wm	Ar	IR	1
			767.7m	Ar	IR	1
			708.3wm	Ar	IR	1
			699.6w	Ar	IR	1
			553.2w	Ar	IR	1
			501.2w	Ar	IR	1

Reference

[1] J. Morawietz and W. Sander, J. Org. Chem. **61**, 4351 (1996).

C_6F_5N:

In an argon matrix,[2] irradiation at 22500 (444 nm) results in isomerization to the azirene (cf. *bicyc*-C_6F_5N).

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1572.4wm	Ar	IR	2
			1575m	N_2	IR	1
			1564.4wm	Ar	IR	2
			1565m	N_2	IR	1
			1502.7vs	Ar	IR	2
			1502vs	N_2	IR	1
			1464.0m	Ar	IR	2
			1462vs	N_2	IR	1
			1455.6ms	Ar	IR	2
			1454vs	N_2	IR	1
			1359.4wm	Ar	IR	2
			1359s	N_2	IR	1
			1334.6w	Ar	IR	2
			1281.4wm	Ar	IR	2
			1284m	N_2	IR	1
			1205.5w	Ar	IR	2
			1204w	N_2	IR	1
			1151.7w	Ar	IR	2
			1149w	N_2	IR	1
			1025.5s	Ar	IR	2
			1029vs	N_2	IR	1
			1008.5wm	Ar	IR	2
			1007s	N_2	IR	1
			1000.6wm	Ar	IR	2
			990m	N_2	IR	1
			982.3vs	Ar	IR	2
			981vs	N_2	IR	1
			916.1w	Ar	IR	2
			610.7vw	Ar	IR	2

References

[1] I. R. Dunkin and P. C. P. Thomson, J. Chem. Soc., Chem. Commun. 1192 (1982).
[2] J. Morawietz and W. Sander, J. Org. Chem. **61**, 4351 (1996).

$C_6H_5N^-$

Threshold for electron detachment from ground-state $C_6H_5N^-$ =11700(160) gas PE[1,2]

$\tilde{X}\ ^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1350T	gas	PE	1
		Ring breathing	500T	gas	PE	1

$C_6D_5N^-$

Threshold for electron detachment from ground-state $C_6D_5N^-$ =11620(160) gas PE[1]PD[2]

$\tilde{X}\ ^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			434HT	gas	PD	1

References

[1] M. J. Travers, D. C. Cowles, E. P. Clifford, and G. B. Ellison, J. Am. Chem. Soc. **114**, 8699 (1992).
[2] R. N. McDonald and S. J. Davidson, J. Am. Chem. Soc. **115**, 10857 (1993).

$C_6H_5NH_2^+$

$\tilde{A}\ ^2A_2$ C_{2v}
T_0=10570(80) gas PE[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1		840(40)	gas	PE	7
	6a		524(10)	gas	PE	7

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	8a[a]		1594	gas	TPE	2,5,6
	19a		1436(10)T	gas	PE	2
	13		1385	gas	TPE	2,5,6
	9a		1188	gas	TPE	2,4–6
	18a		996	gas	TPE	5,6
	12	Ring s-stretch	982	gas	PI,TPE	1,2,4–6
	1		814	gas	PI,TPE	1,2,4,6
	6a	N-ring s-str.	522	gas	PI,TPE	1–6
a_2		C-N torsion	577H	gas	TPE	6
	16a		356	gas	PI,TPE	2–6
b_1	17b		963T[b]	gas	TPE	6
	11		790[b]	gas	TPE	6
		Inversion	658	gas	PI,TPE	2,3,5,6
	16b		629	gas	TPE	6
	4	Ring deform.	445	gas	TPE	6
	10b		179	gas	PI,TPE	3,5,6
b_2	6b		582	gas	TPE	6
	15		550H	gas	TPE	5,6

$C_6D_5ND_2^+$

$\tilde{X}\ ^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_1		Inversion	465(10)	gas	PI	3

[a]Vibrational numbering and assignments parallel those given by Chernoff and Rice [J. Chem. Phys. **70**, 2511 (1979)] for aniline.
[b]From combination band.

References

[1] M. A. Smith, J. W. Hager, and S. C. Wallace, J. Chem. Phys. **80**, 3097 (1984).
[2] J. T. Meek, E. Sekreta, W. Wilson, K. S. Viswanathan, and J. P. Reilly, J. Chem. Phys. **82**, 1741 (1985).
[3] J. Hager, M. A. Smith, and S. C. Wallace, J. Chem. Phys. **84**, 6771 (1986).
[4] M. Takahashi, H. Ozeki, and K. Kimura, J. Chem. Phys. **96**, 6399 (1992).
[5] X. Zhang, J. M. Smith, and J. L. Knee, J. Chem. Phys. **97**, 2843 (1992).
[6] X. Song, M. Yang, E. R. Davidson, and J. P. Reilly, J. Chem. Phys. **99**, 3224 (1993).
[7] B. Kim and P. M. Weber, J. Phys. Chem. **99**, 2583 (1995).

C_6H_5O

$\tilde{C}$ C_{2v}
gas AB[1,2] $\tilde{C}-\tilde{X}$ 380–395 nm
T_0=25175(10) Ar AB[4,5] $\tilde{C}-\tilde{X}$ 351–397 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1462(20)	Ar	AB	4
			1140(20)	Ar	AB	4
			920(20)	Ar	AB	4

$\tilde{B}$ C_{2v}
T_0≅16360 gas AB[2,3] $\tilde{B}-\tilde{X}$ 559–612 nm
Ar AB[4,5] $\tilde{B}-\tilde{X}$ 573–629 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			500T	gas	AB	3
			504(10)	Ar	AB	4

$\tilde{A}$ C_{2v}
T_0=8550(40) gas PE[6]

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1490(25)T	gas	PE	6
			515(15)	gas	PE	6

C_6D_5O

$\tilde{C}$ C_{2v}
T_0=25240(10) Ar AB[4] $\tilde{C}-\tilde{X}$ 349–397 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1349(20)	Ar	AB	4
			809(20)	Ar	AB	4

References

[1] G. Porter and F. J. Wright, Trans. Faraday Soc. **51**, 1469 (1955).
[2] G. Porter and B. Ward, J. Chim. Phys. **61**, 1517 (1964).
[3] B. Ward, Spectrochim. Acta A **24**, 813 (1968).
[4] D. Pullin and L. Andrews, J. Mol. Struct. **95**, 181 (1982).
[5] K. Kesper, F. Diehl, J. G. G. Simon, H. Specht, and A. Schweig, Chem. Phys. **153**, 511 (1991).

[6] R. F. Gunion, M. K. Gilles, M. L. Polak, and W. C. Lineberger, Int. J. Mass Spectrom. Ion Proc. **117**, 601 (1992).

$C_6H_5OH^+$

In an argon matrix, an absorption maximum at 36310 (275 nm) has been attributed[3] to $C_6H_5OH^+$.

$\tilde{B}$ C_s
T_0=21129T gas PE[1,3]PRI[4] $\tilde{B}-\tilde{X}$ 405–465 nm

In an argon matrix, an absorption maximum at 23640 (423 nm) has been attributed[3] to $C_6H_5OH^+$.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			392T	gas	PRI	4
			363T	gas	PRI	4
			347T	gas	PRI	4

$\tilde{A}$ C_s
T^a=7180(230) gas PE[1,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1100(80)	gas	PE	1

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1669(33)	gas	PE	2
			1500(30)	gas	PE	2
			1395(28)	gas	PE	2
			1210(24)	gas	PE	2
			1040(21)	gas	PE	2
			1027(21)	gas	PE	2
			976(20)	gas	PE	2
			815(16)	gas	PE	2
			556(12)	gas	PE	2
			516(12)	gas	PE	2
		Ring torsion ?	169(12)	gas	PE	2

$C_6D_5OD^+$

$\tilde{B}$ C_s
gas PRI[4] $\tilde{B}-\tilde{X}$ 425–442 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			234T	gas	PRI	4

[a]From vertical ionization potential.

References

[1] J. P. Maier and D. W. Turner, J. Chem. Soc. Faraday Trans. 2 **69**, 521 (1973).
[2] S. L. Anderson, L. Goodman, K. Krogh-Jesperson, A. G. Ozkabak, R. N. Zare, and C.-F. Zheng, J. Chem. Phys. **82**, 5329 (1985).
[3] K. Kesper, F. Diehl, J. G. G. Simon, H. Specht, and A. Schweig, Chem. Phys. **153**, 511 (1991).
[4] J. E. LeClaire, R. Anand, and P. M. Johnson, J. Chem. Phys. **106**, 6785 (1997).

9. Molecule Index

In the References column, unprefixed numbers give the page on which the table appears in the monograph.[5] Numbers prefixed by ''A'' give the page number in the present paper.

Formula	*Structure/Name*	*References*
AgAuCu	CuAgAu	60
$AgCu_2$	Cu_2Ag	59
AgO_2	AgOO	A178
Ag_3	Ag_3	60,A161
$AlBr_2$	$AlBr_2$	A193
$AlBr_3^+$	$AlBr_3^+$	203
AlClO	OAlCl	85
$AlCl_2$	$AlCl_2$	90,A193
$AlCl_2H$	$HAlCl_2$	169
$AlCl_3^+$	$AlCl_3^+$	203
AlFO	FAlO	85
AlF_2	AlF_2	A192
AlF_3^+	AlF_3^+	202
AlHO	AlOH	36,A143
AlH_2	AlH_2	17,A129
AlH_2O	HAlOH	139
AlH_3	AlH_3	A212
AlH_4^-	AlH_4^-	A266
AlH_4Si	SiH_3AlH	307
AlI_2	AlI_2	A193
AlO_2	*cyc*-AlO_2	75
AlO_2	OAlO	75,A183
AlO_2^-	$OAlO^-$	A189
AlO_3	OAlOO	190
Al_2H_2	*cyc*-Al_2H_2	A219
Al_2H_2	H(*cyc*-AlHAl)	A219
Al_2H_2	HAlAlH	A220
Al_2O	Al_2O	63
Al_2O_2	$(AlO)_2$	184,A248
$Al_2O_2^-$	$(AlO)_2^-$	A249
Al_2O_3	Al_2O_3	283,A297
$Al_2O_3^-$	$Al_2O_3^-$	A297
Al_2O_4	Al_2O_4	A321
$Al_2O_4^-$	$Al_2O_4^-$	A321
Al_2O_5	Al_2O_5	A331
Al_2S_3	Al_2S_3	A297
Al_3	Al_3	62,A162
ArBeO	ArBeO	A188
$ArBeO_2$	$ArBeO_2$	A253
ArBrKr	ArKrBr	123
ArBrXe	ArXeBr	123
ArClKr	ArKrCl	122
ArDKr	ArKrD	57
ArFKr	ArKrF	121,A210
ArFXe	ArXeF	121
ArHXe	ArXeH	57
Ar_2Cl	Ar_2Cl	122
Ar_2H^+	HAr_2^+	56,A159
Ar_2H	Ar_2H	56

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
Ar_2F	Ar_2F	121,A210	$BF_2H_2N^+$	$NH_2BF_2^+$	332
$AsBr_3^+$	$AsBr_3^+$	221	BF_2O	F_2BO	200
AsClO	ClAsO	104	BF_3^+	BF_3^+	201,A255
$AsCl_3^+$	$AsCl_3^+$	221	BF_3^-	BF_3^-	A261
$AsFH_2$	AsH_2F	152	BF_4^-	BF_4^-	302
AsF_2	AsF_2	109,A203	$BGaH_6^+$	$GaBH_6^+$	A332
AsF_2H	$HAsF_2$	179	BHN	HNB	31,A141
AsF_2H_3	AsH_3F_2	325	BHO	HBO	35
AsF_3^+	AsF_3^+	221	BHO_2	HOBO	162
$AsGa_2$	Ga_2As	A165	BHS^+	HBS^+	31,A141
$AsHO_3$	$HOAsO_2$	273	BHS	HBS	35
AsH_2	AsH_2	23	BH_2	BH_2	17
AsH_3^+	AsH_3^+	129	BH_2N	HBNH	137,A222
AsH_3O	H_3AsO	243	BH_2N	H_2NB	A223
AsH_3O	H_2AsOH	243	BH_3	BH_3	124,A212
$AsIn_2$	In_2As	A165	BH_3^-	BH_3^-	125
As_2Ga	$GaAs_2$	A172	BH_3N	$HBNH_2$	A269
As_4^+	As_4^+	187	BH_3O	H_2BOH	233
As_4O	As_4O	284	BH_3O_3	$B(OH)_3$	A326
As_4O	br-As_4O	284	BH_3S	H_2BSH	233
$AuCu_2$	Cu_2Au	60	BH_4^-	BH_4^-	A266
AuO_2	*cyc*-AuO_2	A178	BH_4K	KBH_4	A308
Au_3	Au_3	60,A161	BH_4Li	$LiBH_4$	305,A307
$BBrH_2$	H_2BBr	142	BH_4N^+	$H_2BNH_2^+$	307
BBrO	BrBO	85	BH_4N	H_2BNH_2	309
BBrS	BrBS	85	BH_4Na	$NaBH_4$	305,A307
BBr_2^+	BBr_2^+	A189	BH_4Sr	$SrBH_4$	306
BBr_2	BBr_2	89,A192	BI_2	BI_2	89
BBr_2H^+	$HBBr_2^+$	166	BI_3^+	BI_3^+	202
BBr_2H	$HBBr_2$	A238	BN_2	NBN	67
$BBr_2H_2N^+$	$NH_2BBr_2^+$	332	BN_2	BNN	69
BBr_3^+	BBr_3^+	202	BN_3	NNBN	184
$BCaH_4$	$CaBH_4$	305	BO_2	BO_2	73
$BClF_3^-$	BF_3Cl^-	302	BO_2^-	BO_2^-	84
$BClH_2$	H_2BCl	142	BO_2S	OBSO	190
BClO	ClBO	84,A189	BS_2	BS_2	74,A182
$BClS^+$	$ClBS^+$	74,A183	$B_2Cl_4^+$	$B_2Cl_4^+$	348
BClS	ClBS	85,A189	$B_2F_4^+$	$B_2F_4^+$	347
BCl_2^+	BCl_2^+	A189	B_2HN	HBNB	A232
BCl_2	BCl_2	89,A192	B_2H_2	HBBH	A219
BCl_2H^+	$HBCl_2^+$	166	$B_2H_2N_2$	HNBBNH	A315
BCl_2H	$HBCl_2$	A238	B_2H_3N	H_2BNBH	A311
$BCl_2H_2N^+$	$NH_2BCl_2^+$	332	$B_2H_4^+$	$B_2H_4^+$	306
BCl_3^+	BCl_3^+	201,A255	$B_2H_5^+$	$B_2H_5^+$	359
BCl_3^-	BCl_3^-	A261	$B_2H_6^+$	$B_2H_6^+$	A332
BCl_4^-	BCl_4^-	302	B_2H_7N	$B_2H_5NH_2$	398
BFH^+	HBF^+	37	B_2N	*cyc*-BBN	62,A165
BFH_2	H_2BF	142	B_2N	BNB	63,A165
BFO	FBO	84,A188	B_2N_2	BBNN	181
BFS^+	FBS^+	74	B_2N_2	BNBN	181
BFS	FBS	85	B_2N_2	*cyc*-$(BN)_2$	181
BF_2^+	BF_2^+	A189	B_2O	BBO	63
BF_2	BF_2	89,A191	B_2O	BOB	63
BF_2H^+	HBF_2^+	165	$B_2O_2^+$	$B_2O_2^+$	183
BF_2H	HBF_2	A238	B_2O_2	B_2O_2	184

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
B_3	B_3	A162	BrF_2^-	$FBrF^-$	118
$B_3F_3H_3N_3^+$	*cyc*-$(FBNH)_3^+$	399	BrF_2^-	$FFBr^-$	118
BaHO	BaOH	30	BrF_2P^+	PF_2Br^+	220
BaH_2N	$BaNH_2$	133	BrF_3^+	BrF_3^+	226
BaH_2O	HBaOH	135	BrF_3Si^+	SiF_3Br^+	295
BaH_2O_2	$Ba(OH)_2$	251	BrF_5^+	BrF_5^+	358
BaO_2	OBaO	A175	BrFeH	HFeBr	35
BaO_2	*cyc*-BaO_2	A175	BrGeH	HGeBr	45
Ba_2O_2	*cyc*-$(BaO)_2$	A243	$BrGeH_2$	H_2GeBr	150
Ba_2O_2	BaOBaO	A243	$BrGeH_3^+$	GeH_3Br^+	241
$BeBr_2$	$BeBr_2$	84	$BrHI^-$	$BrHI^-$	55
$BeCl_2$	$BeCl_2$	84	$BrHO^+$	$HOBr^+$	A155
BeF_2	BeF_2	83	BrHO	HOBr	52,A156
BeHO	BeOH	A138	BrHSi	HSiBr	44,A151
BeH_2	BeH_2	A125	BrHXe	HXeBr	A158
BeH_2O	HBeOH	A222	BrH_2N^+	H_2NBr^+	152
BeH_2O_2	$Be(OH)_2$	A281	BrH_2P	H_2PBr	A229
BeI_2	BeI_2	84	BrH_3Si^+	SiH_3Br^+	241
BeKrO	KrBeO	A188	BrKrXe	KrXeBr	123
BeN_2O_2	$NNBeO_2$	A296	$BrKr_2$	Kr_2Br	123
BeN_4	NNBeNN	A294	$BrNO^+$	$BrNO^+$	94
BeN_4	NN(*cyc*-BeN_2)	A294	$BrNO_2$	$BrNO_2$	213,A260
BeOXe	XeBeO	A188	$BrNO_2$	*t*-BrONO	213,A260
BeO_2^+	$OBeO^+$	A171	$BrNO_3^+$	$BrONO_2^+$	A301
BeO_2	OBeO	A174	$BrNO_3$	$BrONO_2$	289,A303
BeO_3	BeO_3	A250	$BrNS^+$	$NSBr^+$	95
BeO_4	O_2BeO_2	A297	BrNS	NSBr	104
Be_2H	BeBeH	A136	BrN_3^+	BrN_3^+	197
Be_2H_2	HBeBeH	A217	BrNeXe	NeXeBr	123
Be_2H_2O	HBeOBeH	A275	BrOP	BrPO	103
Be_2H_3	HBeHBeH	A267	BrOPS	BrP(O)S	214
Be_2H_4	$HBeH_2BeH$	A308	BrO_2	BrOO	110,A204
Be_2N_2	BeBeNN	A242	BrO_2	OBrO	114,A206
Be_2N_2	BeNNBe	A242	BrO_2P	PO_2Br	214
Be_2N_2	$(BeN)_2$	A242	BrPS	BrPS	104
Be_2N_4	NNBeBeNN	A317	BrS_2	SSBr	111
Be_2O	BeOBe	A163	$BrXe_2$	Xe_2Br	123
Be_2O_2	*cyc*-$(BeO)_2$	A242	Br_2Cl^-	$BrClBr^-$	119
Be_2O_2	BeOBeO	A242	Br_2Cl^-	$ClBrBr^-$	119
Be_2O_3	OBeOBeO	A294	Br_2F	BrBrF	117
Bi_3	Bi_3	82	Br_2F_2	Br_2F_2	227
Bi_4	Bi_4	189	Br_2Ge^+	$GeBr_2^+$	92
Bi_4^-	Bi_4^-	197	$Br_2GeH_2^+$	$GeH_2Br_2^+$	263
$BrClH^-$	$ClHBr^-$	54	Br_2H^-	$BrHBr^-$	55,A157
BrClO	BrClO	A209	Br_2HN^+	$HNBr_2^+$	179
BrClO	ClBrO	A209	$Br_2H_2Si^+$	$SiH_2Br_2^+$	262
BrClO	BrOCl	A207	Br_2N	NBr_2	108
$BrClO_2$	$BrClO_2$	A263	Br_2O	BrOBr	114,A207
$BrClO_2$	BrOClO	A264	Br_2O	BrBrO	116,A209
$BrClO_2$	ClOBrO	A264	Br_2OP	$OPBr_2$	221
$BrCl_2^-$	$ClBrCl^-$	119	Br_2P	PBr_2	109,A203
$BrCl_2^-$	$ClClBr^-$	119	Br_2S^+	SBr_2^+	112
$BrFH^-$	$FHBr^-$	54	Br_2S	SBr_2	115
BrFS	FSBr	A208	$Br_2S_2^+$	$S_2Br_2^+$	224
BrF_2	BrF_2	117	Br_2S_2	$SSBr_2$	226

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
Br_2Se^+	$SeBr_2^+$	113	CCaNO	CaNCO	182
Br_2Si	$SiBr_2$	101	CClF	CFCl	98
Br_3^-	Br_3^-	119	CClFOS	ClFCSO (I)	288
Br_3P^+	PBr_3^+	221	CClFOS	ClFCSO (II)	288
Br_3PO^+	Br_3PO^+	299	$CClFS^+$	$FClCS^+$	205
Br_3PS^+	Br_3PS^+	299	$CClF_2^+$	CF_2Cl^+	210
Br_3Sb^+	$SbBr_3^+$	222	$CClF_2$	CF_2Cl	216
Br_4Ge^+	$GeBr_4^+$	297	$CClF_2NO^+$	CF_2ClNO^+	353
Br_4Si^+	$SiBr_4^+$	296	$CClF_2NO_4$	$CF_2ClOONO_2$	425
CAlO	AlCO	68,A172	$CClF_3^+$	CF_3Cl^+	290
CAl_2	Al_2C	A164	$CClF_3^-$	CF_3Cl^-	303
CAsN	AsCN	71	$CClF_4$	CF_3ClF	356
CBF_2NO	F_2BNCO	A321	$CClN^+$	$ClCN^+$	79
CBO	BCO	68	CClN	ClNC	88
CBO_2	OBCO	186	$CClNO^+$	$ClNCO^+$	193
CBS_2	SBCS	A249	CClNO	ClCNO	199
CBaN	BaCN	62	CClNO	ClNCO	198
$CBeO_2$	OCBeO	A247	$CClNS^+$	$ClSCN^+$	194
$CBeO_2$	COBeO	A248	CClNS	ClSCN	198
CBe_2O	BeBeCO	A241	$CClNSe^+$	$ClSeCN^+$	195
$CBrCl^+$	$CClBr^+$	91	CClO	ClCO	90
CBrCl	CClBr	99	$CClP^+$	$ClCP^+$	81
$CBrCl_2^+$	CCl_2Br^+	211	CClP	ClCP	A190
$CBrCl_2$	CCl_2Br	218	CClS	ClCS	105
$CBrClF_2^-$	CF_2ClBr^-	303	CCl_2^+	CCl_2^+	91
CBrF	CFBr	98	CCl_2	CCl_2	99
$CBrF_2^+$	CF_2Br^+	210	CCl_2^-	CCl_2^-	107
$CBrF_2$	CF_2Br	216	CCl_2F^+	$CFCl_2^+$	210
$CBrF_2^-$	CF_2Br^-	225	CCl_2F	$CFCl_2$	216
$CBrF_3^+$	CF_3Br^+	291	CCl_2FNO^+	$CFCl_2NO^+$	353
$CBrF_3^-$	CF_3Br^-	303	CCl_2FNO_4	$CFCl_2OONO_2$	426
$CBrF_4$	CF_3BrF	356	$CCl_2F_2^+$	$CF_2Cl_2^+$	292,A304
$CBrN^+$	$BrCN^+$	80,A187	$CCl_2F_2^-$	$CF_2Cl_2^-$	303
CBrN	BrNC	88	CCl_2I	CCl_2I	218
$CBrNO^+$	$BrCNO^+$	A252	CCl_2O^+	Cl_2CO^+	204
$CBrNO^+$	$BrNCO^+$	193	CCl_2S^+	Cl_2CS^+	206
CBrNO	BrCNO	199,A253	CCl_2Se	Cl_2CSe	212
CBrNO	BrNCO	198	CCl_3^+	CCl_3^+	210
$CBrNS^+$	$BrSCN^+$	194	CCl_3	CCl_3	217
CBrNS	BrSCN	199	CCl_3F^+	$CFCl_3^+$	293
$CBrNSe^+$	$BrSeCN^+$	195	CCl_3F^-	$CFCl_3^-$	303
CBr_2^+	CBr_2^+	91	CCl_3NO^+	CCl_3NO^+	353
CBr_2	CBr_2	100	CCl_3NO_4	CCl_3OONO_2	426
CBr_2Cl^+	$CClBr_2^+$	211	CCl_3O_2	CCl_3O_2	354
CBr_2Cl	$CClBr_2$	218	CCl_4^+	CCl_4^+	294,A305
CBr_2F^+	$CFBr_2^+$	210	CCl_4	Cl_2CCl-Cl	302
CBr_2F	$CFBr_2$	216	CCoO	CoCO	A167
$CBr_2F_2^+$	$CF_2Br_2^+$	292	CCrO	CrCO	A166
$CBr_2F_2^-$	$CF_2Br_2^-$	303	CCuO	CuCO	A167
CBr_3^+	CBr_3^+	211	CD_3O^+	CD_3O^+	235
CBr_3	CBr_3	218	CFI	CFI	99
CBr_3F^+	$CFBr_3^+$	293	CFI_2^+	CFI_2^+	210
CBr_3F^-	$CFBr_3^-$	303	CFI_2	CFI_2	217
CBr_4^+	CBr_4^+	294	CFN^+	FCN^+	79
CCaN	CaNC	62,A164	CFN	FNC	88

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
CFNO	FNCO	198,A253	CHBrF	HCFBr	177
$CFNO_5$	$FC(O)OONO_2$	A342	CHBrO	HCOBr	170,A239
$CFNS^+$	$FSCN^+$	193	$CHBr_2^+$	$HCBr_2^+$	172
CFN_2	FNCN	192	$CHBr_2$	$HCBr_2$	178
CFO^+	FCO^+	86	$CHBr_3^+$	$HCBr_3^+$	276
CFO	FCO	90,A193	$CHCaO_2$	HCOOCa	268
CFO_2	FCO_2	203,A256	CHCl	HCCl	42,A149
CFO_2^-	FCO_2^-	212,A259	$CHCl^-$	$HCCl^-$	47
CFO_3	$FC(O)O_2$	287	$CHClF^+$	$HCFCl^+$	171
CFP^+	FCP^+	81	CHClF	HCFCl	176
CFP	FCP	A190	$CHClF_2^+$	HCF_2Cl^+	275
CFS	FCS	A194	$CHClO^+$	$HCOCl^+$	169
CF_2^+	CF_2^+	91	CHClO	HCOCl	170,A239
CF_2	CF_2	97,A196	$CHCl_2^+$	$HCCl_2^+$	171
CF_2^-	CF_2^-	107	$CHCl_2$	$HCCl_2$	177
CF_2I^+	CF_2I^+	210	$CHCl_2F^+$	$HCFCl_2^+$	275
CF_2I	CF_2I	216	$CHCl_2NO_4$	$CHCl_2OONO_2$	425
CF_2N	F_2CN	204	$CHCl_3^+$	$HCCl_3^+$	275
CF_2NOP^+	PF_2NCO^+	349	CHF^+	HCF^+	41
CF_2NP^+	PF_2CN^+	285	CHF	HCF	42,A148
CF_2NPS^+	PF_2NCS^+	350	CHF^-	HCF^-	47
$CF_2N_2^+$	$CF_2N_2^+$	285	$CHFI^+$	$HCFI^+$	171
CF_2O^+	F_2CO^+	204	CHFI	HCFI	177
CF_2OS	F_2CSO	288	CHFN	HFCN	168
CF_2O_2	*cyc*-F_2CO_2	A302	$CHFO^+$	$HFCO^+$	168
CF_2S^+	F_2CS^+	205	$CHFS^+$	$HFCS^+$	A237
CF_2Se^+	F_2CSe^+	206	CHF_2^+	HCF_2^+	170
CF_3^+	CF_3^+	210,A258	CHF_2	HCF_2	176
CF_3	CF_3	215,A261	CHF_2N^+	CF_2NH^+	A289
CF_3^-	CF_3^-	A263	CHF_2N	$CF_2{=}NH$	270,A289
CF_3I^+	CF_3I^+	291	CHF_2N	*c*-HFC=NF	271
CF_3I^-	CF_3I^-	303	CHF_2P	$CF_2{=}PH$	271
CF_3IO	CF_3IO	356	CHF_3^+	HCF_3^+	274
CF_3IO	CF_3OI	356	CHI	HCI	43
CF_3NO^+	CF_3NO^+	353	CHI^-	HCI^-	48
CF_3NO_3	CF_3ONO_2	382,A342	CHIO	HCOI	A240
CF_3NO_4	CF_3OONO_2	A368	CHI_2	HCI_2	178
CF_3O	CF_3O	289,A303	CHN^+	HCN^+	33
CF_3O^-	CF_3O^-	302	CHN^+	HNC^+	34
CF_3O_2	CF_3O_2	354	CHN	HNC	38,A145
CF_3S	CF_3S	A303	$CHNO^+$	$HNCO^+$	160
CF_4^+	CF_4^+	290,A303	$CHNO^+$	$HCNO^+$	161
CF_4I	CF_3IF	356	CHNO	HNCO	163,A236
CF_4O^+	CF_3OF^+	355	CHNO	HOCN	163
CF_4OS	CF_3OSF	372	CHNO	HCNO	164
CFeO	FeCO	63,A167	CHNO	HONC	164
$CFeO^-$	$FeCO^-$	67	CHNP	HPCN	160
CGaO	GaCO	A172	$CHNS^+$	$HNCS^+$	160
CGeO	GeCO	A180	CHN_2	HCNN	161,A235
CHBr	HCBr	43,A149	CHN_2	HNCN	160,A235
$CHBr^-$	$HCBr^-$	47	CHO^+	HCO^+	37,A145
$CHBrCl^+$	$HCClBr^+$	171	CHO^+	HOC^+	39
CHBrCl	HCClBr	178	CHO	HCO	40,A146
$CHBrClF^+$	$HCFClBr^+$	A292	CHOP	HPCO	165
$CHBrF^+$	$HCFBr^+$	171	$CHOS^+$	$HOCS^+$	165,A236

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
CHO_2^+	$HOCO^+$	165	CH_2NO	H_2CNO	A283
CHO_2	*c*-HOCO	167	CH_2NOSr	HCONHSr	326
CHO_2	*t*-HOCO	167,A236	CH_2NO_2	CH_2NO_2	331,A316
CHO_2	HCO_2	A237	$CH_2NO_2^-$	$CH_2NO_2^-$	337
CHO_2^-	HCO_2^-	A239	$CH_2N_2^+$	$CH_2N_2^+$	253
CHO_2Sr	HCOOSr	268	$CH_2N_2^+$	*cyc*-$CH_2N_2^+$	254
CHO_3	HC(O)OO	270	$CH_2N_2^+$	NH_2CN^+	253
CHP^+	HCP^+	34	CH_2N_2	HN=C=NH	254,A282
CHS^+	HCS^+	38,A145	CH_2N_2	HCNNH	A282
CHS_2	*t*-HSCS	167	CH_2N_2O	H_2NNCO	331
CHS_2	HCS_2	168	CH_2Ni	$NiCH_2$	A219
CHTi	TiCH	A137	CH_2O^+	H_2CO^+	140,A223
CHV	VCH	A137	CH_2OS^+	H_2CSO^+	258
CHW	WCH	A137	CH_2OS	H_2CSO	259,A284
CH_2^+	CH_2^+	18	$CH_2O_2^+$	$HCOOH^+$	257
CH_2	CH_2	18,A130	CH_2O_2	*cyc*-H_2CO_2	A283
CH_2^-	CH_2^-	21	CH_2O_3	HC(O)OOH	336
CH_2B	HBCH	A221	CH_2S^+	H_2CS^+	141
CH_2B_2	HBCBH	245,A275	CH_2S	H_2CS	143,A224
CH_2Br^+	H_2CBr^+	147	CH_2S^-	H_2CS^-	149
CH_2Br	H_2CBr	150,A228	CH_2S_2	*t*-HCSSH	259
CH_2BrCl	H_2CCl-Br	264	CH_2S_2	*c*-HCSSH	259
CH_2BrF^+	CH_2FBr^+	261	CH_2Se^+	H_2CSe^+	141
CH_2BrI	H_2CBr-I	265	CH_2Se	H_2CSe	145,A226
$CH_2Br_2^+$	$CH_2Br_2^+$	261	CH_2Si	H_2CSi	138,A223
CH_2Br_2	H_2CBr-Br	264	CH_2Zn	$ZnCH_2$	131
CH_2CaNO	HCONHCa	326	CH_2Zn	HZnCH	131
CH_2Cl^+	H_2CCl^+	147	CH_3^+	CH_3^+	124,A213
CH_2Cl	H_2CCl	149,A228	CH_3	CH_3	125,A214
CH_2ClF^+	CH_2FCl^+	261	CH_3^-	CH_3^-	129
CH_2ClI	H_2CCl-I	264	CH_3Al	$AlCH_3$	A268
CH_2ClN	CH_2=NCl	258	CH_3B	H_2C=BH	A268
CH_2ClNO_4	$CH_2ClOONO_2$	425	CH_3BO^+	BH_3CO^+	312
CH_2ClP	CH_2=PCl	258	CH_3BaO	$BaOCH_3$	315
$CH_2Cl_2^+$	$CH_2Cl_2^+$	261,A285	CH_3Br^+	CH_3Br^+	239,A274
CH_2Cl_2	H_2CCl-Cl	263	CH_3Br^+	H_2CBrH^+	A274
CH_2Cl_2O	$HCCl_2OH$	339	CH_3BrF	CH_3BrF	324
$CH_2Cl_2O_2$	$CHCl_2OOH$	368	CH_3Ca	$CaCH_3$	230,A267
CH_2Cl_2Si	CH_2=$SiCl_2$	337	CH_3CaO	$CaOCH_3$	314
CH_2Co	$CoCH_2$	A219	CH_3CaS	$CaSCH_3$	315
CH_2Cr	$CrCH_2$	A218	CH_3Cd	$CdCH_3$	231,A268
CH_2Cu	$CuCH_2$	132	CH_3Cl^+	CH_3Cl^+	239,A273
CH_2F^+	H_2CF^+	147	CH_3Cl^+	H_2CClH^+	A274
CH_2F	H_2CF	149	CH_3ClF	CH_3ClF	324
CH_2FI^+	CH_2FI^+	261	CH_3ClO^+	CH_3OCl^+	322
CH_2FO_2	CH_2FO_2	339	CH_3ClO	$ClCH_2OH$	323
$CH_2F_2^+$	$CH_2F_2^+$	260,A284	CH_3ClO_2	CH_2ClOOH	368
CH_2Fe	$FeCH_2$	131	CH_3ClSi	CH_2=SiHCl	321
CH_2Fe	HFeCH	132	CH_3ClSi	CH_3SiCl	321
CH_2I	H_2CI	150	CH_3F^+	CH_3F^+	238
$CH_2I_2^+$	$CH_2I_2^+$	262	CH_3F^+	H_2CFH^+	A273
CH_2I_2	H_2CI-I	265	CH_3FI	CH_3IF	324
CH_2N^+	$HCNH^+$	138	CH_3FO^+	CH_3OF^+	322
CH_2N	H_2CN	140	CH_3FO	CH_3OF	322
CH_2N^-	H_2CN^-	143	CH_3I^+	CH_3I^+	239

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
CH_3IO	CH_3IO	323	CH_4OSi	HCH_3SiO	363
CH_3IO	CH_3OI	323	CH_4O_2	$CH_2(OH)_2$	A325
CH_3IO	ICH_2OH	323	CH_4O_3	HO_2CH_2OH	379
CH_3K	KCH_3	230	CH_4S^+	CH_3SH^+	310
CH_3Mg	$MgCH_3$	A267	CH_4Si^+	$CH_2{=}SiH_2^+$	308
CH_3N^+	CH_2NH^+	233	CH_4Si	$CH_2{=}SiH_2$	309,A310
CH_3N	CH_3N	234,A269	CH_4Si	CH_3SiH	309
CH_3N	CH_2NH	234	CH_4Zn	CH_3ZnH	A309
CH_3NO^+	CH_3NO^+	318	CH_5BO	$H_2B{=}OCH_3$	374
CH_3NO^+	CH_2NOH^+	318	CH_5BS	H_2BSCH_3	A335
CH_3NO^+	$HCONH_2^+$	318	CH_6BN	$H_2B{=}NHCH_3$	398
CH_3NO	CH_3NO	320	CH_6OSi	CH_3SiH_2OH	416
CH_3NO	CH_2NOH	320,A314	CIN^+	ICN^+	81
CH_3NO_2	*c*-$CH_2(NO)OH$	367	CIN	INC	A191
CH_3NO_2	*t*-$CH_2(NO)OH$	367	$CINO^+$	$INCO^+$	193
CH_3NO_4	CH_3OONO_2	425	CINO	INCO	198
CH_3NO_5	$HOCH_2OONO_2$	425	$CINS^+$	$ISCN^+$	195
CH_3NS^+	$HCSNH_2^+$	319	CINS	ISCN	199
CH_3Na	$NaCH_3$	229	CI_3	CI_3	218
CH_3O^+	CH_2OH^+	235,A270	CMgN	MgCN	A164
CH_3O	CH_3O	236,A271	CMgN	MgNC	62,A164
CH_3O	CH_2OH	237,A272	CNO^+	NCO^+	71
CH_3O^-	CH_3O^-	242	CNO	CNO	82
CH_3OSr	$SrOCH_3$	315	CNO	NCO	76,A184
CH_3O_2	CH_3O_2	321	CNO^-	NCO^-	85
CH_3O_3	$HOCH_2O_2$	368	CNOSr	SrNCO	182
CH_3P^+	CH_2PH^+	233	CNP	PCN	70
CH_3S^+	CH_3S^+	235,A270	CNS	NCS	77
CH_3S^+	CH_2SH^+	235	CNS^-	NCS^-	86
CH_3S	CH_3S	237,A272	CNSr	SrNC	62
CH_3S	CH_2SH	238	CN_2	NCN	70,A180
CH_3S^-	CH_3S^-	242	CN_2	CNN	71
CH_3SSr	$SrSCH_3$	315	CN_2O^+	$ONCN^+$	186
CH_3S_2	CH_3S_2	322	CN_2O	NCNO	188
$CH_3S_2^-$	$CH_3S_2^-$	322	CN_2S^+	$NSCN^+$	A249
CH_3Si	CH_2SiH	232	CN_2S	NSCN	A252
CH_3Si	CH_3Si	232	CN_4^+	N_3CN^+	278
CH_3Si^-	CH_2SiH^-	233	CNiO	NiCO	A167
CH_3Si^-	CH_3Si^-	233	$CNiO^-$	$NiCO^-$	A171
CH_3Sr	$SrCH_3$	230,A267	COP	PCO	77
CH_3Te	CH_3Te	238	COPd	PdCO	A167
CH_3Zn	$ZnCH_3$	230,A267	COPt	PtCO	A167
CH_4^+	CH_4^+	227	COS^+	OCS^+	78,A185
CH_4B	H_2CBH_2	A309	COSc	ScCO	A166
CH_4B	CH_3BH	A310	COSi	SiCO	70
CH_4Cd	CH_3CdH	A309	COSn	SnCO	A180
CH_4Co	CH_3CoH	A308	COTa	TaCO	A166
CH_4Fe	CH_3FeH	306	COTi	TiCO	A166
CH_4Ga	CH_3GaH	307,A310	COU	CUO	A168
CH_4Hg	CH_3HgH	A309	COU	UCO	A168
CH_4N^+	$CH_2NH_2^+$	310	COV	VCO	A166
CH_4Ni	CH_3NiH	306	CO_2^+	CO_2^+	77,A185
CH_4NiO	$HNiOCH_3$	362	CO_2^-	CO_2^-	90,A193
CH_4NiO	CH_3NiOH	362	CO_2Ti	OTiCO	A248
CH_4O^+	CH_3OH^+	310	CO_2U	OUCO	A248

Formula	*Structure/Name*	*References*
CO_3	CO_3	199
CO_3^-	CO_3^-	203
CO_3Ti	O_2TiCO	A296
CO_3U	O_2UCO	A297
CO_4^-	CO_4^-	287
CS_2^+	CS_2^+	79,A186
CS_2^-	CS_2^-	A194
CSi_2	Si_2C	67
CSi_3	Si_3C	181
C_2Al_2	AlCCAl	A242
C_2B	*cyc*-BCC	62,A164
$C_2BFN_2O_2$	$FB(NCO)_2$	A341
C_2BeO_2	$Be(CO)_2$	A293
C_2BrCl^+	$ClCCBr^+$	191
C_2BrF_3	CF_3CBr	354
C_2BrN	BrCCN	189
$C_2Br_2^+$	$C_2Br_2^+$	191
$C_2ClF_3^+$	$CF_2{=}CFCl^+$	352
C_2ClF_3	CF_3CCl	354
C_2ClN	ClCCN	189
$C_2Cl_2^+$	$C_2Cl_2^+$	190
$C_2Cl_2F_2^+$	$CF_2{=}CCl_2^+$	352
$C_2Cl_2O^+$	Cl_2CCO^+	285
C_2Cl_2O	Cl_2CCO	285
$C_2Cl_2O_2^+$	*t*-$(ClCO)_2^+$	348
$C_2Cl_4^+$	$C_2Cl_4^+$	353
$C_2F_2^+$	$C_2F_2^+$	190
C_2F_2	FCCF	197
C_2F_2	$F_2C{=}C$:	197
$C_2F_2^-$	$F_2C{=}C:^-$	203
$C_2F_2N_2$	$F_2C{=}C{=}N{=}N$	347
$C_2F_2O_2^+$	*t*-$(FCO)_2^+$	348
C_2F_3	C_2F_3	287
C_2F_3O	CF_3CO	A322
$C_2F_4^+$	$C_2F_4^+$	351
C_2F_4	CF_3CF	354
C_2F_5	C_2F_5	371
C_2F_5P	$CF_2{=}PCF_3$	382
C_2Fe	FeCC	A164
C_2Fe^-	$FeCC^-$	A164
C_2DFe	FeCCD	A232
C_2H	HCC	32,A142
C_2H^-	HCC^-	37
C_2HAl	HCCAl	A233
C_2HB	HBCC	A232
C_2HB	HCCB	A232
C_2HB	*cyc*-HBC_2	A232
C_2HBe	BeCCH	A231
C_2HBr^+	$HCCBr^+$	158
C_2HCa	CaCCH	155,A231
C_2HCl^+	$HCCCl^+$	158
$C_2HClF_2^+$	$CHCl{=}CF_2^+$	340
C_2HClO	HClCCO	269
$C_2HCl_3^+$	$CHCl{=}CCl_2^+$	341
$C_2HF_3^+$	$CHF{=}CF_2^+$	340
C_2HF^+	$HCCF^+$	158
C_2HF	$HFC{=}C$:	162
C_2HF^-	$HFC{=}C:^-$	168
C_2HFO	HFCCO	269,A288
C_2HFe^-	$FeCCH^-$	A232
C_2HI^+	$HCCI^+$	159
C_2HMg	MgCCH	A231
C_2HN	HCCN	156,A234
C_2HNO	HCOCN	269,A287
C_2HNO_2	$O{=}C{=}C{=}NOH$	A317
C_2HNS^+	$HCSCN^+$	A287
C_2HNS	HCSCN	A288
$C_2HN_2^+$	$HNCCN^+$	268
C_2HO	HCCO	156,A234
C_2HS	HCCS	157,A234
C_2HS	HSCC	157
C_2HSi	HCCSi	A233
C_2HSr	SrCCH	155,A231
$C_2H_2^+$	$HCCH^+$	133,A221
C_2H_2	$H_2C{=}C$:	137
$C_2H_2^-$	$H_2C{=}C:^-$	139
C_2H_2Al	*cyc*-$HC{=}CHAl$	A276
C_2H_2Al	HCCAlH	A276
C_2H_2Al	$(C_2H_2)Al$	A277
C_2H_2B	*cyc*-$HC{=}CHB$	A276
C_2H_2B	*cyc*-$HC{=}CBH$	A276
C_2H_2B	HCCBH	A276
C_2H_2Be	HBeCCH	A275
C_2H_2Br	$CHBr{=}CH$	257
$C_2H_2ClF^+$	$CH_2{=}CFCl^+$	334
$C_2H_2ClF^+$	*c*-$CHF{=}CHCl^+$	334
$C_2H_2ClF^+$	*t*-$CHF{=}CHCl^+$	334
$C_2H_2ClN^+$	CH_2ClCN^+	331
$C_2H_2Cl_2^+$	$CH_2{=}CCl_2^+$	335
$C_2H_2Cl_2^+$	*c*-$CHCl{=}CHCl^+$	335
$C_2H_2Cl_2^+$	*t*-$CHCl{=}CHCl^+$	336
C_2H_2F	*t*-$CHF{=}CH$	257
$C_2H_2FN^+$	CH_2FCN^+	330
C_2H_2FO	CH_2CFO	A316
$C_2H_2FO^-$	CH_2COF^-	337
$C_2H_2F_2^+$	$CH_2{=}CF_2^+$	332
$C_2H_2F_2^+$	*c*-$CHF{=}CHF^+$	333
$C_2H_2F_2^+$	*t*-$CHF{=}CHF^+$	333
C_2H_2Fe	HFeCCH	245
C_2H_2Ga	$(C_2H_2)Ga$	A277
C_2H_2In	$(C_2H_2)In$	A277
C_2H_2Li	LiC_2H_2	244
C_2H_2N	H_2CCN	250,A280
C_2H_2N	H_2CNC	250
$C_2H_2N^-$	H_2CCN^-	252
$C_2H_2N^-$	H_2CNC^-	252
$C_2H_2N_2^+$	$HN{=}CHCN^+$	327
$C_2H_2N_2^+$	$H_2C{=}NCN^+$	327
$C_2H_2N_2$	*c*-$HN{=}CHCN$	327
$C_2H_2N_2$	*t*-$HN{=}CHCN$	328

Formula	*Structure/Name*	*References*
$C_2H_2N_2$	$H_2C{=}NCN$	328
$C_2H_2N_2O_2$	$HON{=}CHCNO$	381
$C_2H_2N_2O_2$	$HON{=}CHNCO$	381
C_2H_2Ni	$(C_2H_2)Ni$	245
C_2H_2Ni	$NiC{=}CH_2$	245
$C_2H_2O^+$	H_2CCO^+	250,A280
C_2H_2O	HCCOH	255
C_2H_2OS	CHOCHS	330
$C_2H_2O_2^+$	$(HCO)_2^+$	329
$C_2H_2O_2$	$HOC{\equiv}COH$	A315
$C_2H_2O_3$	$(HCO)_2O$	368
$C_2H_2S^+$	H_2CCS^+	253
C_2H_2S	H_2CCS	255,A282
C_2H_2S	HCCSH	256
C_2H_2S	*cyc*-C_2H_2S	256
$C_2H_2S_2$	$HS\text{-}CH{=}C{=}S$	331
C_2H_2Se	H_2CCSe	A283
C_2H_2Si	*cyc*-$HC{=}CHSi$	A278
C_2H_2Si	HCCSiH	A279
C_2H_2Si	$H_2C{=}C{=}Si$:	A279
C_2H_2Si	*cyc*-H_2SiCC	A279
$C_2H_3^+$	$C_2H_3^+$	232,A268
C_2H_3	C_2H_3	232,A269
C_2H_3As	$HCCAsH_2$	A313
C_2H_3As	CH_3CAs	A313
$C_2H_3CaO_2$	CH_3COOCa	379
$C_2H_3Cl^+$	$CH_2{=}CHCl^+$	319
C_2H_3ClO	CH_3OCCl	366
$C_2H_3F^+$	$CH_2{=}CHF^+$	319
$C_2H_3F_2$	CH_3CF_2	A327
$C_2H_3N^+$	CH_3CN^+	312
$C_2H_3N^+$	CH_3NC^+	313
$C_2H_3N^+$	$CH_2{=}C{=}NH^+$	313
$C_2H_3N^+$	*cyc*-$(HC{=}NCH_2)^+$	A311
C_2H_3N	$CH_2{=}C{=}NH$	316,A312
C_2H_3N	$HCNCH_2$	A312
C_2H_3N	*cyc*-$(HC{=}NCH_2)$	A313
C_2H_3NO	CH_3CNO	366
C_2H_3NO	CH_3OCN	A326
C_2H_3NO	$HOCH_2CN$	366
$C_2H_3NO_2$	CH_3ONCO	380
C_2H_3O	CH_3CO	317
C_2H_3O	CH_2CHO	317,A313
$C_2H_3O^-$	CH_2CHO^-	320,A314
$C_2H_3O_2Sr$	CH_3COOSr	380
$C_2H_3O_3$	CH_3COO_2	380,A339
$C_2H_3P^+$	CH_3CP^+	314
C_2H_3P	CH_3CP	316
$C_2H_4^+$	$C_2H_4^+$	307
C_2H_4Al	AlC_2H_4	361
C_2H_4F	FCH_2CH_2	364,A325
C_2H_4Fe	$HFeC_2H_3$	360
C_2H_4FeO	$CH_2{=}CHFeOH$	378
C_2H_4FeO	*cyc*-C_2H_4OFe	378
C_2H_4In	InC_2H_4	361
C_2H_4Li	C_2H_4Li	360
$C_2H_4Li_2$	1,2-$C_2H_4Li_2$	377
$C_2H_4N^+$	CH_3CNH^+	362
$C_2H_4O^+$	$CH_2{=}CHOH^+$	362,A324
C_2H_4O	$CH_2{=}CHOH$	363
$C_2H_4O_3$	1,2,3-*cyc*-$C_2H_4O_3$	422,A366
$C_2H_4O_3$	1,2,4-*cyc*-$C_2H_4O_3$	422,A367
$C_2H_4O_3$	*c*-$HCOOCH_2OH$	423
$C_2H_4O_3$	*t*-$HCOOCH_2OH$	423
$C_2H_4S^+$	CH_3CHS^+	363
C_2H_4S	CH_3CHS	363,A324
C_2H_4Si	*cyc*-C_2SiH_4	A324
$C_2H_5^+$	$C_2H_5^+$	359
C_2H_5	C_2H_5	359,A323
C_2H_5BrS	CH_3SBrCH_2	418
C_2H_5ClS	CH_3SClCH_2	418
C_2H_5IO	C_2H_5IO	A364
C_2H_5IO	C_2H_5OI	A364
$C_2H_5IO_2$	$C_2H_5IO_2$	A364
C_2H_5IS	CH_3SICH_2	418
C_2H_5N	*c*-$CH_3CH{=}NH$	374,A336
C_2H_5N	*t*-$CH_3CH{=}NH$	374
C_2H_5N	$C_2H_3NH_2$	375,A336
C_2H_5N	$H_2C{=}NCH_3$	375
$C_2H_5NO_2$	*c*-$CH_3CH(NO)OH$	424
$C_2H_5NO_4$	$C_2H_5OONO_2$	425
C_2H_5O	C_2H_5O	376,A337
C_2H_5O	CH_3CHOH	376
C_2H_5O	$HOCH_2CH_2$	376,A337
$C_2H_5O_2$	$C_2H_5O_2$	420
$C_2H_5O_3$	$HOCH_2CH_2O_2$	424
$C_2H_5S^+$	$CH_3SCH_2^+$	A336
C_2H_5S	C_2H_5S	376,A337
C_2H_6Ge	$(CH_3)_2Ge$	400
C_2H_6Hg	C_2H_5HgH	A357
$C_2H_6N_2O$	CH_3NHCH_2NO(A)	424
$C_2H_6N_2O$	CH_3NHCH_2NO(B)	424
C_2H_6OSi	$(CH_3)_2SiO$	416
C_2H_6OSi	$CH_2{=}Si(OH)CH_3$	417
C_2H_6OSi	CH_3OSiCH_3	417
C_2H_6OSi	$CH_3OSiH{=}CH_2$	417
$C_2H_6O_2Si$	$(CH_3O)_2Si$	421
$C_2H_6O_2Si$	$CH_3SiOOCH_3$	421
$C_2H_6O_2Si$	$CH_3SiHOHCHO$	A365
$C_2H_6O_3$	$HOCH_2CH_2OOH$	424
$C_2H_6O_4$	$CH_3O_4CH_3$	424
C_2H_6Si	$(CH_3)_2Si$	399
C_2H_6Si	$CH_3SiH{=}CH_2$	399
C_2H_6Sn	$(CH_3)_2Sn$	400
$C_2H_6Zn^+$	$(CH_3)_2Zn^+$	A357
$C_2H_7^+$	$C_2H_7^+$	383
$C_2H_7^+$	*br*-$C_2H_7^+$	383
C_2H_7BO	$H_2B{=}OC_2H_5$	408
C_2H_7BS	$H_2BSC_2H_5$	A361
C_2H_8BN	$H_2B{=}N(CH_3)_2$	399

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
C_2H_8OSi	$(CH_3)_2SiHOH$	417	C_3HFe	FeC=C=CH	A286
$C_2I_2^+$	$C_2I_2^+$	192	C_3HFe	FeCCCH	A286
C_2N^+	CNC^+	67	C_3HFe^-	$FeC=C=CH^-$	A286
C_2N	CCN	68,A173	C_3HFe^-	$FeCCCH^-$	A286
C_2N	CNC	69	C_3HN^+	$HCCCN^+$	266
$C_2N_2^+$	$NCCN^+$	183	C_3HN^+	$HCCNC^+$	267
$C_2N_2^+$	$CNCN^+$	184	C_3HN	HNCCC	267
C_2N_2	CNCN	185,A248	C_3HN	HCCNC	267
C_2N_2	CNNC	185	C_3HF_3S	CF_3H(*cyc*-CCS)	381
$C_2N_2O^+$	$NCCNO^+$	A295	C_3HO	HCCCO	268,A286
$C_2N_2O^+$	$NCNCO^+$	279	C_3HS	HCCCS	A287
C_2N_2O	NCCNO	283,A297	$C_3H_2^+$	*cyc*-$C_3H_2^+$	248
C_2N_2O	NCNCO	283	C_3H_2	HCCCH	249,A278
$C_2N_2O_2^+$	$ONCCNO^+$	A320	C_3H_2	*cyc*-C_3H_2	248
$C_2N_2O_2$	ONCCNO	A321	C_3H_2	$H_2C=C=C$:	248,A277
$C_2N_2S^+$	$S(CN)_2^+$	280	C_3H_2	HCCH=C:	249
$C_2N_2S^+$	$NCNCS^+$	280	$C_3H_2^-$	$H_2C=C=C:^-$	A280
C_2N_2S	NCNCS	284	$C_3H_2N^+$	$HCCCNH^+$	326,A315
$C_2N_2S_2^+$	$(SCN)_2^+$	346	$C_3H_2O^+$	$H_2C=C=C=O^+$	327
$C_2N_2Se^+$	$Se(CN)_2^+$	281	C_3H_2O	HC≡CC-OH	328
C_2O	CCO	69,A179	C_3H_2O	$H_2C=C=C=O$	328
C_2O^-	CCO^-	76,A183	$C_3H_2O_2$	*t*-HCCCHOO	A327
$C_2O_2^+$	*t*-$OCCO^+$	186	$C_3H_2O_2$	*c*-HCCCHOO	A327
$C_2O_2^-$	*t*-$OCCO^-$	190	$C_3H_2O_2$	HCC(*cyc*-CHOO)	A328
C_2O_2Si	$Si(CO)_2$	283	$C_3H_2O_3$	*cyc*-(HOC=COHC)=O	A340
C_2S	CCS	70	C_3H_2S	$H_2C=C=C=S$	329
C_2S_2	SCCS	188	C_3H_2Se	$H_2C=C=C=Se$	329
C_2S_3	$S(CS)_2$	284	C_3H_2Se	HCC-CHSe	329
C_2Si	SiCC	66,A170	$C_3H_3^+$	CH_2CCH^+	312
C_2Si_2	Si_2C_2	181,A245	C_3H_3	CH_2CCH	312,A311
C_2Si_3	Si_3C_2	A293	$C_3H_3^-$	CH_2CCH^-	A311
C_2Y	YCC	A164	$C_3H_3^-$	CH_3CC^-	A312
C_3	C_3	65,A168	$C_3H_3Br^+$	CH_3CCBr^+	365
C_3^-	C_3^-	68,A173	$C_3H_3Cl^+$	CH_3CCCl^+	365
C_3BrN^+	$BrCCCN^+$	282	$C_3H_3N^+$	$C_2H_3CN^+$	A325
C_3ClN^+	$ClCCCN^+$	281	C_3H_3N	$H_2C=$(*cyc*-CN=CH)	A326
C_3Cl_2	*cyc*-C_3Cl_2	A299	$C_3H_4^+$	$H_2CCCH_2^+$	362,A323
C_3Cl_2	ClCCCCl	A299	C_3H_4Li	CH_3CCHLi	377
C_3Cl_2	$Cl_2C=C=C$:	A299	$C_3H_4NO_2$	$CH_3C(=NO)CHO$	A367
C_3FN^+	$FCCCN^+$	281	C_3H_4O	*cyc*-$(H_2COC)=CH_2$	379
C_3F_2	*cyc*-C_3F_2	A299	C_3H_4O	CH_3CCOH	A338
C_3F_2	FCCCF	A299	C_3H_4S	HCH_3(*cyc*-CCS)	379
C_3F_2	$F_2C=C=C$:	A299	$C_3H_5^+$	$CH_2CHCH_2^+$	372
C_3F_2O	$F_2C=C=C=O$	347	$C_3H_5^+$	*cyc*-$C_3H_5^+$	372
C_3F_2O	*cyc*-(CF=CFC)=O	347	C_3H_5	CH_2CHCH_2	372,A334
$C_3F_6^+$	$C_3F_6^+$	405	$C_3H_5^-$	$CH_2CHCH_2^-$	A335
C_3F_7	*n*-C_3F_7	405	C_3H_5N	$H_2C=CH-CH=NH$	408
C_3F_7	*i*-C_3F_7	406	C_3H_5N	$H_2C=C=NCH_3$	408
C_3Fe	FeCCC	A242	C_3H_5N	$H_2C=CHN=CH_2$	409
C_3Fe^-	$FeCCC^-$	A242	C_3H_5N	*cyc*-C_3H_5N	409
C_3H	HC_3	156,A233	C_3H_6O	*t*-CH_3C-OCH_3	415
C_3H	*cyc*-HC_3	156,A233	C_3H_6O	*c*-CH_3C-OCH_3	415
C_3HCl	*cyc*-C_3HCl	A288	C_3H_6S	$(CH_3)_2CS$	415
C_3HCl	HCCCCl	A288	$C_3H_7^+$	1-$C_3H_7^+$	383
C_3HCl	HClC=C=C:	A288	$C_3H_7^+$	2-$C_3H_7^+$	383

Formula	*Structure/Name*	*References*
C_3H_7	$CH_3CH_2CH_2$	383
C_3H_7	$(CH_3)_2CH$	383
C_3H_7N	$C_2H_3NHCH_3$	409
C_3H_7O	*n*-C_3H_7O	416
C_3H_7O	$(CH_3)_2CHO$	416
$C_3H_7O_2$	$(CH_3)_2CHO_2$	420
$C_3H_8O_2Si$	$(CH_3)_2SiOHCHO$	A365
$C_3H_8Si^+$	$(CH_3)_2Si\text{-}CH_2^+$	400
C_3H_8Si	$(CH_3)_2Si{=}CH_2$	401
C_3H_9Al	$(CH_3)_3Al$	400
C_3H_9NSi	$(CH_3)_3SiN$	410
C_3IN^+	$ICCCN^+$	282
C_3N	CCCN	183,A247
C_3N_2	$C(CN)_2$	278,A295
$C_3N_2O^+$	$CO(CN)_2^+$	343
$C_3N_2O_2$	$(CN)_2COO$	A330
C_3O	CCCO	186
$C_3O_2^+$	$C_3O_2^+$	279
C_3S	CCCS	186,A249
C_3Si_2	SiCCCSi	278,A293
C_4	C_4	181,A245
C_4^-	C_4^-	183,A246
$C_4Br_2^+$	$Br(CC)_2Br^+$	345
$C_4Cl_2^+$	$Cl(CC)_2Cl^+$	345
$C_4F_2^+$	$F(CC)_2F^+$	344
C_4F_6O	CF_3CCOCF_3	418
C_4F_6O	$(CF_3)_2$(*cyc*-CCO)	418
C_4Fe^-	FeC_4^-	A292
C_4H	C_4H	266,A286
C_4HBr^+	$H(CC)_2Br^+$	339
C_4HCl^+	$H(CC)_2Cl^+$	339
C_4HF^+	$H(CC)_2F^+$	339
C_4HFe^-	$FeCCCCH^-$	A316
C_4HI^+	$H(CC)_2I^+$	340
C_4HO	HCCCCO	A316
C_4HS	HCCCCS	A317
$C_4H_2^+$	$C_4H_2^+$	325
C_4H_2	H_2CCCC:	326,A315
$C_4H_4^+$	*cyc*-$C_4H_4^+$	377,A337
$C_4H_4^+$	$H_2C{=}$(*cyc*-C_3H_2)$^+$	377
C_4H_4	*cyc*-C_4H_4	378,A338
C_4H_4	$H_2C{=}$(*cyc*-C_3H_2)	377
C_4H_4	$C_2H_3CH{=}C$:	A338
$C_4H_4^-$	$C_2H_3CH{=}C{:}^-$	A338
C_4H_4CaN	$Ca(C_4H_4N)$	410
C_4H_4CdN	$Cd(C_4H_4N)$	412
C_4H_4MgN	$Mg(C_4H_4N)$	410
C_4H_4NSr	$Sr(C_4H_4N)$	411
C_4H_4NZn	$Zn(C_4H_4N)$	411
C_4H_5N	$H_2C{=}$(*cyc*-$CN{=}CCH_3$)	A361
$C_4H_6^+$	*t*-$H_2C{=}CH\text{-}CH{=}CH_2^+$	A342
C_4H_6	$C(CH_2)_3$	A343
$C_4H_6^-$	$C(CH_2)_3^-$	A343
C_4H_6Ge	*cyc*-$C_4H_4GeH_2$	A359
C_4H_6Ge	*cyc*-C_4H_6Ge:	A359
C_4H_6Ge	*cyc*-C_4H_5GeH(1,3)	A360
C_4H_6Ge	*cyc*-C_4H_5GeH(1,4)	A360
C_4H_6S	$(CH_3)_2$(*cyc*-CCS)	419
C_4H_6Si	*cyc*-$C_4H_4SiH_2$	A358
C_4H_6Si	*cyc*-C_4H_6Si:	A358
C_4H_6Si	*cyc*-C_4H_5SiH(1,3)	A358
C_4H_6Si	*cyc*-C_4H_5SiH(1,4)	A359
$C_4H_7^+$	$H_2CC(CH_3)CH_2^+$	A343
$C_4H_7^+$	*cyc*-$C_4H_7^+$	A343
C_4H_7	$CH_3CHCH{=}CH_2$	A343
C_4H_7	$H_2CC(CH_3)CH_2$	A343
$C_4H_7^-$	$H_2CC(CH_3)CH_2^-$	A344
C_4H_7N	$(CH_3)_2C{=}C{=}NH$	412
C_4H_7N	$CH_3CC\text{-}NHCH_3$	412
C_4H_8Si	*cyc*-$C_2H_2Si(CH_3)_2$	A358
$C_4H_9^+$	*t*-$C_4H_9^+$	384
C_4H_9	*n*-C_4H_9	384,A344
C_4H_9	*i*-C_4H_9	384
C_4H_9	*t*-C_4H_9	384
$C_4H_9O_2$	*t*-$C_4H_9O_2$	421
$C_4H_{10}Si$	$(CH_3)_2Si{=}CHCH_3$	401
$C_4I_2^+$	$I(CC)_2I^+$	345
$C_4N_2^+$	$NCC{\equiv}CCN^+$	343,A319
C_4N_2	NCCCNC	343,A320
C_4N_2	CNCCNC	343
C_4N_2O	$(CN)_2CCO$	A330
C_4O	C_4O	278,A294
C_4OS	C_4OS	344
C_4O_2	C_4O_2	344
C_4S	C_4S	278,A294
C_4S_2	C_4S_2	344
C_4Si	C_4Si	277,A293
C_4Si_2	SiC_4Si	A318
C_5^+	*cyc*-C_5^+	277
C_5	C_5	277,A292
C_5^-	C_5^-	278,A293
C_5Br_4	*cyc*-C_5Br_4	A357
$C_5Br_4O_2$	*cyc*-C_5Br_4O-1-O	A366
C_5Cl_4	*cyc*-C_5Cl_4	A357
$C_5Cl_4O_2$	*cyc*-C_5Cl_4O-1-O	A365
$C_5F_4^+$	$CF_3(CC)_2F^+$	407
C_5F_6O	$(CF_3)_2$(*cyc*-CCO)	418
C_5F_8O	CF_3(*cyc*-CCO)C_2F_5	419
C_5H	C_5H	A316
C_5HN^+	$H(CC)_2CN^+$	369,A328
$C_5H_2^+$	$C_5H_2^+$	A327
C_5H_2	HC_5H	A327
$C_5H_3Br^+$	$CH_3(CC)_2Br^+$	406
$C_5H_3Cl^+$	$CH_3(CC)_2Cl^+$	406
$C_5H_3F_2N^+$	*cyc*-$C_5H_3F_2N^+$	412
C_5H_3N	*cyc*-C_5H_3N	412
$C_5H_4^+$	$CH_3(CC)_2H^+$	385
C_5H_4	*cyc*-C_5H_4	385
C_5H_4Cl	*cyc*-C_5H_4Cl	407
C_5H_4F	*cyc*-C_5H_4F	407

Formula	*Structure/Name*	*References*
C_5H_4O	(cyc-C_5H_4)O	419
$C_5H_4O_2$	cyc-C_5H_4O-1-O	422,A365
C_5H_5	cyc-C_5H_5	385,A344
C_5H_5Ca	CaC_5H_5	402,A360
C_5H_5Cd	CdC_5H_5	403
C_5H_5Mg	MgC_5H_5	401
C_5H_5Sr	SrC_5H_5	402
C_5H_5Zn	ZnC_5H_5	402
$C_5H_6^+$	cyc-$C_5H_6^+$	A345
C_5H_6Se	$(CH_2)_3C{=}C{=}Se$	419
$C_5H_6Si^+$	$C_5SiH_6^+$	404
C_5H_6Si	C_5SiH_6	404
C_5H_6Si	C_5SiH_6 (Dewar)	405
C_5H_{11}	n-C_5H_{11}	386,A346
C_5H_{11}	$(CH_3)_3CCH_2$	386
C_5N	C_5N	A319
C_5N_2	C_5N_2	A330
C_5O	C_5O	A320
C_5OS	C_5OS	370
C_5O_2	C_5O_2	370
C_5S	C_5S	343
C_5S_2	C_5S_2	370
C_6	C_6	342,A317
C_6^-	C_6^-	342,A318
$C_6Br_3F_3^+$	sym-$C_6F_3Br_3^+$	439
$C_6ClF_5^+$	$C_6F_5Cl^+$	439
$C_6Cl_3F_3^+$	sym-$C_6F_3Cl_3^+$	439
C_6F_5N	C_6F_5N:	442,A371
C_6F_5N	$bicyc$-C_6F_5N	A361
$C_6F_6^+$	$CF_3(CC)_2CF_3^+$	307
$C_6F_6^+$	$C_6F_6^+$	438
C_6H	C_6H	369,A328
$C_6HF_5^+$	$C_6HF_5^+$	437
$C_6HF_5O^+$	$C_6F_5OH^+$	445
C_6HN^+	HC_5CN^+	A340
$C_6H_2^+$	$C_6H_2^+$	380,A339
C_6H_2	HC_6H	A340
$C_6H_2F_4^+$	1,2,3,4-$C_6H_2F_4^+$	435
$C_6H_2F_4^+$	1,2,3,5-$C_6H_2F_4^+$	436
$C_6H_2F_4^+$	1,2,4,5-$C_6H_2F_4^+$	437
$C_6H_2F_4O^+$	2,3,5,6-$F_4C_6HOH^+$	445
$C_6H_3ClF_2^+$	1,3,5-$C_6H_3ClF_2^+$	434
$C_6H_3Cl_2F^+$	1,3,5-$C_6H_3Cl_2F^+$	434
$C_6H_3Cl_3^+$	1,3,5-$C_6H_3Cl_3^+$	434
$C_6H_3F_2N$	2,6-$C_6H_3F_2N$:	A371
$C_6H_3F_2N$	$bicyc$-$C_6H_3F_2N$	A361
$C_6H_3F_3^+$	1,2,3-$C_6H_3F_3^+$	432
$C_6H_3F_3^+$	1,2,4-$C_6H_3F_3^+$	432
$C_6H_3F_3^+$	1,3,5-$C_6H_3F_3^+$	433
$C_6H_3F_3O^+$	2,3,4-$F_3C_6H_2OH^+$	445
$C_6H_3F_3O^+$	2,4,5-$F_3C_6H_2OH^+$	445
$C_6H_3N^+$	$CH_3(CC)_2CN^+$	413
$C_6H_4^+$	$C_6H_4^+$	386
C_6H_4	o-C_6H_4	386
C_6H_4	m-C_6H_4	A346
$C_6H_4^-$	$C_6H_4^-$	387
C_6H_4Br	o-C_6H_4Br	428
C_6H_4Br	m-C_6H_4Br	428
C_6H_4Br	p-C_6H_4Br	428
C_6H_4Cl	o-C_6H_4Cl	427
C_6H_4Cl	m-C_6H_4Cl	427
C_6H_4Cl	p-C_6H_4Cl	427
$C_6H_4Cl_2^+$	1,3-$C_6H_4Cl_2^+$	431
$C_6H_4Cl_2^+$	1,4-$C_6H_4Cl_2^+$	431
C_6H_4F	o-C_6H_4F	427
C_6H_4F	m-C_6H_4F	427
C_6H_4F	p-C_6H_4F	427
$C_6H_4F_2^+$	1,2-$C_6H_4F_2^+$	429
$C_6H_4F_2^+$	1,3-$C_6H_4F_2^+$	429
$C_6H_4F_2^+$	1,4-$C_6H_4F_2^+$	430,A369
$C_6H_4F_2O^+$	2,5-$F_2C_6H_3OH^+$	444
$C_6H_4F_2O^+$	3,5-$F_2C_6H_3OH^+$	444
C_6H_4I	o-C_6H_4I	428
C_6H_4N	(cyc-C_5H_4)CN	413
$C_6H_4N_2O_2$	1,2-$C_6H_4(NO)_2$	446
C_6H_4O	2,4-C_6H_3OH	426
$C_6H_4S_2$	p-$C_6H_4S_2$	422
$C_6H_5^+$	$C_6H_5^+$	387
C_6H_5	C_6H_5	388,A346
$C_6H_5^-$	$C_6H_5^-$	388
$C_6H_5Cl^+$	$C_6H_5Cl^+$	428,A368
$C_6H_5F^+$	$C_6H_5F^+$	428
C_6H_5N	C_6H_5N	442,A370
C_6H_5N	3-CH(cyc-C_5H_4N)	413
C_6H_5N	cyc-C_6H_5N	413
$C_6H_5N^-$	$C_6H_5N^-$	442,A371
C_6H_5O	C_6H_5O	443,A372
$C_6H_5O^-$	$C_6H_5O^-$	446
C_6H_5S	C_6H_5S	443
$C_6H_6^+$	$C_6H_6^+$	388,A347
$C_6H_6^+$	$CH_3(CC)_2CH_3^+$	390
C_6H_6F	C_6H_6F	440
C_6H_6Li	LiC_6H_6	440
C_6H_6N	C_6H_5NH	443
$C_6H_6O^+$	$C_6H_5OH^+$	444,A373
C_6H_7	CH_3(cyc-C_5H_4)	391
C_6H_7Ca	$CaC_5H_4CH_3$	403
C_6H_7Cd	$CdC_5H_4CH_3$	404
C_6H_7Mg	$MgC_5H_4CH_3$	403
C_6H_7Zn	$ZnC_5H_4CH_3$	404
$C_6H_7N^+$	$C_6H_5NH_2^+$	443,A372
$C_6H_8^+$	t-CH2$(CH)_4CH_2^+$	391
C_6H_8Si	1-$CH_3C_5SiH_5$	405
C_6H_{10}	$(CH_3)_3CCH{=}C$:	A348
$C_6H_{10}^-$	$(CH_3)_3CCH{=}C^-$	A348
$C_6N_2^+$	$NC(CC)_2CN^+$	414,A341
C_6O	C_6O	370,A330
$C_6O_2S_4$	$C_6S_4O_2$	426
C_6S_6	C_6S_6 (A)	426
C_6S_6	C_6S_6 (B)	427

Formula	*Structure/Name*	*References*
C_7	C_7	369,A329
C_7^-	C_7^-	370,A329
$C_7F_8^+$	$C_6F_5CF_3^+$	442
C_7H	C_7H	A340
C_7HN^+	$H(C{\equiv}C)_3CN^+$	A362
$C_7H_2^+$	$C_7H_2^+$	A349
C_7H_2	HC_7H	A349
$C_7H_3F_5^+$	$C_6F_5CH_3^+$	441
C_7H_4O	$(cyc\text{-}C_5H_4)CCO$	419
C_7H_4O	$cyc\text{-}C_6H_4C{=}O$	419
C_7H_5Cl	C_6H_5CCl	441
C_7H_5Cl	$(2\text{-}ClC_6H_4)CH$	441
C_7H_5Cl	$cyc\text{-}1\text{-}C_7H_5Cl$	408
C_7H_5ClO	C_6H_5OCCl	446
C_7H_5F	C_6H_5CF	440
C_7H_5F	$cyc\text{-}1\text{-}C_7H_5F$	407
$C_7H_5F_3^+$	$sym\text{-}C_6H_2F_3CH_3^+$	441
$C_7H_5N^+$	$C_2H_5(CC)_2CN^+$	414
C_7H_6	C_6H_5CH	391
C_7H_6	$cyc\text{-}C_7H_6$	391
C_7H_6	$cyc\text{-}C_7H_6$:	392
C_7H_6Cl	$(4\text{-}ClC_6H_4)CH_2$	A370
C_7H_6F	$(2\text{-}FC_6H_4)CH_2$	A369
C_7H_6F	$(3\text{-}FC_6H_4)CH_2$	A369
C_7H_6F	$(4\text{-}FC_6H_4)CH_2$	A370
$C_7H_7^+$	$cyc\text{-}C_7H_7^+$	392
$C_7H_7^+$	$C_6H_5CH_2^+$	392,A349
C_7H_7	$C_6H_5CH_2$	392,A349
C_7H_7	$cyc\text{-}C_7H_7$	394
$C_7H_7^-$	$C_6H_5CH_2^-$	394
$C_7H_8^+$	$C_6H_5CH_3^+$	394
$C_7N_2^+$	NCC_5CN^+	A362
C_7O	C_7O	A341
C_7O_2	C_7O_2	422
C_8	C_8	381,A340
C_8^-	C_8^-	381,A340
C_8H	C_8H	A351
C_8HN^+	HC_7CN^+	A362
$C_8H_2^+$	$C_8H_2^+$	A351
C_8H_6N	$(4\text{-}NC\text{-}C_6H_4)CH_2$	A370
C_8H_8	$o\text{-}(CH_2)_2C_6H_4$	396
C_8H_8	$m\text{-}(CH_2)_2C_6H_4$	A351
C_8H_8	$p\text{-}(CH_2)_2C_6H_4$	A352
C_8H_8	$C_6H_5CCH_3$	396
C_8H_8	$m\text{-}CH_3C_6H_4CH$:	395
C_8H_8	$o\text{-}CH_3C_6H_4CH$:	395
C_8H_8	$p\text{-}CH_3C_6H_4CH$:	395
C_8H_8	$1\text{-}CH_3(cyc\text{-}C_7H_5)$	396
C_8H_8	$4\text{-}CH_3(cyc\text{-}C_7H_5)$	397
C_8H_8	$5\text{-}CH_3(cyc\text{-}C_7H_5)$	397
$C_8H_8^-$	$m\text{-}(CH_2)_2C_6H_4$	A352
$C_8N_2^+$	$NC(C{\equiv}C)_3CN^+$	A362
C_8O	C_8O	A364
C_9	C_9	398,A352
C_9^-	C_9^-	398,A352
C_9H	C_9H	A353
C_9HN^+	$H(C{\equiv}C)_4CN^+$	A362
$C_9H_2^+$	$C_9H_2^+$	A353
C_9H_2	HC_9H	A353
$C_9N_2^+$	NCC_7CN^+	A363
C_9O	C_9O	A364
C_{10}	C_{10}	A353
C_{10}^-	C_{10}^-	A354
$C_{10}H$	$C_{10}H$	A354
$C_{10}HN^+$	HC_9CN^+	A363
$C_{10}H_2^+$	$C_{10}H_2^+$	A354
$C_{10}N_2^+$	$NC(C{\equiv}C)_4CN^+$	A363
C_{11}	C_{11}	398,A354
C_{11}^-	C_{11}^-	398
$C_{11}H$	$C_{11}H$	A354
$C_{11}HN^+$	$H(C{\equiv}C)_5CN^+$	A363
$C_{11}H_2^+$	$C_{11}H_2^+$	A355
$C_{11}H_2$	$HC_{11}H$	A355
$C_{11}N_2^+$	NCC_9CN^+	A363
C_{12}	C_{12}	A355
C_{12}^-	C_{12}^-	A355
$C_{12}H$	$C_{12}H$	A355
$C_{12}HN^+$	$HC_{11}CN^+$	A363
$C_{12}H_2^+$	$C_{12}H_2^+$	A355
$C_{12}N_2^+$	$NC(C{\equiv}C)_5CN^+$	A363
C_{13}	C_{13}	A356
$C_{13}HN^+$	$H(C{\equiv}C)_6CN^+$	A363
$C_{13}H_2^+$	$C_{13}H_2^+$	A356
$C_{13}H_2$	$HC_{13}H$	A356
C_{14}^-	C_{14}^-	A356
$C_{14}H$	$C_{14}H$	A356
$C_{14}H_2^+$	$C_{14}H_2^+$	A356
C_{15}	C_{15}	A357
C_{16}^-	C_{16}^-	A357
CaHO	CaOH	27,A139
CaHS	CaSH	28,A140
CaH_2	CaH_2	14
CaH_2N	$CaNH_2$	132,A220
CaH_2O	HCaOH	134
CaH_2O_2	$Ca(OH)_2$	251
CaN_3	CaN_3	182
CaO_2	OCaO	A174
CaO_2	$cyc\text{-}CaO_2$	A174
CaO_4	O_2CaO_2	A298
Ca_2H_2	Ca_2H_2	130
Ca_2H_2O	HCaOCaH	246
Ca_2H_2O	HCa_2OH	247
Ca_2H_4	$HCaH_2CaH$	305
Ca_2O_2	$cyc\text{-}(CaO)_2$	A243
Ca_2O_2	CaOCaO	A243
Ca_3H_2	Ca_3H_2	244
CdH_2	CdH_2	A127
CdH_2O	HCdOH	A222
CdO_2	OCdO	A179
Cd_2H	CdCdH	A136

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
Cd_2O_2	CdOCdO	A244	ClO_2	OClO	113,A205
CeO_2	OCeO	A179	ClO_2	ClOO	110,A204
$ClFH^-$	$FHCl^-$	53	ClO_2^-	$OClO^-$	115
ClFN	NFCl	108,A201	ClO_2P	PO_2Cl	213
ClFO	FClO	116	ClO_3	ClO_3	A262
$ClFO_2S^+$	$FClSO_2^+$	301	ClO_4	$OClO_3$	A306
$ClFO_3^+$	$FClO_3^+$	300	ClPS	ClPS	104
ClFS	FSCl	115,A208	ClS_2	SSCl	111,A205
ClFXe	XeClF	121	$ClXe_2$	Xe_2Cl	122
ClF_2	ClF_2	116	Cl_2F	ClClF	116
ClF_2^-	$FClF^-$	117	Cl_2F^-	$ClFCl^-$	118
ClF_2^-	$FFCl^-$	118	Cl_2F^-	$FClCl^-$	118
ClF_2P^+	PF_2Cl^+	220	Cl_2F_2	Cl_2F_2	227
ClF_3^+	ClF_3^+	226	Cl_2F_2S	SCl_2F_2	304
ClF_3P^-	$PClF_3^-$	304	$Cl_2F_2Si^+$	$SiF_2Cl_2^+$	295
ClF_3S	$SClF_3$	304	$Cl_2F_3Si^-$	$SiF_3Cl_2^-$	357
ClF_3Si^+	SiF_3Cl^+	295	Cl_2Ga	$GaCl_2$	90
ClF_4Si^-	SiF_4Cl^-	357	Cl_2GaH	$HGaCl_2$	169
ClFeH	HFeCl	35	$Cl_2Ga_2H_4$	$H_2GaCl_2GaH_2$	A339
$ClGaH_2$	GaH_2Cl	143	Cl_2Ge^+	$GeCl_2^+$	92
ClGeH	HGeCl	45	Cl_2Ge	$GeCl_2$	102,A198
$ClGeH_2$	H_2GeCl	150	$Cl_2GeH_2^+$	$GeH_2Cl_2^+$	263
$ClGeH_3^+$	GeH_3Cl^+	241	Cl_2GeS	Cl_2GeS	211
$ClHI^-$	$ClHI^-$	55	Cl_2H^-	$ClHCl^-$	54,A157
ClHKr	HKrCl	A158	Cl_2HN^+	$HNCl_2^+$	179
$ClHO^+$	$HOCl^+$	51	$Cl_2H_2Si^+$	$SiH_2Cl_2^+$	262
ClHO	HOCl	52,A155	Cl_2Mn^+	$MnCl_2^+$	73
$ClHO_2$	HOClO	A241	Cl_2N	NCl_2	108
$ClHO_2$	$HClO_2$	A241	Cl_2Ni^+	$NiCl_2^+$	73
ClHSSi	HClSi=S	172	Cl_2O^+	Cl_2O^+	111
ClHSi	HSiCl	44,A150	Cl_2O	ClClO	116,A208
ClHXe	HXeCl	A158	Cl_2OP	$OPCl_2$	220
ClH_2^+	H_2Cl^+	26	Cl_2OS^+	Cl_2SO^+	223
ClH_2N^+	H_2NCl^+	152	Cl_2OSi	Cl_2SiO	211
ClH_2P	H_2PCl	A229	Cl_2O_2	ClOOCl	225,A263
ClH_3Si^+	SiH_3Cl^+	240	Cl_2O_2	$ClClO_2$	225,A263
ClIO	OICl	116	Cl_2O_2	ClOClO	A264
$ClIO_2$	$ClIO_2$	226	$Cl_2O_2S^+$	$Cl_2SO_2^+$	301
$ClIO_2$	$IClO_2$	A264	Cl_2O_2Si	*cyc*-Cl_2SiO_2	287
$ClIO_2$	IOClO	A264	Cl_2O_3	Cl_2O_3	302,A307
ClKrNe	NeKrCl	122	Cl_2O_4	$ClOClO_3$	355,A322
ClKrXe	KrXeCl	122	Cl_2O_6	$O_3ClOClO_2$	382
$ClKr_2$	Kr_2Cl	122	Cl_2P	PCl_2	108,A203
$ClNO^+$	$ClNO^+$	93	Cl_2S^+	SCl_2^+	112
$ClNO_2^+$	$ClNO_2^+$	208	Cl_2SSi	Cl_2SiS	211
$ClNO_2$	$ClNO_2$	212,A259	$Cl_2S_2^+$	$S_2Cl_2^+$	224
$ClNO_2$	*c*-ClONO	213,A259	Cl_2S_2	$SSCl_2$	226
$ClNO_2$	*t*-ClONO	213,A259	Cl_2Se^+	$SeCl_2^+$	112
$ClNO_3^+$	$ClONO_2^+$	A301	$Cl_2Se_2^+$	$Se_2Cl_2^+$	224
$ClNO_3$	$ClONO_2$	288,A302	Cl_2Si^+	$SiCl_2^+$	92
$ClNO_5$	O_2ClONO_2	371	Cl_2Si	$SiCl_2$	101,A197
$ClNS^+$	$NSCl^+$	95	Cl_2Xe	$XeCl_2$	121
ClN_3^+	ClN_3^+	196	Cl_2Zn^+	$ZnCl_2^+$	72
ClOP	ClPO	103	Cl_3^-	Cl_3^-	119
ClO_2^+	$OClO^+$	106	Cl_3FS	SCl_3F	304

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
Cl_3FSi^+	$SiFCl_3^+$	296	FFeH	HFeF	35
$Cl_3F_2Si^-$	$SiF_2Cl_3^-$	357	FFe_2H	HFe_2F	155
Cl_3Ge	$GeCl_3$	219	FGaO	OGaF	85
Cl_3HOSi	$SiCl_3OH$	342	$FGeH_3^+$	GeH_3F^+	241
Cl_3HSi^+	$HSiCl_3^+$	276	FHI^-	FHI^-	54
Cl_3N^+	NCl_3^+	219	FHN	HNF	48,A152
Cl_3NO_3Si	$SiCl_3ONO_2$	382	FHO^+	HOF^+	51
Cl_3NO_4Si	$SiCl_3OONO_2$	426	FHO	HOF	51
Cl_3OP^+	Cl_3PO^+	298	FHSi	HSiF	43,A150
Cl_3O_2P	$OPCl_2OCl$	355	FH_2^+	H_2F^+	26
Cl_3P^+	PCl_3^+	220	FH_2N^+	NH_2F^+	151
Cl_3PS^+	Cl_3PS^+	299	FH_2N	NH_2F	153
Cl_3Sb^+	$SbCl_3^+$	222	FH_2P	H_2PF	153,A228
Cl_3Si^+	$SiCl_3^+$	211	FH_3N_2	NH_2NHF	324
Cl_3Si	$SiCl_3$	218	FH_3Si^+	SiH_3F^+	240
Cl_4FSi^-	$SiFCl_4^-$	358	FI_2	IIF	117
Cl_4Ge^+	$GeCl_4^+$	297,A306	FKrXe	KrXeF	121,A211
Cl_4Si^+	$SiCl_4^+$	296,A306	FKr_2	Kr_2F	121,A210
Cl_4SiO	$SiCl_3OCl$	356	FNO^+	FNO^+	93
Cl_5P^+	PCl_5^+	357	FNO	FON	104
CoH_2	CoH_2	15,A127	FNO_2^+	FNO_2^+	208
CoH_2^-	CoH_2^-	17	FNO_2	FONO	212
CoH_2O	HCoOH	136	FNO_3^+	$FONO_2^+$	A301
CrH_2	CrH_2	15	FNO_3	$FONO_2$	A302
CrH_2O	HCrOH	136	FNS^+	NSF^+	94
CrH_3	CrH_3	123	FN_2^+	FNN^+	87
CrH_3O_2	$HCr(OH)_2$	316	FN_3^+	FN_3^+	196
CrO_2	OCrO	A175	FN_3	FN_3	199
CrO_2^-	$OCrO^-$	A182	FNeXe	NeXeF	121
Cr_2H	CrCrH	26	FNe_2	Ne_2F	121
Cr_2H^-	$CrCrH^-$	26	FOP	FPO	103
CuHO	CuOH	31	FOS	FSO	111
CuH_2N	$CuNH_2$	133	FO_2	FOO	109
CuH_2O	HCuOH	137	FO_2S^-	FSO_2^-	225
CuH_3N	$HCuNH_2$	232	FO_3S^+	FSO_3^+	289
CuO_2^+	$CuOO^+$	A172	FO_3S	FSO_3	300
CuO_2	OCuO	A178	FPS	FPS	104
CuO_2	CuOO	A178	FS_2	SSF	A205
CuO_2^-	$OCuO^-$	A182	FXe_2	Xe_2F	122,A211
CuO_2^-	$CuOO^-$	A182	F_2Ga	GaF_2	A193
CuO_3	CuO_3	A251	F_2Ge^+	GeF_2^+	92
CuO_3^-	CuO_3^-	A252	F_2Ge	GeF_2	101,A198
CuO_4	O_2CuO_2	A299	$F_2GeH_2^+$	$GeH_2F_2^+$	263
Cu_2H_2	Cu_2H_2	131	F_2GeO	F_2GeO	212
Cu_2O	CuOCu	A163	F_2H^-	FHF^-	53,A156
Cu_2O^-	$CuOCu^-$	A166	F_2HN^+	HNF_2^+	178
Cu_2O_2	Cu_2O_2	A244	F_2HP^+	HPF_2^+	179
$Cu_2O_2^-$	$Cu_2O_2^-$	A246	$F_2H_2Si^+$	$SiH_2F_2^+$	262
Cu_2O_3	Cu_2O_3	A294	F_2H_3P	PH_3F_2	324,A315
$Cu_2O_3^-$	$Cu_2O_3^-$	A295	F_2I^-	FIF^-	118
Cu_2O_4	Cu_2O_4	A320	F_2I^-	FFI^-	118
$Cu_2O_4^-$	$Cu_2O_4^-$	A320	F_2I_2	I_2F_2	227
Cu_3	Cu_3	59,A161	F_2Kr^+	KrF_2^+	117
Cu_3H_2	Cu_3H_2	244	F_2Kr	KrF_2	120,A209
DOSc	ScOD	30	F_2Mg^+	MgF_2^+	A181

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
F_2Mg	MgF_2	84	F_6S^+	SF_6^+	A331
F_2N^+	NF_2^+	103,A199	FeHI	HFeI	35
F_2N	NF_2	107,A201	FeH_2	FeH_2	15,A126
F_2N^-	NF_2^-	A207	FeH_2^-	FeH_2^-	17
$F_2N_2^+$	t-$N_2F_2^+$	207	FeH_2O	HFeOH	136
F_2O^+	OF_2^+	111	FeH_2O_2	$Fe(OH)_2$	251
F_2OS^+	F_2SO^+	223	FeH_3	FeH_3	A211
F_2OSi	F_2SiO	211	FeH_3N	$HFeNH_2$	231
F_2O_2	FOOF	225	FeNO	NFeO	A171
$F_2O_2S^+$	$F_2SO_2^+$	300	FeNO	FeNO	A171
F_2O_2Si	cyc-F_2SiO_2	287	$FeNO_2$	$NFeO_2$	A249
F_2O_2Xe	XeO_2F_2	304	FeN_2	NFeN	A166
F_2O_3Xe	XeO_3F_2	358	FeN_2	FeNN	A167
F_2P^+	PF_2^+	104	FeN_2O	N_2FeO	A248
F_2P	PF_2	108,A202	FeN_2O_2	N_2FeO_2	A296
F_2S^+	SF_2^+	112	FeO_2	OFeO	A176
F_2S	SF_2	114,A207	FeO_2	FeOO	A176
$F_2S_2^+$	F_2SS^+	223	FeO_2	cyc-FeO_2	A177
$F_2S_2^+$	$FSSF^+$	224	FeO_2^-	$OFeO^-$	A182
F_2Se^+	SeF_2^+	112	FeO_3	FeO_3	A250
F_2Se	SeF_2	A208	FeO_3	(cyc-O_2Fe)O	A251
F_2Se_2	FSeSeF	A264	FeO_3^-	FeO_3^-	A252
F_2Se_2	$SeSeF_2$	A264	FeO_4	(cyc-O_2Fe)O_2	A298
F_2Si^+	SiF_2^+	91	FeO_4	(cyc-O_2Fe)OO	A298
F_2Si	SiF_2	100,A197	Fe_2H_2O	HFeOFeH	247
F_2Xe^+	XeF_2^+	117	Fe_2H_2O	HFe_2OH	247
F_2Xe	XeF_2	120,A209	Fe_2H_3N	HFe_2NH_2	311
F_3^-	F_3^-	117	Fe_2N	cyc-Fe_2N	A162
F_3HSi^+	$HSiF_3^+$	276	Fe_2N	FeFeN	A162
F_3N^+	NF_3^+	219,A262	Fe_2O	FeOFe	A163
F_3NO^+	F_3NO^+	298	Fe_2O^-	$FeOFe^-$	A166
F_3NS^+	F_3NS^+	298	Fe_2O_2	$(FeO)_2$	A244
F_3OP^+	F_3PO^+	298	$Fe_2O_2^-$	$Fe_2O_2^-$	A246
F_3OS^-	SOF_3^-	304	Fe_2O_3	Fe_2O_3	A294
$F_3O_2S^-$	$SO_2F_3^-$	358	$Fe_2O_3^-$	$Fe_2O_3^-$	A295
F_3P^+	PF_3^+	219	Fe_2O_4	Fe_2O_4	A320
F_3PS^+	F_3PS^+	299	$Fe_2O_4^-$	$Fe_2O_4^-$	A320
F_3S	SF_3	226	GaHO	GaOH	36
F_3Sb^+	SbF_3^+	222	GaH_2	GaH_2	18,A129
F_3Si^+	SiF_3^+	A258	GaH_2O	HGaOH	139,A223
F_3Si	SiF_3	218,A262	GaH_3	GaH_3	A213
F_3Si^-	SiF_3^-	A263	GaInO	InGaO	64
F_4Ge^+	GeF_4^+	297	GaO_2	cyc-GaO_2	75
F_4OXe^+	$XeOF_4^+$	359	GaO_2	OGaO	75
F_4P^-	PF_4^-	304	GaO_3	OGaOO	190
$F_4P_2^+$	$P_2F_4^+$	355	GaP_2	GaP_2	A172
F_4P_2	$PF_3{=}PF$	355	$GaSb_2$	$GaSb_2$	A172
F_4S^+	SF_4^+	A307	Ga_2H_2	cyc-Ga_2H_2	A220
F_4Si^+	SiF_4^+	294,A305	Ga_2H_2	HGaGaH	A220
F_4Xe^+	XeF_4^+	305	$Ga_2H_6^+$	$Ga_2H_6^+$	A333
F_5I^+	IF_5^+	358	Ga_2H_6	Ga_2H_6	372,A333
F_5P^+	PF_5^+	356	Ga_2O	Ga_2O	64
F_5S	SF_5	358	Ga_2O_2	GaOGaO	185
F_5S^-	SF_5^-	359	Ga_2O_2	cyc-GaO_2Ga	185
F_5Si^-	SiF_5^-	357	Ga_2O_3	Ga_2O_3	283

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
Ga_2P	Ga_2P	A165	HNO_4	$HOONO_2$	341,A317
Ga_2Sb	Ga_2Sb	A165	HNSc	ScNH	A138
Ga_3H_2	HGa_3H	A275	HNSi	HNSi	38,A146
GeH_2	GeH_2	2,A132	HNSi	HSiN	A145
$GeH_2I_2^+$	$GeH_2I_2^+$	263	HNY	YNH	27
GeH_2O	H_2GeO	146	HN_2^+	HN_2^+	39
GeH_2O	HGeOH	146	HN_2O^+	$HONN^+$	165
GeH_2O_3	H_2GeO_3	338	HN_3^+	HN_3^+	161
GeH_3^+	GeH_3^+	125	$HNaO^+$	$NaOH^+$	27
GeH_3	GeH_3	128	HNiO	NiOH	30
GeH_3I^+	GeH_3I^+	242	HOP	HPO	46
GeH_4^+	GeH_4^+	228	HOS^+	HSO^+	A152
GeH_4O	GeH_3OH	311	HOS	HSO	50,A154
GeH_4S^+	GeH_3SH^+	311	$HOSi^+$	$HOSi^+$	39
GeI_2^+	GeI_2^+	92	HOSr	SrOH	29,A140
GeOS	OGeS	86	HOXe	XeOH	53
GeO_2	GeO_2	86	HOZn	ZnOH	31,A141
GeO_2^-	GeO_2^-	A194	HO_2^+	HO_2^+	47
GeS_2	GeS_2	86	HO_2	HO_2	49,A153
Ge_2H_2O	HGe_2OH	256	HO_2^-	HO_2^-	51
Ge_2O_2	Ge_2O_2	188,A251	HO_2P	*c*-HOPO	174
$Ge_2O_2^-$	$Ge_2O_2^-$	A252	HO_3P	$HOPO_2$	273
$Ge_2O_3^-$	$Ge_2O_3^-$	A300	HO_3P	HOOPO	273
Ge_3	Ge_3	A171	HO_3P	$HP(O_2)O$	273
Ge_3^-	Ge_3^-	A173	HO_3S	$HOSO_2$	277
Ge_3O_3	$(GeO)_3$	346	HO_3Sb	$HSbO_3$	274
Ge_4	Ge_4	A246	HO_3Sb	$HOSbO_2$	274
HIO^+	HOI^+	A155	HPS_2	HPSS	A241
HIO	HOI	52,A156	HPS_3	$HSPS_2$	A292
HISi	HSiI	44	HSSr	SrSH	29
HIXe	HXeI	A158	HS_2	HS_2	50,A154
HI_2^-	IHI^-	55,A158	HS_2^-	HS_2^-	53
HInO	InOH	37,A144	HXe_2^+	HXe_2^+	56
HKO^+	KOH^+	27	HXe_2	Xe_2H	57
HKrXe	KrXeH	57	HZn_2	ZnZnH	A136
HKr_2^+	HKr_2^+	56,A159	H_2Hf	HfH_2	A126
HKr_2	Kr_2H	57	H_2Hg	HgH_2	16,A128
HLi_2	Li_2H	26,A136	H_2Hg_2	HHgHgH	A218
HMgO	MgOH	27,A138	H_2IP	H_2PI	A229
HNO^+	HNO^+	41	$H_2I_2Si^+$	$SiH_2I_2^+$	263
HNO	HNO	45,A151	H_2In	InH_2	A129
HNO^-	HNO^-	48	H_2InO	HInOH	139
$HNOS^+$	$HNSO^+$	169	H_2Mg	MgH_2	14,A125
HNOS	*t*-HONS	174	H_2MgO	HMgOH	134
HNOS	*t*-HSNO	174	H_2MgO_2	$Mg(OH)_2$	A282
HNOS	*c*-HSNO	174	H_2Mg_2	HMgMgH	A217
HNOS	*c*-HNSO	175,A240	H_2Mg_2	br-$(MgH)_2$	A218
HNOS	*t*-HNSO	175	H_2Mg_2O	HMgOMgH	246
HNOS	*c*-HOSN	176	H_2Mg_2O	HMg_2OH	246
HNO_2	*t*-HONO	172	H_2Mn	MnH_2	15
HNO_2	*c*-HONO	173	H_2Mn^-	MnH_2^-	17
HNO_3^+	HNO_3^+	270	H_2MnO	HMnOH	136
HNO_3	$HONO_2$	271,A289	H_2Mn_2O	HMn_2OH	247
HNO_3	*c*,*c*-HOONO	A291	H_2Mn_2O	HMnOMnH	247
HNO_3	*t*,perp-HOONO	272,A291	H_2Mo	MoH_2	16

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
H_2N^+	NH_2^+	20,A132	H_2U_2	*cyc*-U_2H_2	A218
H_2N	NH_2	21,A133	H_2V	VH_2	14
H_2N^-	NH_2^-	26	H_2Xe	HXeH	A136
H_2NO^+	H_2NO^+	148	H_2Zn	ZnH_2	16,A127
H_2NO	H_2NO	151	H_2Zn_2	HZnZnH	130,A218
H_2NSr	$SrNH_2$	133	H_2Zr	ZrH_2	A126
$H_2N_2^+$	*t*-$N_2H_2^+$	142	H_3^+	H_3^+	11,A123
H_2N_2	*t*-N_2H_2	147,A227	H_3	H_3	12,A123
H_2N_2	H_2NN	148	H_3Hf	HfH_3	A211
H_2N_2O	NH_2NO	260	H_3ISi^+	SiH_3I^+	241
$H_2N_2O_2$	NH_2NO_2	337	H_3In	InH_3	A213
H_2Nb	NbH_2	A128	H_3Mo	MoH_3	124
H_2Ni	NiH_2	16,A127	H_3N^+	NH_3^+	128,A217
H_2Ni^-	NiH_2^-	17	H_3NNi	$HNiNH_2$	231
H_2NiO	HNiOH	136	H_3NO^+	NH_2OH^+	242
H_2NiO_2	$Ni(OH)_2$	252	H_3NSi	$HSiNH_2$	235
H_2Ni_2O	HNi_2OH	248	H_3NSi	SiH_2NH	A270
H_2O^+	H_2O^+	24,A134	$H_3N_2^+$	$N_2H_3^+$	236
H_2OP	H_2PO	151,A228	H_3O^+	H_3O^+	129
H_2OP	HPOH	151	H_3OP	PH_3O	242
H_2OS	HSOH	154	H_3OP	*c*-H_2POH	243
H_2OSc	HScOH	135	H_3OSb	H_3SbO	243
H_2OSi	HSiOH	146	H_3OSb	H_2SbOH	244
H_2OSi	H_2SiO	145,A226	H_3O_3P	$(HO)_2HPO$	368
H_2OSn	HSnOH	146	H_3P^+	PH_3^+	129
H_2OSn_2	HSn_2OH	257	H_3PS	H_2PSH	A275
H_2OSr	HSrOH	134	H_3S^+	H_3S^+	130,A217
H_2OTi	HTiOH	135	H_3Sb^+	SbH_3^+	129
H_2OV	HVOH	135	H_3Si^+	SiH_3^+	124,A213
H_2OZn	HZnOH	A222	H_3Si	SiH_3	126,A215
$H_2O_2^+$	$HOOH^+$	152	H_3Si^-	SiH_3^-	129
H_2O_2	HOOH	153,A229	H_3Th	ThH_3	A212
H_2O_2S	HSO_2H	265	H_3Ti	TiH_3	A211
H_2O_2Si	HSiOOH	260	H_3U	UH_3	A212
H_2O_3Si	H_2SiO_3	338	H_3Zr	ZrH_3	A211
H_2P^+	PH_2^+	21	H_4Hf	HfH_4	A265
H_2P	PH_2	22,A134	H_4Mg_2	$HMgH_2MgH$	A308
H_2PS	HPSH	A228	H_4N^+	NH_4^+	229,A266
H_2Pt	PtH_2	A127	H_4N	NH_4	229,A266
H_2S^+	H_2S^+	24,A135	$H_4N_2^+$	$N_2H_4^+$	311
$H_2S_2^+$	$HSSH^+$	153	H_4N_2O	NH_2NHOH	364
H_2S_2	HSSH	155,A230	H_4OSi	SiH_3OH	311
H_2S_3	*c*-HSSSH	A285	$H_4P_2^+$	$P_2H_4^+$	311
H_2S_3	*t*-HSSSH	A285	H_4SSi^+	SiH_3SH^+	310
H_2Sb	SbH_2	23	H_4Si^+	SiH_4^+	228
H_2Se^+	H_2Se^+	25	H_4Th	ThH_4	A265
H_2Si^+	SiH_2^+	18,A130	H_4Ti	TiH_4	227,A265
H_2Si	SiH_2	19,A131	H_4U	UH_4	A265
H_2Si^-	SiH_2^-	21	H_4U_2	U_2H_4	A308
H_2Si_2	*br*-Si_2H_2	138,A223	H_4Zr	ZrH_4	A265
H_2Si_2	Si(H)SiH	138	H_5^+	H_5^+	227
H_2Te^+	H_2Te^+	25	H_5NSi	SiH_3NH_2	360
H_2Th	ThH_2	A128	$H_5O_2^+$	$H_5O_2^+$	360,A323
H_2Ti	TiH_2	14,A126	H_5Si^+	SiH_5^+	A307
H_2U	UH_2	A128	H_6OSi_2	SiH_3SiH_2OH	417

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
$H_7O_3^+$	$H_7O_3^+$	414	NOS_2	SSNO	A258
$H_9O_4^+$	$H_9O_4^+$	414,A364	NOSe	SeNO	A195
HfO_2	OHfO	A176	NOU	NUO	A172
HfO_2^-	$OHfO^-$	A182	NOU	UNO	A172
HfO_3	OHfOO	A250	NO_2^+	NO_2^+	87,A190
Hf_2O_2	*cyc*-$(HfO)_2$	A244	NO_2^-	NO_2^-	102
IKrXe	KrXeI	123	NO_2U	NUO_2	A249
INO	INO	102	NO_3^+	NO_3^+	A255
INO_2	INO_2	213	NO_3	NO_3	207,A257
INO_3	$IONO_2$	289	NO_3^-	NO_3^-	A259
INS^+	NSI^+	95	NP_2	PNP	A187
INS	NSI	105	NS_2^+	SNS^+	A191
IO_2	OIO	114,A207	NS_2	NS_2	94,A195
IO_2	IOO	A204	NS_2	NSS	94
IO_2^-	OIO^-	115	NS_2^-	NS_2^-	102
IXe_2	Xe_2I	123	NS_3	NSSS	208
I_2S	SI_2	115	NSe_2^+	$SeNSe^+$	A191
I_2Si^+	SiI_2^+	92	NSe_2	NSe_2	A195
I_3^-	I_3^-	119	NSe_2	SeSeN	A195
InO_2	*cyc*-InO_2	75	NSe_3	SeSeNSe	A258
InO_2	OInO	75	NSe_3	SeSeSeN	A258
In_2O	In_2O	64	NSi_2	SiNSi	A174
In_2O_2	InOInO	185	N_2O^+	N_2O^+	83,A187
In_2O_2	*cyc*-InO_2In	185	N_2OS	SNNO	A254
In_2O_3	In_2O_3	283	$N_2O_2^+$	*t*-$(NO)_2^+$	195,A252
In_2P	In_2P	A165	N_2O_2	*c*-$(NO)_2$	200,A254
In_2Sb	In_2Sb	A165	N_2O_2	*t*-$(NO)_2$	200,A254
KNO_2	*cyc*-KNO_2	A247	N_2O_2	NNO_2	A254
KNO_2	*t*-KNO_2	A247	$N_2O_2^-$	NNO_2^-	207,A256
KNO_3	*c*-KOONO	A296	$N_2O_2^-$	*t*-$(NO)_2^-$	207,A257
KNO_3	*t*-KOONO	A296	N_2O_2S	ON-NSO	286
$LiNO_3$	*c*-LiOONO	A295	N_2O_2S	ONSNO	286
$LiNO_3$	*t*-LiOONO	A295	N_2O_2Ti	O_2TiN_2	A296
$LiNa_3$	$LiNa_3$	180	$N_2O_2U_2$	$(NUO)_2$	A320
Li_2Na_2	Li_2Na_2	180	N_2O_3	O_2N-NO	286,A300
Li_3	Li_3	58,A159	N_2O_3	O=N-O-N=O	286,A300
Li_4	Li_4	180	$N_2O_4^+$	$N_2O_4^+$	349
Li_6	Li_6	342	N_2O_4	N_2O_4	350,A321
Li_7	Li_7	369	N_2O_4	N_2O_4 (V_d)	350
Li_8	Li_8	381	N_2O_4	ONO-NO_2 (D)	351
MgO_2	OMgO	A174	N_2O_4	ONO-NO_2 (D′)	351
MgO_2	*cyc*-MgO_2	A174	N_2O_5	O_2N-O-NO_2	370,A331
MgO_4	O_2MgO_2	A298	N_2Pu	NPuN	A168
Mg_2O_2	MgOMgO	A243	N_2S^+	NNS^+	83
Mn_3	Mn_3	61	N_2S	NNS	88
MoO_2	OMoO	A175	$N_2S_2^+$	$N_2S_2^+$	196
MoO_3	MoO_3	A250	N_2S_2	NS-SN	200
$NNaO_2$	*cyc*-$NaNO_2$	A247	$N_2S_4^+$	$N_2S_4^+$	349
$NNaO_2$	*t*-NaONO	A247	N_2S_4	*cyc*-N_2S_4	351
$NNaO_3$	*c*-NaOONO	A295	N_2Se_2	NSeNSe	A255
$NNaO_3$	*t*-NaOONO	A296	N_2Si	SiNN	72
NOP	PNO	88	N_2Ti	TiNN	A166
NOS^+	SNO^+	A191	N_2U	NUN	63
NOS	SNO	93,A194	N_3^+	N_3^+	72,A181
NOS	NSO	94	N_3	N_3	82

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
N_3^-	N_3^-	87	O_2Si	SiO_2	86
N_3P_3	$(PN)_3$	346	O_2Si^-	SiO_2^-	A194
$N_3S_3^+$	$S_3N_3^+$	347	O_2Si_2	Si_2O_2	188
N_3Sr	SrN_3	183	O_2Sn	OSnO	A189
N_4^+	N_4^+	187,A250	O_2Sn_2	Sn_2O_2	A251
Na_3	Na_3	58,A160	O_2Sr	OSrO	A174
Na_4	Na_4	180	O_2Sr	*cyc*-SrO_2	A175
Na_5	Na_5	277	O_2Sr_2	*cyc*-$(SrO)_2$	A243
Na_6	Na_6	342	O_2Ta	OTaO	A176
Na_7	Na_7	369	O_2Tb	OTbO	A179
Na_8	Na_8	381	O_2Th	OThO	A179
Nb_3	Nb_3	A162	O_2Ti	OTiO	A176
NiO_2	ONiO	A177	O_2Ti^-	$OTiO^-$	A181
NiO_2	*cyc*-NiO_2	A177	O_2Ti_2	*cyc*-$(TiO)_2$	A243
NiO_2	NiOO	A177	O_2U	OUO	A179
NiO_2^-	$ONiO^-$	A182	O_2W	OWO	A175
NiO_2^-	*cyc*-NiO_2^-	A182	O_2Zn	OZnO	A178
NiO_3	ONiOO	A251	O_2Zn_2	ZnOZnO	A244
NiO_3	*cyc*-$(O_2Ni)O$	A251	O_2Zr	OZrO	A176
NiO_4	O_2NiO_2	A298	O_2Zr^-	$OZrO^-$	A182
Ni_2O	NiNiO	A163	O_2Zr_2	*cyc*-$(ZrO)_2$	A243
Ni_2O_2	*cyc*-$(NiO)_2$	A244	O_3^+	O_3^+	95
Ni_2O_2	NiONiO	A244	O_3^-	O_3^-	109,A203
Ni_3	Ni_3	61	O_3P	PO_3	209
OP_2	P_2O	88,A191	O_3Pb	$OPb(O_2)$	A253
OP_4	P_4O	284	O_3S^+	SO_3^+	209
OP_4	*br*-P_4O	284	O_3S	OSOO	A260
OPb_2	PbOPb	A181	O_3S^-	SO_3^-	223
OSSi	OSiS	86	O_3Se	SeO_3	214,A260
OS_2^+	SSO^+	97	O_3Se	OSeOO	A261
OS_2	SSO	105,A199	O_3Si	SiO_3	A253
OS_2^-	SSO^-	110	$O_3Si_2^-$	$Si_2O_3^-$	A300
OSeSi	OSiSe	A189	O_3Si_3	$(SiO)_3$	346
OSe_2	SeSeO	A201	O_3Ti	OTiOO	A250
OTi_2	TiOTi	A163	O_3U	UO_3	A251
OTl_2	Tl_2O	65	O_3W	WO_3	A250
O_2P	PO_2	93,A194	O_3Zr	OZrOO	A250
O_2P^-	PO_2^-	103,A199	O_4^+	*t*-O_4^+	209,A258
O_2P_2	$(PO)_2$	200	O_4^+	*cyc*-O_4^+	209,A258
O_2Pb	OPbO	A190	O_4^-	*t*-O_4^-	222
O_2Pb	*cyc*-PbO_2	A190	O_4Pd	O_2PdO_2	A298
O_2Pb_2	Pb_2O_2	A252	O_4Pt	O_2PtO_2	A298
O_2Pb_2	$PbPb(O_2)$	A252	O_4Rh	O_2RhO_2	A298
O_2Pd	*cyc*-PdO_2	A177	O_4S	SO_4	289
O_2Pr	OPrO	A179	O_4Si_2	Si_2O_4	A321
O_2Pt	*cyc*-PtO_2	A177	$O_4Si_2^-$	$Si_2O_4^-$	A321
O_2Pu	OPuO	A179	O_5P_2	P_2O_5	371
O_2Rh	*cyc*-RhO_2	A177	PS_2	PS_2	95
O_2S^+	SO_2^+	96,A195	PS_2^-	PS_2^-	104
O_2S	SOO	A199	P_2S	P_2S	88
O_2S^-	SO_2^-	110	P_2S_4	P_2S_4	351
O_2Se	SeO_2	A200	P_3	P_3	82
O_2Se	SeOO	A201	P_4^+	P_4^+	187
O_2Se^-	SeO_2^-	A204	P_4S	*cyc*-P_4S	284
O_2Se_2	*cyc*-(SeOSe)=O	A261	Pd_3	Pd_3	61

Formula	*Structure/Name*	*References*
Pt_3	Pt_3	61
S_2Si	SiS_2	86
S_3	S_3	105,A200
S_3^-	S_3^-	110
S_4	S_4	214,A260
S_4	SS_3	214
Sb_3	Sb_3	82
Sb_3^-	Sb_3^-	88
Sb_4	Sb_4	189
Sb_4^-	Sb_4^-	197
Sc_3	Sc_3	61
Se_2Si	$SiSe_2$	A189
Se_3	Se_3	106
Se_4	Se_4	214
Se_4	$SeSe_3$	215
Si_3	Si_3	67,A170
Si_3^-	Si_3^-	68,A173
Si_4	Si_4	182,A245
Si_4^-	Si_4^-	183,A247
Si_6	Si_6	A318
Si_7	Si_7	A329
Ta_4	Ta_4	A241
Te_3	Te_3	106
Te_4	Te_4	215
Te_4	$TeTe_3$	215