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

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A summary is presented of recently published, critically evaluated experimental vibrational and electronic energy level data for approximately 1700 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, and several thousand references are cited. The types of measurement surveyed include conventional and laser-based absorption and emission techniques, laser absorption with mass analysis, and photoelectron spectroscopy. [DOI: 10.1063/1.1497629]

Key words: *ab initio* calculations; density functional calculations; 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.

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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 selection 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. In 1998, a supplement to that monograph appeared,[6] adding data for approximately 900 molecules, more than half of which were not in the monograph. Electronic band origins, vibrational fundamentals in the ground and excited electronic states, and radiative lifetimes were given in both the monograph and its supplement. To aid in spectral identification, the principal rotational constants were also given in cm^{-1} to three decimal places. The vibrational and electronic energy level data from these tables forms a part of the material available from the Internet-based NIST Chemistry WebBook ⟨http://WebBook.nist.gov/chemistry/⟩. The WebBook format permits relatively frequent updates and several different types of data search.

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 late 1997 cutoff in the data evaluation for the 1998 supplement,[6] substantive new spectroscopic data have been published for many species included in it, and the first data have become available for more than 1200 other molecules. Progress in the spectroscopic characterization of transient species produced by the reaction of metal atoms with oxygen and other small molecules has continued. This paper attempts to provide a comprehensive, critically evaluated summary of these new data for the vibrational and electronic energy levels of small polyatomic transient molecules, in order to support further research and technologies such as plasma processing and chemical vapor deposition.

2. Scope of Review

This review provides a critical evaluation of the vibrational and electronic spectral data available at the end of 2001 (or, for a few species, in early 2002) for approximately 1700 small polyatomic transient molecules. Of these, about 1225 are new; the remaining approximately 475 molecules were included in the monograph and/or the earlier supplement but have since been more extensively studied. 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 remain to be discovered.

Data have been selectively included for some molecules which are important in environmental and industrial chemical reaction systems but which can be studied only with difficulty using conventional sampling techniques because of the ease with which they decompose, rearrange, or polymerize. 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. These species include a number of binary and some ternary complexes involving a metal atom and a small inorganic molecule (H_2, N_2, O_2, CO, NO). Examples of unusual chemical bonding, including side bonding to produce a cyclic intermediate, are found. Such complexes are expected to play important roles in catalysis. Because of the ubiquity of atmospheric impurities, these complexes may contribute widely to the chemistry of metal–atom reaction systems. A number of other molecules included in this database are among the first inorganic species to exhibit aromatic behavior. Moreover, there is a growing number of entries for small molecular cations and anions.

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.

During the past few years, the power of *ab initio* and density functional calculations for obtaining ground-state vibrational frequencies has grown dramatically. Relatively so-

phisticated calculations are now feasible for molecules in the size range covered by this compilation. Recently, Byrd and co-workers[7] have compared the positions of 84 ground-state vibrational fundamentals for 33 small free radicals calculated at several different levels (e.g., Hartree–Fock, MP2, CCSD, B3LYP) using a variety of common basis sets with the experimentally determined positions. The results are expressed as averages of the numerical and absolute deviations and as the standard deviation for each calculational procedure. These deviations generally amount to several percent. Since anharmonicity is expected to be a major contributor to these deviations, Byrd and co-workers also attempted a comparison for the small set of frequencies for which the harmonic values are available. They reported the results only for the most sophisticated basis set, cc-pVTZ, used in their study. Their results for three different calculations are summarized in Fig. 1. The deviations obtained at the CCSD level and using the B3LYP density functional procedure are approximately 4%. The more sophisticated CCSD(T) calculations overcorrected for the anharmonicity by approximately 0.9%. Moreover, the spread in the deviations, expressed by the standard deviation, was greater than for the other two types of calculation. Of course, these conclusions may change as a larger data set of experimentally determined harmonic vibrational frequencies becomes available.

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 neutral and ionic reaction intermediates has recently been reviewed.[8] 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 bandwidths between 0.1 cm^{-1} and 1 cm^{-1}. Rotational structure is, with few exceptions, quenched. Multiple trapping sites occur, often resulting in the appearance of several absorption maxima—usually one or two of which predominate—over a range of a few cm^{-1}.

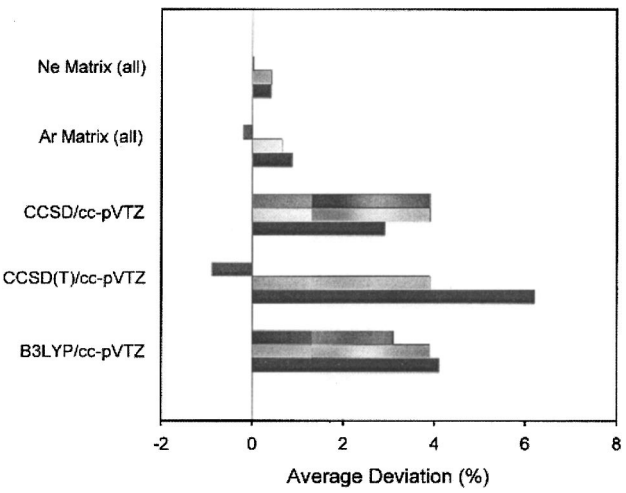

FIG. 1. Comparison of average deviations (matrix—gas, %) of transient molecules from 2 to 16 atoms trapped in neon and argon matrices with average deviations (calculated—observed, %) reported by Byrd *et al.*[7] for harmonic vibrational fundamentals of small free radicals. In each group, top=num. av., middle=abs. av., and bottom=std. dev.

Matrix shifts for covalently bonded molecules trapped in solid neon or argon often are quite small. A comparison[9] of the positions of the ground-state vibrational fundamentals of over 200 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. This comparison has been updated—with similar conclusions—in the recent review[8] for diatomic oxides, an important class of molecules for which considerable new data have become available since the earlier comparison. 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 less than 2%, and shifts for the molecules isolated in solid neon are even smaller. Similar conclusions result from the comparison of neon- and argon-matrix shifts for the ground-state vibrational fundamentals of larger molecules.[8] Figure 1 includes a comparison of the observed average deviations (by analogy with the computational deviations, expressed as matrix value minus gas-phase value, in percent) for all of the the ground-state fundamental vibrations of transient molecules with from 2 to 16 atoms trapped in solid neon and argon for which the positions of the gas-phase band centers have been determined. These comparisons included 168 fundamental vibrations for the neon matrix and 426 for the argon matrix. The numerical average deviation of the neon-matrix band centers from their gas-phase counterparts is very small, and both the absolute average deviation and the standard deviation are well within 1%. The deviations for argon-matrix measurements are somewhat larger, and the average fundamental frequency is approximately 0.2% smaller than the gas-phase value. As is shown in Fig. 1, the average deviations obtained from the *ab initio* and density functional calculations are several times as large. While the results of such calculations are demonstrated to be a useful guide, where neon- or argon-matrix values for the ground-state vibrational frequencies of small transient molecules have been determined they are likely to provide a significantly better approximation to the gas-phase band centers. Interaction between both gas-phase and matrix-isolation spectroscopists and scientists developing new computational strategies for molecules with unpaired electrons, for which configuration interaction is important, promises to be mutually helpful.

For molecular ions, neon is the matrix of choice. Data for many small cation species trapped in solid neon are consistent with the matrix shift generalizations given above. How-

ever, some ions react with even the lighter rare gases. An extreme example is provided by HF^+, the ground-state vibrational fundamental of which is shifted by some 700 cm^{-1} because of reaction to form $NeHF^+$.[10] Vibrational frequency shifts which result from proton sharing between rare-gas atoms or clusters and small protonated molecules have recently been reviewed by Bieske and Dopfer.[11] Because the proton affinity of helium is 80% as great as that of neon, such shifts can be appreciable even for helium. Although specific examples are not yet available, it is anticipated that some nonprotonated species may also interact strongly with neon. Polarization and charge-transfer interactions become successively more important for molecules isolated in the heavier rare gases. Moreover, charge delocalization sometimes occurs for ionic species trapped in the rare gases.[12,13] The anomalously large matrix shift for ν_3 of $ClHCl^-$ may be attributed to this phenomenon. Only a few comparisons are available for molecular cations observed both in the gas phase and trapped in solid argon. The absolute values of almost half of the observed matrix shifts are greater than 1%. Very few comparisons are possible for molecular anions. Where the frequency of a cation or an anion vibrational fundamental is similar in both argon- and neon-matrix observations, it is suggested that the deviation from the gas-phase band center is small. However, data are insufficient to confirm this generalization. A number of molecular anions 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 molecular 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 most molecular cations with more than six atoms. Those who need such data for larger molecules may find the reviews by Turner *et al.*,[14] Rabalais,[15] and Kimura *et al.*[16] 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 ioniza-

tion 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[17,18] (also available in the NIST Chemistry WebBook) 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.[19] 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. This generalization is supported by the recent study by Maier[20] of the electronic spectra of mass-selected carbon-chain species. In that work, neon-matrix spectra were used as a guide in the search for $\pi-\pi$ electronic transitions of the gas-phase species. For these transitions of neutral and charged species of formula C_n, HC_n, HC_nH, HC_nN, and NC_nN, Maier found that almost all of the neon-matrix shifts were to longer wavelengths, with a magnitude less than approximately 150 cm^{-1}. 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 blueshift of the phonon maximum from the zero-phonon line in absorption measurements, and the red shift in emission measurements, typically amount to approximately 1%–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.[3,20,21]

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.[22] 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 December 2001; 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[23] remain extremely useful. At the time of those compilations, it was difficult to ascertain the positions of band centers for very prominent fundamentals of molecules with dense rotational structure, such as the small inorganic halides. For such absorptions, it is important to seek more recent high resolution infrared measurements. 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. To check on the possibility of reassignment, check the Molecule Index (Sec. 9) to see whether the previously listed molecule is still included. Candidate molecules or energy levels may also have been inadvertently omitted. The NIST Chemistry WebBook is inherently more responsive than any archival publication can be, and should be checked for more recent information. 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,[24] 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 meV 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. However, in matrix isolation absorption and laser excitation studies only the lowest component is accessible. Except for transitions with relatively small values of A, this is also likely to be true for studies using cooled molecular beams. Often these latter studies give T_0 values for the lowest energy component with a precision better than that to which A is known.

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

The format of the vibrational tables is similar to that used in the earlier compilations. The vibrational numbering convention is that used by Herzberg.[1] Within a given symmetry species, vibrations are numbered starting with the highest frequency. The same convention is followed for deuterated species. Therefore, a given type of vibration may be numbered differently for the deuterated than for the unsubstituted molecule. For triatomic molecules, the bending vibration is always designated as ν_2. For aromatic molecules, an alternate vibrational numbering scheme developed by Wilson[25] 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
DM	degenerate four-wave mixing
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 ionization
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

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7. General References

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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	1,4,15,22,23
			2109.7T	H_2	IR	24

$B_0=43.510$; $C_0=20.698$ 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
$\tau = 37(4)$ 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}
$\tau = 1.1(+0.2,-1.0)$ 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]
$\tau_{00} = 640(+300,-100)$ ns; $\tau_{10} = 740(+300,-100)$ 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

$3p\ ^2B_1$ C_{2v}
$T_0^a = 17806.5$ gas EM[30]
$\tau = 29(3)$ ns gas EM[20]
$A = 42.75(50)$; $B = 28.6(5)$; $C = 16.5(5)$ EM[30]

$3s\ ^2A_1$ C_{2v}
$T_0^a = 16609.25$ gas EM[31]
$\tau \cong 4$ ns gas EM[20]
$A = 43.99$; $B = 29.439$; $C = 16.954$ EM[31]

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

$2p\ ^2A_2$ C_{2v}
$A = 44.125$; $B = 29.486$; $C = 16.841$ EM[31]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		2300(30)T	gas	EM	30
b_2	3		2450(30)T	gas	EM	30

$\tau \geqslant 0.4(2)$ ps gas EM[30]
$A = 45.3(5)$; $B = 30.3(5)$; $C = 17.5(5)$ EM[30]

D_2H

$3p\ ^2B_1$ C_{2v} Structure: EM[9]
$T_0^a = 17834.4$ gas EM[9,30] $3p^2B_1-2s^2A_1$ 560–673 nm
$\tau_1 = 31.5(3.2)$ ns; $\tau_2 \cong 8.9$ ns gas EM[20]
$A = 37.8(4)$; $B = 22.6(4)$; $C = 13.9(4)$ EM[30]

$3s\ ^2A_1$ C_{2v}
$T_0^a = 16602.51$ gas EM[31]
$\tau \cong 5$ ns gas EM[20]
$A = 37.7$; $B = 22.17$; $C = 13.69$ EM[31]

$3p\ ^2A_1$, $^2B_2$ C_{2v}
gas EM[30] $3p^2(B_2,A_1)-2s^2A_1$ 709–860 nm
$\tau = 5.0(7)$ ns gas EM[21]

$2p\ ^2A_2$ C_{2v}

$A = 36.9$; $B = 22.07$; $C = 13.58$ EM[31]

$2s\ ^2A_1$ 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
	2		2125(80)	gas	EM	30
b_2	3		2358(50)	gas	EM	30

$\tau \geqslant 0.5(2)$ ps gas EM[30]
$A = 39.14(40)$; $B = 23.4(4)$; $C = 14.4(4)$ EM[30]

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]LD[33] $3d-3p^2E'$ 3772–4517 cm^{-1}
$\tau = 12(1)$ 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]LD[33] $3d-3p^2E'$ 3772–4517 cm^{-1}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Ring breathing	2296.1	gas	PI	32

$\tau = 12(1)$ 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]LD[33] $3d-3p^2E'$ 3772–4517 cm^{-1}
$\tau=12(1)$ 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[2,3,8,30]LF[7] $3p^2A_2''-2s^2A_1'$ 553–651 nm
$\tau_0=29(1)$ 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]LD[33] $3s^2A_1'-3p^2E'$ 3382–3768 cm^{-1}
$\tau\cong10$ 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[2,4,21,30]LF[7] $3p^2E'-2s^2A_1'$ 700–860 nm
EM[6]LD[33] $3s^2A_1'-3p^2E'$ 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

$\tau=17.5(2.0)$ 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	29,32
e'	2	Deformation	1900.9	gas	PI	29,32

$B_0=22.112$; $C_0=11.056$ 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	2470(22)	gas	EM	4,20,21, 30
e'	2	Deformation	1884(22)	gas	EM	21,30

$B_0=23.09$; $C_0=11.544(6)$ 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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CeH_2^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CeH_2 s-stretch	1486.3	Ar	IR	1
b_2	3	CeH_2 a-stretch	1445.9	Ar	IR	1

CeD_2^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CeD_2 s-stretch	1059.8	Ar	IR	1
b_2	3	CeD_2 a-stretch	1035.3	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **104**, 1640 (2000).

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]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	335	Ar	IR	2
			322	Kr	IR	1
			323	Xe	IR	1
Σ_g^+	3	FeH a-stretch	1674.72	gas	LMR	5,7
			1660.8	Ar	IR	2,4
			1647	Kr	IR	1,2
			1636	Xe	IR	1,2

$B_0=3.075$ LMR[5,7]

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]

$\tilde{X}\,^5\Delta_g$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	221.14[a]	gas	LMR	6
			235	Ar	IR	2
			232	Xe	IR	1
Σ_u^+	3	FeD a-stretch	1204.2	Ar	IR	2,4
			1195	Kr	IR	2
			1188	Xe	IR	1

$B_0=1.542$ LMR[6]

[a] $^5\Pi_3-{}^5\Delta_4$ component. $^5\Phi_3-{}^5\Delta_2$ component at 226.06.[6]

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cyc-PdH_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	HH stretch	2971.4	Ar	IR	2,3
	2	PdH s-stretch	871.8	Ne	IR	3
			865.3			
			950.0s	Ar	IR	2,3
			960	Kr	IR	1
			894.5	Xe	IR	1
			885.5			
b_2	3	PdH a-stretch	1507.5w	Ar	IR	2,3

cyc-PdD_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	DD stretch	2169	Ar	IR	2,3
	2	PdD s-stretch	670.9	Ne	IR	3
			714.4	Ar	IR	2,3
			714	Kr	IR	1
b_2	3	PdD a-stretch	1098.0	Ar	IR	2,3

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[1] G. A. Ozin and J. García-Prieto, J. Am. Chem. Soc. **108**, 3099 (1986).
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PtH_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PtH s-stretch	2365.7	Ar	IR	2
b_2	3	PtH a-stretch	2355.2	Ne	IR	2
			2348.9	Ar	IR	1,2
			2314	Kr	IR	1

PtD_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PtD s-stretch	1697.7	Ar	IR	2
b_2	3	PtD a-stretch	1688.2	Ne	IR	2
			1683.3	Ar	IR	2

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CeH_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CeH_2 s-stretch	1330.7	Ar	IR	1
b_2	3	CeH_2 a-stretch	1281.7	Ar	IR	1

CeD_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CeD_2 s-stretch	943.7	Ar	IR	1
b_2	3	CeD_2 a-stretch	916.9	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **104**, 1640 (2000).

PrH_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		PrH_2 stretch	1286.6	Ar	IR	1

PrD_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		PrD_2 stretch	917.2	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **104**, 1640 (2000).

NdH_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	NdH_2 a-stretch	1148.4	Ar	IR	1

NdD_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	NdD_2 a-stretch	822.4	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **104**, 1640 (2000).

SmH_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SmH_2 s-stretch	1213.0	Ar	IR	1
b_2	3	SmH_2 a-stretch	1156.5	Ar	IR	1

SmD_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SmD_2 s-stretch	864.3	Ar	IR	1
b_2	3	SmD_2 a-stretch	827.2	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **104**, 1640 (2000).

EuH_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	EuH_2 s-stretch	1211.7	Ar	IR	1
b_2	3	EuH_2 a-stretch	1155.6	Ar	IR	1

EuD_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	EuD_2 s-stretch	863.6	Ar	IR	1
b_2	3	EuD_2 a-stretch	827.0	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **104**, 1640 (2000).

GdH_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	GdH_2 s-stretch	1399.0	Ar	IR	1
b_2	3	GdH_2 a-stretch	1359.3	Ar	IR	1

GdD_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	GdD_2 s-stretch	998.8	Ar	IR	1
b_2	3	GdD_2 a-stretch	973.0	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **104**, 1640 (2000).

TbH_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	TbH_2 s-stretch	1445.3	Ar	IR	1
b_2	3	TbH_2 a-stretch	1391.1	Ar	IR	1

TbD_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	TbD_2 s-stretch	1031.4	Ar	IR	1
b_2	3	TbD_2 a-stretch	996.0	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **104**, 1640 (2000).

DyH_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	DyH_2 s-stretch	1247.1	Ar	IR	1
b_2	3	DyH_2 a-stretch	1193.1	Ar	IR	1

DyD_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	DyD_2 s-stretch	888.6	Ar	IR	1
b_2	3	DyD_2 a-stretch	853.8	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **104**, 1640 (2000).

HoH_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	HoH_2 s-stretch	1255.8	Ar	IR	1
b_2	3	HoH_2 a-stretch	1203.6	Ar	IR	1

HoD_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	HoD_2 s-stretch	895.1	Ar	IR	1
b_2	3	HoD_2 a-stretch	861.3	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **104**, 1640 (2000).

ErH_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ErH_2 s-stretch	1271.0	Ar	IR	1
b_2	3	ErH_2 a-stretch	1217.3	Ar	IR	1

ErD_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ErD_2 s-stretch	905.7	Ar	IR	1
b_2	3	ErD_2 a-stretch	871.3	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **104**, 1640 (2000).

TmH_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	TmH_2 s-stretch	1281.2	Ar	IR	1
b_2	3	TmH_2 a-stretch	1222.2	Ar	IR	1

TmD_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	TmD_2 s-stretch	913.3	Ar	IR	1
b_2	3	TmD_2 a-stretch	874.8	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **104**, 1640 (2000).

YbH_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	YbH_2 s-stretch	1276.1	Ar	IR	1
b_2	3	YbH_2 a-stretch	1218.6	Ar	IR	1

YbD_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	YbD_2 s-stretch	910.0	Ar	IR	1
b_2	3	YbD_2 a-stretch	872.1	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **104**, 1640 (2000).

LuH_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	LuH_2 s-stretch	1486.4	Ar	IR	1
b_2	3	LuH_2 a-stretch	1426.4	Ar	IR	1

LuD_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	LuD_2 s-stretch	1061.3	Ar	IR	1
b_2	3	LuD_2 a-stretch	1021.5	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **104**, 1640 (2000).

PdH_2^-

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	PdH a-stretch	1247.0	Ar	IR	1

PdD_2^-

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	PdD a-stretch	912.9	Ne	IR	1
			908.5	Ar	IR	1

Reference

[1] L. Andrews, X. Wang, M. E. Alikhani, and L. Manceron, J. Phys. Chem. A **105**, 3052 (2001).

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]
$T_0 = 11497(10)$ gas $\tilde{b}-\tilde{a}$ 465–1049 nm
AB[1,3,27,44]LMR[21]LF[33,38,40,42,43]DL[47–50]

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]
$3.8(3)\ \mu s$ LF[39]
$B_{010} = 8.59(4)$ DL[47]
Barrier to linearity = 1617[29]

$\tilde{a}\ ^1A_1$[b] C_{2v} Structure: AB[3,29,31]
$T_0 = 3147(5)$ gas $\tilde{b}-\tilde{a}$ 465–1049 nm
AB[1,3,27,28,44]LMR[21,26,30]PE[23,24]LF[32,38,40,42,43,45]SEP[32,34]DL[47–50]

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	10,20,31
					IR	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

$A_0 = 37.787;\ 1/2(B+C)_0 = 3.962;\ 1/2(B-C)_0 = 0.267$ 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[1,2,16]

$T_0 = 15547.77$ gas AB[1,2,16] 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

$\tau_0 = 1.10(17)$ μs gas LF[6,7,11]

$A_0 = 18.324(2)$; $B_0 = 4.900$; $C_0 = 3.766$ AB[2]

Barrier to linearity $\cong 8000$[3]

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

$T_0 = 7340(240)$[b] 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	1995.93[c]	gas	LF,DL	10,13,15, 18
			1992.8[c]	Ar	IR	5
			2013.8T	Kr	IR	17
	2	Bend	999.03	gas	AB,LF	2,4,9,13
					DL	15
			994.8	Ar	IR	5
			998.5	Kr	IR	17
b_2	3	Asym. stretch	1992.82	gas	DL	18
			1973.3	Ar	IR	5
			1993.7T	Kr	IR	17

$A_0 = 8.099$; $B_0 = 7.024$; $C_0 = 3.703$ AB[2,16] DL[9,17]

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]

$\tau_0 = 0.93(38)$ μs gas LF[11]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1444.6[c]	Ar	IR	5
			1456.3T	Kr	IR	17
	2	Bend	731[d]	gas	LF	11
			719.8	Ar	IR	5
			721	Kr	IR	17
b_2	3	Asym. stretch	1439.1	Ar	IR	5
			1447T	Kr	IR	17

$A_0 = 4.334$; $B_0 = 3.519$; $C_0 = 1.919$ 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] Possibly 6290(240).[8]

[c]In Fermi resonance with $2\nu_2$, observed for SiH_2 at 1987.69 (gas) and 1964.4 (Ar) and for SiD_2 at 1426.9 (Ar), adopting the reanalysis proposed by Ref. 18.
[d]ω.

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GeH_2

$\tilde{A}\,^1B_1$ C_{2v} Structure: LF[5,7]AB[7]
$T_0 = 16325.54$ gas LF[3–5,7]AB[6,7] $\tilde{A}-\tilde{X}$ 489–850 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1798.4	gas	LF	5
	2	Bend	783.0	gas	LF	3–5

$\tau_0 = 2.29(7)$ μs gas LF[4,5]
$A_0 = 16.363(11)$; $B_0 = 4.522$; $C_0 = 3.458(2)$ LF[5]AB[7]

$\tilde{X}\,^1A_1$ C_{2v} Structure: LF[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1856	gas	LF	7
			1864wmT	Ar	IR	1,2
	2	Bend	916	gas	LF	3,7
			920wm	Ar	IR	1,2
b_2	3	Asym. stretch	1887wmT	Ar	IR	1,2

$A_0 = 7.019(6)$; $B_0 = 6.529(3)$; $C_0 = 3.330(2)$ LF[5]AB[6,7]

GeD_2

$\tilde{A}\,^1B_1$ C_{2v}
$T_0 = 16324.34$ gas LF[3,4,7] $\tilde{A}-\tilde{X}$ 500–850 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1304	gas	LF	7
	2	Bend	561	gas	LF	3,4,7

$\tau_0 = 2.5(5)$ μs gas LF[4]
$A_0 = 8.348(3)$; $B_0 = 2.269$; $C_0 = 1.756$ LF[7]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1335	gas	LF	7
			1329vsT	Ar	IR	1
			1325vsT			
	2	Bend	657	gas	LF	3,7
			658m	Ar	IR	1
b_2	3	Asym. stretch	1338msT	Ar	IR	1

$A_0 = 3.618(4)$; $B_0 = 3.273$; $C_0 = 1.699$ LF[7]

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PH_2^+

$\tilde{a}\,^3B_1$ C_{2v}
$T_0 \cong 5650$ gas PE[1–3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	888(80)	gas	PE	3

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

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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]
$T_0 = 11122.23(5)$ gas AB[1,8,22,31]LF[6,21,25,26]EM[25,31,33] $\tilde{A}-\tilde{X}$ 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	1157.8	gas	AB,EM	31

$\tau_{090\Sigma} = 10.0(1.7)$ μs gas LF[7]
$\tau_{080\Pi} = 10(3)$ μs gas LF[17]

Approximate ν^3 dependence.[7,17] In another LF study,[12] τ varied from 25 to 46 μs for relatively unperturbed rotational sublevels, and there was a weaker

~100 μs component associated with levels which are substantially perturbed.
$B_0 = 8.776(4)$ AB[1,31]EM[31]
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	16,21
					IR	23

$A_0 = 23.693$; $B_0 = 12.952$; $C_0 = 8.173$ AB[1,8]LMR[13]IR[20,29,30]MW[28,32]
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

$B_0 = 4.41$ 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 redshifted 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

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

$\tilde{X}\,^2B_1$[a] C_{2v} Structure: AB[4]MW[24]

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

$A_0 = 4.855$; $B_0 = 4.048$; $C_0 = 2.180$ AB^9MW^{24}

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

AsH_2

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

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

Predissociated above 23300[1]

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

$\tau = 130(20)$ ns gas EM^2

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

$\tilde{X}\,^2B_1$ C_{2v} Structure: AB^1MW^4

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

$A_0 = 7.550$; $B_0 = 7.163$; $C_0 = 3.615$ $AB^1MW^3LMR^5$

AsD_2

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

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

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

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

$A_0 = 3.881$; $B_0 = 3.587$; $C_0 = 1.842$ MW^4

H_2O^+

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

$T_0 = 36757(12)$ gas PE^9

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

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$\tilde{A}\,^2A_1(\Pi_u)$[b] $D_{\infty h}$ Structure: PE[4,7]EM[7]
$T_{070}=13409.3$ gas EM[1,5,17]AB[14,18] $\tilde{A}-\tilde{X}$ 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

$\tau=10.5(1.0)$ μs gas EF[6]
$B_{070}=8.57$ EM[5]

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

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

$A_0=29.036(2)$; $B_0=12.423$; $C_0=8.469$ LMR[8]LD[11]DL[12]CC[15]
Barrier to linearity $\leqslant 9187$[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_2Cl^+

$\tilde{X}$ C_{2v} Structure: DL[1]MW[2,4]LD[3]

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

$A_0=11.253$; $B_0=9.124$; $C_0=4.941$ DL[1]MW[2,4]LD[3]

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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	1,4
Σ_u^+	3	Asym. stretch	1170.0T	Ne	IR	6
			1163.2T			
			1180.6	Xe	IR	1–5
			1165.9			

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	1,4

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8.2. Triatomic Monohydrides

NaCH

$\tilde{X}\,^3\Sigma^-$ $C_{\infty v}$ Structure: MW[1,2]
$B_0 = 0.378$ MW[1,2]

NaCD

$\tilde{X}\,^3\Sigma^-$ $C_{\infty v}$
$B_0 = 0.334$ MW[1,2]

References

[1] J. Xin and L. M. Ziurys, Astrophys. J. **508**, L109 (1998).
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KCH

$\tilde{X}\,^3\Sigma^-$ $C_{\infty v}$ Structure: MW[1]
$B_0 = 0.250$ MW[1]

KCD

$\tilde{X}\,^3\Sigma^-$ $C_{\infty v}$
$B_0 = 0.221$ MW[1]

Reference

[1] J. Xin and L. M. Ziurys, J. Chem. Phys. **110**, 3360 (1999).

YNH

$\tilde{B}\,^2\Sigma^+$ $C_{\infty v}$ Structure: LF[2,3]
$T_0 = 16992.60$ gas LF[1–3] $\tilde{B}$–$\tilde{X}$ 585–650 nm
$B_0 = 0.330$ LF[2,3]

$\tilde{A}\,^2\Pi$ $C_{\infty v}$ Structure: LF[3]
$T_0 = 15425.61$ gas LF[3] $\tilde{A}$–$\tilde{X}$ 636–660 nm
$A_0 = 443.76$ gas LF[3]
$B_0 = 0.331$ LF[3]

$\tilde{A}''\,^2\Pi_{1/2}$ $C_{\infty v}$ Structure: LF[3]
$T_0 = 14742.77$ gas LF[3] $\tilde{A}''$–$\tilde{X}$ 675–680 nm
$\tau = 260(10)$ ns gas LF[3]
$B_0 = 0.330$ LF[3]

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

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

$B_0 = 0.340$ gas LF[2,3]

YND

$\tilde{B}\,^2\Sigma^+$ $C_{\infty v}$
$T_0 = 16949.25$ gas LF[1–3] $\tilde{B}$–$\tilde{X}$ 585–650 nm
$B_0 = 0.285$ LF[2,3]

$\tilde{A}\,^2\Pi$ $C_{\infty v}$
$T_0 = 15396.05$ gas LF[3]
$B_0 = 0.292$ LF[3]

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

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

$B_0 = 0.300$ LF[2,3]

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HCC^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	549.5	Ar	IR	1
Σ^+	3	CC stretch	1832.2	Ne	IR	1
			1820.4	Ar	IR	1

DCC^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2496.0	Ar	IR	1
Π	2	Bend	433.8	Ar	IR	1
Σ^+	3	CC stretch	1735.1	Ne	IR	1
			1724.6	Ar	IR	1

Reference

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MgOH

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

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

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]

[a] Analysis[4] of rotational transitions which arise from states of MgOH and MgOD in which ν_2 is vibrationally excited indicates that these species are quasilinear.

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MgSH

$\tilde{X}$ C_s Structure: MW[1]

$A_0 = 9.640(8)$; $B_0 = 0.227$; $C_0 = 0.221$ MW[1]

Reference

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SrOH

$\tilde{F}\,^2\Pi$ $C_{\infty v}$

$T_0 = 32985$ gas LF[16] $\tilde{F}-\tilde{X}$ 297–304 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	SrO stretch	592T	gas	LF	16

$A = 22$ gas LF[16]

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

$T_0 = 29990$ gas LF[16] $\tilde{E}-\tilde{X}$ 308–334 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	SrO stretch	612T	gas	LF	16

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

$T_0 = 27698$T gas LF[16] $\tilde{D}-\tilde{X}$ 353–361 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	SrO stretch	630T	gas	LF	16

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

$T_0 = 27303$ gas LF[16] $\tilde{C}-\tilde{X}$ 354–383 nm

		Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	255T (ω)	gas	LF	16

$A = 24.52(4)$ gas LF[16]
$B = 0.256$ LF[16]

$\tilde{B}\,^2\Sigma^+$ $C_{\infty v}$ 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]
$\epsilon = -0.0791$ 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	3,6,11,16
Σ^+	3	SrO stretch	526.99	gas	LF	3,6,13,16
			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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SrSH

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

$T_0 = 15026$ gas LF[1] $\tilde{C}-\tilde{X}$ 642–690 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	SrS stretch	269	gas	LF	1

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

$T_0 = 14815$ gas LF[1] $\tilde{B}-\tilde{X}$ 675–688 nm

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

$T_0 = 14293$ gas LF[1] $\tilde{A}-\tilde{X}$ 686–727 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	SrS stretch	270	gas	LF	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	SrS stretch	270	gas	LF	1

$A_0 = 9.709(3)$; $B_0 = 0.096$; $C_0 = 0.095$ MW^2

SrSD

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

$A_0 = 4.993$; $B_0 = 0.094$; $C_0 = 0.092$ MW^2

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BaOH

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

$T_0 = 23057$ gas LF[8] $\tilde{D}-\tilde{X}$ 413–454 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	290T	gas	LF	8
Σ^+	3	BaO stretch	563	gas	LF	8

$B_0 = 0.255(5)$ LF[8]

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

James and Sugden[1] first proposed the assignment to the $\tilde{C}\,^2\Pi - \tilde{X}\,^2\Sigma^+$ transition of BaOH emission bands near 500 nm in flames produced in the $Ba/H_2/O_2/N_2$ system. Laser-excited fluorescence studies on the jet-cooled molecule by Ref. 8 support this identification, but a detailed assignment of the BaOH bands in this spectral region has not yet been achieved.

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

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

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

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

$B_0 = 0.213$ LF[4]

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

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

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

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

$A = 635(1)$ LF[4]

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

gas LF[5] $\tilde{A}'-X$ 848–888 nm

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

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

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

$B_0 = 0.217$ LF^4MW^7

BaOD

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

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

$B_0 = 0.19$ gas LF[4]

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

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

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

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

gas LF[5] $\tilde{A}'-X$ 886–889 nm

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

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

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

$B_0 = 0.196$ LF^4MW^7

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HScO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ScH stretch	1391.1	Ar	IR	1
	3	ScO stretch	922.3	Ar	IR	1

DScO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ScD stretch	1004.2	Ar	IR	1
	3	ScO stretch	922.3	Ar	IR	1

Reference

[1] L. Zhang, J. Dong, and M. Zhou, J. Phys. Chem. A **104**, 8882 (2000).

ScOH

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	ScO stretch	765.6	Ar	IR	1

ScOD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	3	ScO stretch	750.5	Ar	IR	1

Reference

[1] L. Zhang, J. Dong, and M. Zhou, J. Phys. Chem. A. **104**, 8882 (2000).

HYO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	YH stretch	1316.2	Ar	IR	1
	3	YO stretch	809.6	Ar	IR	1

DYO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	YD stretch	945.8	Ar	IR	1
	3	YO stretch	807.9	Ar	IR	1

Reference

[1] L. Zhang, L. Shao, and M. Zhou, Chem. Phys. **272**, 27 (2001).

YOH

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

$T_0 = 18508.6$ gas LF[1] $\tilde{C}-\tilde{X}$ 508–540 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	457	gas	LF	1
Σ^+	3	YO stretch	575	gas	LF	1

$B_0 = 0.271$ LF[1]

$\tilde{B}\,^1\Pi$[a] $C_{\infty v}$

$T_0 = 16448.5$ gas LF[1] $\tilde{B}-\tilde{X}$ 539–613 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	YO stretch	565.20	gas	LF	1

$B_0 = 0.270$ LF[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	313.73	gas	LF	1
Σ^+	3	YO stretch	673.83(2)	gas	LF	1
			662.2wT	Ar	IR	2

$B_0 = 0.290$ LF[1]

YOD

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

$T_0 = 18472.5$ gas LF[1] $\tilde{C}-\tilde{X}$ 510–542 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	339	gas	LF	1
Σ^+	3	YO stretch	568	gas	LF	1

$B_0 = 0.247$ LF[1]

$\tilde{B}\,^1\Pi$[a] $C_{\infty v}$

$T_0 = 16464.0$ gas LF[1] $\tilde{B}-\tilde{X}$ 569–612 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	YO stretch	550.86	gas	LF	1

$B_0 = 0.246$ LF[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	237.43(2)	gas	LF	1
Σ^+	3	YO stretch	655.34(3)	gas	LF	1
			651.2wT	Ar	IR	2

$B_0 = 0.261$ LF[1]

[a] At equilibrium, the molecule is bent and this state is split into A' and A'' states, but with a small barrier to linearity.

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HLaO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	LaH stretch	1180.2	Ar	IR	1
	3	LaO stretch	758.6	Ar	IR	1

DLaO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			753.1	Ar	IR	1

Reference

[1] L. Zhang, L. Shao, and M. Zhou, Chem. Phys. **272**, 27 (2001).

HTiO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	TiH stretch	1483.3	Ar	IR	1
	3	TiO stretch	968.8	Ar	IR	1

DTiO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	TiD stretch	1071.1	Ar	IR	1
	3	TiO stretch	967.9	Ar	IR	1

Reference

[1] M. Zhou, L. Zhang, J. Dong, and Q. Qin, J. Am. Chem. Soc. **122**, 10680 (2000).

HZrO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	ZrH stretch	1544.7	Ar	IR	1
	3	ZrO stretch	908.8	Ar	IR	1

DZrO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	ZrD stretch	1110.1	Ar	IR	1
	3	ZrO stretch	907.4	Ar	IR	1

Reference

[1] M. Zhou, L. Zhang, J. Dong, and Q. Qin, J. Am. Chem. Soc. **122**, 10680 (2000).

HHfO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	HfH stretch	1626.5	Ar	IR	1
	3	HfO stretch	902.9	Ar	IR	1

DHfO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	3	HfO stretch	900.9	Ar	IR	1

Reference

[1] M. Zhou, L. Zhang, J. Dong, and Q. Qin, J. Am. Chem. Soc. **122**, 10680 (2000).

CuOH

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

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

$A_0 = 25.898$; $B_0 = 0.382$; $C_0 = 0.376$ $LF^{1,3}$

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

$T_0 = 15911.546$ gas LF^4

$A_0 = 18.316$; $B_0 = 0.388$; $C_0 = 0.378$ LF^4

$\tilde{X}\,^1A'$ C_s Structure: $LF^{1,3}MW^{5,6}$

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

$A_0 = 23.039$; $B_0 = 0.392$; $C_0 = 0.385$ $LF^{1,3}MW^5$

CuOD

$\tilde{B}\,^1A''$ C_s
$T_0 = 18422.335$ gas LF[1,3] $\tilde{B}-\tilde{X}$ 500–560 nm
$A_0 = 14.235$; $B_0 = 0.354$; $C_0 = 0.344$ LF[1,3]

$\tilde{A}\,^1A'$ C_s
$T_0 = 15911.095(3)$ gas LF[4]
$A_0 = 10.714$; $B_0 = 0.361$; $C_0 = 0.346$ LF[4]

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

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

$A_0 = 12.426$; $B_0 = 0.366$; $C_0 = 0.354$ LF[1,3]MW[6]

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AgOH

$\tilde{X}$ C_s Structure: MW[1,2]
$A = 22.22(3)$; $B = 0.277$; $C = 0.273$ MW[1]

AgOD

$\tilde{X}$ C_s
$A = 11.92$; $B = 0.259$; $C = 0.253$ MW[2]

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[2] C. J. Whitham, H. Ozeki, and S. Saito, J. Chem. Phys. **112**, 641 (2000).

YbOH

$\tilde{A}\,^2\Pi$ $C_{\infty v}$
$T_0 = 17998.62$ gas LF[1] $\tilde{A}-\tilde{X}$ 520–580 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	357(5)	gas	LF	1
Σ^+	3	YbO stretch	573(5)	gas	LF	1

$A = 1350$T gas LF[1]
$B_0 = 0.253$ 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	339(5)	gas	LF	1
Σ^+	3	YbO stretch	529.34	gas	LF	1

$B_0 = 0.245$ LF[1]

Reference

[1] T. C. Melville and J. A. Coxon, J. Chem. Phys. **115**, 6974 (2001).

HCC

$3p\sigma$ 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

$\tilde{B}\,^2A'$ C_s Structure: LF[46]
$T_0 \leqslant 39157.4$ gas LF[35,36,40,46]EM[39] $\tilde{B}-\tilde{X}$ 250–313 nm
Approximately 30 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 excited ground-state vibrational levels. However, a definitive assignment of the upper-state energy levels has not been achieved.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	775T	gas	LF	46
	3	CC stretch	1221T	gas	LF	46

$\tau_0 = 287(13)$ ns gas LF[47]
$A_T = 18.82(3)$; $B_T = 1.278$; $C_T = 1.195$ LF[46]
$T_0 \leqslant 29360$ 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[32,43]
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[10,14,19,26,27,32,37,40–42,46] 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 ca. 5 μs near 500 nm to ca. 60 μs near 4000. Unstructured HCC emission between 400 and 500 nm has also been observed[15] on vacuum UV irradiation of C_2H_2 isolated in the solid rare gases.

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	38,45
			1846.2m	Ar	IR	1,3,20,21,45

$A \cong 10$ IR[14]
$B_{000} = 1.457$ MW[4,6,7,9,48]LMR[12]
$B_{020} = 1.451$ LMR[28]

DCC

$3p\sigma$ 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, probably $\tilde{B}\,^2A'$.

$\tilde{A}\,^2\Pi$ $C_{\infty v}$
$T_0 = 3594(50)$T gas PE[43]
<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[22,29,33,44] and photoelectron spectroscopy.[43]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2537.1	Ne	IR	38
Π	2	Bend	288.21	gas	PE,LMR	32,44
Σ^+	3	CC stretch	1743.18	gas	DL	25
			1739.6	Ne	IR	38,45
			1746.3m	Ar	IR	1,3,20,21,45

$B_0 = 1.203$ 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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HCSi

$\tilde{A}\,^2\Sigma^+$ $C_{\infty v}$ Structure: $LF^{4,5}$
$T_0 = 11766.72$ gas $AB^3LF^{4,5,7,8}EM^6$ $\tilde{A}-\tilde{X}$ 605–1300 nm
11749(3)[a] Ne AB^1 $\tilde{A}-\tilde{X}$ 656–852 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	715	gas	LF	4,5
Σ^+	3	CSi stretch	1167.7	gas	AB,LF,EM	3,5,6
			1170(5)	Ne	AB	1

$B_0 = 0.635$ $AB^3LF^5EM^6$

$\tilde{X}\,^2\Pi$ $C_{\infty v}$ Structure: $LF^{4,5}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend (ω)	508.0(4)	gas	LF	7
		($\kappa\,^2\Sigma$)	606.9	gas	LF	7
		($^2\Delta_{3/2}$)	576.0(2)	gas	LF	7
		($^2\Delta_{5/2}$)	505.4(2)	gas	LF	7
		($\mu\,^2\Sigma$)	442.7(2)	gas	LF	7
Σ^+	3	CSi stretch	1014.29	gas	AB,EM	3,6
			1010.4	Ar	IR	2

$A_0 = -69.81$ gas $AB^3LF^{4,5}$
$B_0 = 0.580$ $AB^3LF^{4,5}EM^6$

DCSi

$\tilde{A}\,^2\Sigma^+$ $C_{\infty v}$
$T_0 = 11709.47$ gas $LF^{5,7}$ $\tilde{A}-\tilde{X}$ 617–1290 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	558	gas	LF	5
Σ^+	3	SiC stretch	1127	gas	LF	5

$B_0 = 0.543$ LF^5

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend (ω)	391.0(5)	gas	LF	7
		($\kappa\,^2\Sigma$)	482.9	gas	LF	7
		($^2\Delta_{3/2}$)	460.3(2)	gas	LF	7
		($^2\Delta_{5/2}$)	389.8(2)	gas	LF	7
		($\mu\,^2\Sigma$)	350.2(2)	gas	LF	7
Σ^+	3	CSi stretch	980.5	gas	LF	7
			977.4	Ar	IR	2

$A_0 = -69.94$ gas LF^5
$B_0 = 0.499$ LF^5

[a] Reassigned to HCSi by Ref. 3.

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HCGe

$\tilde{A}\,^2\Sigma^+$ $C_{\infty v}$ Structure: LF^2
$T_0 = 13901.83$ gas $LF^{1,2}$ $\tilde{A}-\tilde{X}$ 555–730 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	638	gas	LF	2
Σ^+	3	CGe stretch	990	gas	LF	2

$B_0 = 0.480$ LF^2

$\tilde{X}\,^2\Pi$ $C_{\infty v}$ Structure: LF^2
$A = -334.7$ gas $LF^{1,2}$
$B_0 = 0.429$ LF^2

DCGe

$\tilde{A}\,^2\Sigma^+$ $C_{\infty v}$
$T_0 = 13845.33$ gas LF^2 $\tilde{A}-\tilde{X}$ 555–730 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	497	gas	LF	2
Σ^+	3	CGe stretch	952	gas	LF	2

$B_0 = 0.409$ LF^2

$\tilde{X}\,^2\Pi$ $C_{\infty v}$
$B_0 = 0.368$ LF^2

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cyc-HSi_2

$\tilde{A}\,^2B_1$ C_{2v}
$T_0 = 160T$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	SiSi stretch	520(20)	gas	PE	1

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

Reference

[1] C. Xu, T. R. Taylor, G. R. Burton, and D. M. Neumark, J. Chem. Phys. **108**, 7645 (1998).

HCN^+

$\tilde{B}$ C_s
$T_0 = 44140(10)$ gas PE[2,4,7]
PEPICO measurements[7] indicate that this state is strongly predissociated. H^+ and, at higher energies, CN^+ have been detected.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	1194(10)	gas	PE	7
	2	Bend	331(10)	gas	PE	7

$\tilde{A}\,^2\Sigma^+$ $C_{\infty v}$
$T_0 = 3260(30)$ gas PE[2]TPE[6]
The $\tilde{A}$ and $\tilde{X}$ states of HCN^+ are strongly coupled by vibronic interaction. A band assignment based on *ab initio* calculations[3] is supported by the results of the TPE study.[6]

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

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3070(30)	gas	PE	1
			3049.9	Ne	IR	5
Π	2	Bend	760(30)T[a]	gas	PE	1
Σ^+	3	CN stretch	1800(30)	gas	PE	1,2

DCN^+

$\tilde{B}$ C_s
$T_0 = 44400(10)$ gas PE[2,7]
PEPICO measurements[7] indicate that this state is strongly predissociated.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CD stretch	984(10)	gas	PE	7
	2	Bend	250(10)	gas	PE	7

$\tilde{A}\,^2\Sigma^+$ $C_{\infty v}$
$T_0 = 3114(30)$ gas PE[2]

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

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2374.1	Ne	IR	5
Σ^+	3	CN stretch	1686(30)	gas	PE	2

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

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HHgCl

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	HgH stretch	2091.9	Ar	IR	1
			2076.0	Kr	IR	1
			2096.0	N_2	IR	1
	2	Bend	546.9	Ar	IR	1
			543.1			
			540.8	Kr	IR	1
			537.3			
			546.7	N_2	IR	1
			541.1			

DHgCl

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	HgD stretch	1500.5	Ar	IR	1
			1503.5	N_2	IR	1

Reference

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$HTiO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	TiH stretch	1341.8	Ar	IR	1
	3	TiO stretch	933.4	Ar	IR	1

$DTiO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	TiD stretch	978.3	Ar	IR	1
	3	TiO stretch	931.1	Ar	IR	1

Reference

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HBO

$\tilde{X}$ $C_{\infty v}$ Structure: MW[3,4,8]IR[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	754.42	gas	DL	5
			756.1m	Ar	IR	1,6,7
Σ^+	3	BO stretch	1825.56	gas	DL	2
			1822.3s	Ar	IR	1,6,7

$B_0 = 1.308$ DL[2]MW[3,4]

DBO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BD stretch	2253.53	gas	DL,EM	8
			2258.9w	Ar	IR	1,7
Π	2	Bend	608.36	gas	EM	8
			607.6m	Ar	IR	1,7
Σ^+	3	BO stretch	1647.69	gas	DL,EM	8
			1650.2m	Ar	IR	1,7

$B_0 = 1.049$ gas MW[4,8]

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$HBCl^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	BCl stretch	1121.57	gas	DL	1

$B_0 = 0.631$ DL[1]

Reference

[1] N. T. Hunt, Z. Liu, and P. B. Davies, Mol. Phys. **97**, 205 (1999).

$HBBr^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	BBr stretch	937.57	gas	DL	1

$B_0 = 0.462$ DL[1]

Reference

[1] N. T. Hunt, D. Collet, Z. Liu, and P. B. Davies, J. Chem. Phys. **111**, 5905 (1999).

HCC^-

Threshold for electron detachment from ground-state $HCC^- = 23950(50)$ gas PE[1,3]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3318.5	Ar	IR	4
Π	2	Bend	505(20)	gas	PE	1
Σ^+	3	CC stretch	1800(20)	gas	PE	1
			1773.0	Ne	IR	2,4
			1770.5	Ar	IR	4

DCC^-

Threshold for electron detachment from ground-state $DCC^- = 23990(50)$ gas PE[1,3]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	395(40)	gas	PE	1
Σ^+	3	CC stretch	1705(20)	gas	PE	1
			1675.7	Ne	IR	4
			1676.7	Ar	IR	4

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cyc-HSi_2^-

Threshold for electron detachment from ground-state *cyc*-HSi_2^- = 18640(80) gas PE[1]

Reference

[1] C. Xu, T. R. Taylor, G. R. Burton, and D. M. Neumark, J. Chem. Phys. **108**, 7645 (1998).

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,MPI	10,11,18
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	666.0	gas	PE,MPI	1,13,19,20
Σ^+	3	CO stretch	1904.06	gas	DL	9

$B_0 = 1.201$ MW[2–4]

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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]

Higher vibrational levels of HNC ($\tilde{X}$) have been analyzed by Ref. 13.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NH stretch	3652.66	gas	IR,EM	3,6,8,11,15–17
			3643.1	Ne	IR	10
			3620s	Ar	IR	2
			3583s N_2	Ar	IR	1,2
			3598.6	Kr	IR	14
			3577.0	Xe	IR	14
			3567s	N_2	IR	2
Π	2	Bend	462.72	gas	IR,EM	8,17
			477s	Ar	IR	2
			535s N_2	Ar	IR	1
			478.2	Kr	IR	14
			477.0	Xe	IR	14
			559s	N_2	IR	2
Σ^+	3	NC stretch	2023.86	gas	IR,EM	8,15,17
			2025.4	Ne	IR	10
			2029w	Ar	IR	2
			2032w N_2	Ar	IR	1
			2024.7	Kr	IR	14
			2021.0	Xe	IR	14
			2035w	N_2	IR	2

$B_0 = 1.512$ MW[4,18]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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HOC^+

$\tilde{X}$ $C_{\infty v}$ Structure: MW[1–3]

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

$B_0 = 1.492$ MW[1,2,5]LD[4]

DOC^+

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

$B_0 = 1.274$ MW[3,5]

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HCO

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

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

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

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

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

$\tilde{B}\ ^2A'$ C_s Structure: MPI,LF[40,46]
$T_0 = 38695.48$ 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 MPI	6,25,29, 30,33
			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

$A_0 = 15.976$; $1/2(B_0 + C_0) = 1.151$; $1/4(B_0 - C_0) = 0.021$ LF[35,43]
$\tau_0 = 89(2)$ 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

$\tau_{090} = 46(4)$ 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
			2442.3	Xe	IR	45
			2488m	CO	IR	4
	2	Bend	1080.76	gas	UV,LS	1,3,8
					LMR	9,10
					LF	25,26
			1087s	Ar	IR	5
			1076.5	Xe	IR	44,45
			1090s	CO	IR	2,4
	3	CO stretch	1868.17	gas	IR	12,23
					LMR	13,25
			1863vs	Ar	IR	5
			1858.4	Xe	IR	44,45
			1856.6			
			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

$A = 0.9(3)$; $\epsilon = 0.069$ MPI[28]

$B = 1.221(12)$ MPI[28]

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

$T_0 = 38629.50(3)$ gas MPI[29]LF[34,40,46] $\tilde{B}-\tilde{X}$ 236–450 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)	gas	MPI,LF	29,40,42,46
	2	CO stretch+bend	1211.8(8)	gas	MPI,LF	29,40,42,46
			1150(35)	Ar	AB	5
			1150(35)	CO	AB	5
	3	Bend+CO stretch	921.6(8)	gas	MPI,LF	29,40,42,46
			925(35)	Ar	AB	5
			925(35)	CO	AB	5

$A_0 = 9.172$; $B_0 = 1.093$; $C_0 = 0.974$ LF[40,46]

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

$T_0 = 9162(3)$ 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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HCS

$\tilde{X}\,^2A'$ C_s
$B_{eff}=0.672$ MW[1]

Reference

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$HCCl^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1078	Ar	IR	1

Reference

[1] T. D. Fridgen, X. K. Zhang, J. M. Parnis, and R. E. March, J. Phys. Chem. A **104**, 3487 (2000).

HSC

$\tilde{X}$ C_s Structure: MW[1]
$A_0=9.841$; $B_0=0.702$; $C_0=0.652$ MW[1]

DSC

$\tilde{X}$ C_s
$A_0=5.201$; $B_0=0.682$; $C_0=0.600$ MW[1]

Reference

[1] H. Habara and S. Yamamoto, J. Chem. Phys. **112**, 10905 (2000).

HSiO

$\tilde{X}$ C_s Structure: MW[1]
$A_0=10.411$; $B_0=0.663$; $C_0=0.621$ MW[1]

Reference

[1] M. Izuha, S. Yamamoto, and S. Saito, J. Mol. Struct. **413/414**, 527 (1997).

HSiS

$\tilde{X}\,^2A'$ C_s Structure: MW[1]
$A_0=10.197$; $B_0=0.281$; $C_0=0.272$ MW[1]

Reference

[1] F. X. Brown, S. Yamamoto, and S. Saito, J. Mol. Struct. **413/414**, 537 (1997).

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 $AB^1CL^3LF^{5,10,16}$ $\tilde{A}-\tilde{X}$ 414–635 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'	1	CH stretch	2852(2)T	gas	LF	16
	2	Bend	1021.26	gas	AB,LF	1,7
			1000(20)	Ar	AB	2
	3	CF stretch	1260(2)	gas	LF	16

$A_0=25.69$; $B_0=1.162$; $C_0=1.107$ AB^1LF^5

$\tau_0=2.45(10)$ μs gas LF^4

$\tau_1=2.57(16)$ μs; $\tau_2=12.5(8)$ 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

$A_0=15.563$; $B_0=1.223$; $C_0=1.130$ $AB^1LF^5SEP^{11}DR^{17}$

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 $AB^{1,8,9}LF^{4,7,13}$ $\tilde{A}-\tilde{X}$ 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: $AB^1LF^{3,13}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	1195	gas	LF	13
			1201wm	Ar	IR	2,11
			1201	Kr	IR	11
	3	CCl stretch	811.60	gas	DL,LF	10,13
			815s	Ar	IR	2,11
			817	Kr	IR	11

$A_0=15.759$; $B_0=0.605$; $C_0=0.581$ $AB^1LF^3MW^{12}$

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

$T_0=11972.43$ gas $LF^3AB^{4-6,8,10}$ $\tilde{A}-\tilde{X}$ 550–955 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	828.7	gas	LF	3,6
	3	CBr stretch	783T	gas	LF	3

Barrier to linearity approximately 13590 above $\tilde{X}(000)$.[3]

$B_{av}=0.437$ AB^8

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

$T_0=2006(8)$ gas LF^9

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	994	gas	LF	9
	3	CBr stretch	733	gas	PE,LF	2,9

$\tilde{X}\,^1A'$ C_s Structure: $AB^{4,5,8}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	1117.2	gas	LF,AB	9,10
	3	CBr stretch	676	gas	PE,LF	1,2,9

$A_0=15.534$; $B_0=0.429$; $C_0=0.417$ $AB^{4-6,8,10}$

DCBr

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

$T_0=11966.28$ gas $LF^3AB^{5,6,8,10}DL^7$ $\tilde{A}-\tilde{X}$ 550–970 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	608	gas	LF	3,6
	3	CBr stretch	737T	gas	LF	3,6

$A_0=17.99(3)$ AB^6DL^7

$B_{av}=0.383$ AB^8

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	832.75	gas	AB,DL,LF	6,7,10,11
	3	CBr stretch	663	gas	LF	11

$A_0=8.618$; $B_0=0.394$; $C_0=0.376$ $AB^{5,6,8,10}$

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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

$\tau_0 = 175(6)$ ns gas LF[2,3]
$A_0 = 9.319$; $B_0 = 0.549$; $C_0 = 0.516$ LF[3–5]
Barrier to linearity = 9130(20) LF[5]

$\tilde{X}\,^1A'$ C_s Structure: LF[3,4,6,7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SiH stretch	1930(3)	gas	LF	7
			1913s	Ar	IR	1
	2	Bend	860.8(6)	gas	LF	2,7
			859m	Ar	IR	1
	3	SiF stretch	838(2)	gas	LF	7
			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	1402(4)	gas	LF	7
			1387m	Ar	IR	1
	2	Bend	640.7(5)	gas	LF	6,7
			638w	Ar	IR	1
	3	SiF stretch	839.6(6)	gas	IR	7
			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^1LF^2

$T_0 = 20717.77$ gas $UV^1LF^{2,3}$ $\tilde{A}-\tilde{X}$ 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

$\tau_0 = 432(20)$ ns gas LF^2
$A_0 = 9.840(2)$; $B_0 = 0.247$; $C_0 = 0.240$ UV^1LF^2

$\tilde{X}\,^1A'$ C_s Structure: $UV^1LF^{2,4}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SiH stretch	1968.6(8)	gas	LF	2,4
	2	Bend	806.6(2)	gas	UV,LF	1,2,4
	3	SiCl stretch	522.6(4)	gas	UV,LF	1,2,4

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

$\tau_0 = 437(20)$ 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	gas	LF	2,4
	2	Bend	593.4	gas	LF	2,4
	3	SiCl stretch	518.2(5)	gas	LF	2,4

$A_0 = 3.970$; $B_0 = 0.240$; $C_0 = 0.226$ 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
$\tau_0 = 598(18)$ ns gas LF^2

$\tilde{X}\,^1A'$ C_s Structure: $UV^1LF^{2,3}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SiH stretch	1976	gas	LF	2,3
	2	Bend	772.4(3)	gas	UV,LF	1–3
	3	SiBr stretch	412.7(5)	gas	UV,LF	1–3

$A_0 = 7.576(8)$; $B_0 = 0.158$; $C_0 = 0.155$ 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

$\tau_0 = 586(21)$ 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	1440	gas	LF	2,3
	2	Bend	562.8(2)	gas	LF	3
	3	SiBr stretch	407.8(7)	gas	LF	2,3

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

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HSiI

$\tilde{A}\,^1A''$ C_s Structure: AB^1
$T_0 = 18259.02$ gas AB^1LF^2 $\tilde{A}-\tilde{X}$ 460–560 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SiH stretch	1852.5	gas	LF	2
	2	Bend	485.0	gas	AB,LF	1,2
	3	SiI stretch	335.7	gas	LF	2

$\tau_0 = 1.23(3)$ μs gas LF^2
$A_0 = 9.807$; $B_0 = 0.118$; $C_0 = 0.116$ AB^1LF^2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	727	gas	AB	1
	2	SiI stretch	350.0	gas	LF	2

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

DSiI

$\tilde{A}\,^1A''$ C_s
$T_0 = 18302.96$ gas AB^1LF^2 $\tilde{A}-\tilde{X}$ 460–560 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SiD stretch	1356T	gas	LF	2
	2	Bend	368	gas	AB,LF	1,2
	3	SiI stretch	325	gas	LF	2

$\tau_0 = 1.22(9)$ μs gas LF^2
$A_0 = 5.198$; $B_0 = 0.112$; $C_0 = 0.110$ LF^2

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HGeCl

$\tilde{A}\,^1A''$ C_s Structure: $LF^{3,4}$
$T_0 = 21514.68$ gas $CL^2LF^{3,4}$ $\tilde{A}-\tilde{X}$ 439–520 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	GeH stretch	1262.9(2)	gas	LF	4
	2	Bend	431.2(2)	gas	CL,LF	2–4
	3	GeCl stretch	398.8(2)	gas	LF	4

$\tau_0 = 548(19)$ ns gas LF^4
$A_0 = 7.961(3)$; $B_0 = 0.151$; $C_0 = 0.147$ LF^4

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

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

$A_0=6.748(15)$; $B_0=0.149$; $C_0=0.146$ LF[4]

DGeCl

$\tilde{A}\,^1A''$ C_s
$T_0=21614.48$ gas LF[4] $\tilde{A}-\tilde{X}$ 441–462 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	GeD stretch	979.6(2)	gas	LF	4
	2	Bend	321.7(2)	gas	LF	4
	3	GeCl stretch	398.9(2)	gas	LF	4

$\tau_0=527(26)$ ns gas LF[4]
$A_0=4.145(3)$; $B_0=0.149$; $C_0=0.142$ LF[4]

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

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

$A_0=3.435(14)$; $B_0=0.148$; $C_0=0.143$ LF[4]

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HGeBr

$\tilde{A}\,^1A''$ C_s Structure: LF[2,3]
$T_0=20660.30$ gas LF[2,3] $\tilde{A}-\tilde{X}$ 450–500 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	GeH stretch	1380.8(2)	gas	LF	3
	2	Bend	419.3(2)	gas	LF	2,3
	3	GeBr stretch	280.3(2)	gas	LF	3

$\tau_0=736(24)$ ns gas LF[3]
$A_0=8.184(4)$; $B_0=0.082$; $C_0=0.081$ LF[3]

$\tilde{X}\,^1A'$ C_s Structure: LF[2,3]

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

$A_0=6.736(14)$; $B_0=0.081$; $C_0=0.080$ LF[3]

DGeBr

$\tilde{A}\,^1A''$ C_s
$T_0=20746.43$ gas LF[3] $\tilde{A}-\tilde{X}$ 462–482 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	GeD stretch	1047.6(2)	gas	LF	3
	2	Bend	312.1(2)	gas	LF	3
	3	GeBr stretch	278.5(2)	gas	LF	3

$\tau_0=733(37)$ ns gas LF[3]
$A_0=4.210(4)$; $B_0=0.080$; $C_0=0.079$ LF[3]

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

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

$A_0=3.305(13)$; $B_0=0.080$; $C_0=0.078$ LF[3]

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HGeI

$\tilde{A}\,^1A''$ C_s Structure: LF[1]
$T_0=18929.29$ gas LF[1] $\tilde{A}-\tilde{X}$ 482–529 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	GeH stretch	1542.5(2)	gas	LF	1
	2	Bend	337.1(2)	gas	LF	1
	3	GeI stretch	203.4(2)	gas	LF	1

$\tau_0=1.515(4)$ μs gas LF[1]
$A_0=8.052$; $B_0=0.055$; $C_0=0.055$ LF[1]

$\tilde{X}\,^1A'$ C_s Structure: LF[1]
$A_0=6.714$; $B_0=0.056$; $C_0=0.056$ LF[1]

DGeI

$\tilde{A}\,^1A''$ C_s
$T_0=19001.76$ gas LF[1] $\tilde{A}-\tilde{X}$ 496–527 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	GeD stretch	1144.2(2)	gas	LF	1
	2	Bend	259.7(2)	gas	LF	1
	3	GeI stretch	205.0(2)	gas	LF	1

$\tau_0=1.52(3)$ μs gas LF[1]
$A_0=4.158$; $B_0=0.055$; $C_0=0.054$ LF[1]

$\tilde{X}\,^1A'$ C_s
$A_0=3.424$; $B_0=0.056$; $C_0=0.055$ LF[1]

Reference

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HON

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3467.2wm	Ar	IR	1
	2	Bend	1095.6vs	Ar	IR	1

DON

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2563.6wm	Ar	IR	1
	2	Bend	868.8s	Ar	IR	1
	3	ON stretch	1149.0vs	Ar	IR	1

Reference

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BiOH

$\tilde{A}\,{}_1A'$[a] C_s
$T_0 = 22782$ gas LF[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	BiO stretch	272	gas	LF	2

$\tau_0 = 0.92(3)\ \mu s$ gas LF[2]
$A_0 - 1/2(B_0 + C_0) = 23.99(5)$ LF[2]

$\tilde{a}\,{}_1A'$[a] C_s
$T_0 = 11326(50)$ gas LF[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	BiO stretch	520(70)	gas	LF	2

$\tilde{X}\,{}_3A'$[a] C_s
$T_0 = 6183.8(3)$ gas CL[1,2]

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

$A_0 - 1/2(B_0 + C_0) = 23.09$ LF[2]

$\tilde{X}\,{}_2A''$[a] C_s
$T_0 = 6171.4$ gas CL[1] $\tilde{X}_2A'' - \tilde{X}_1A'$ 1580–1677 nm
$A_0 - 1/2(B_0 + C_0) = 22.6$ CL[1]

$\tilde{X}\,{}_1A'$[a] C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3669(50)	gas	LF	2
	3	BiO stretch	504.7(4)	gas	CL,LF	1,2

$A_0 - 1/2(B_0 + C_0) = 23.47(6)$ CL[1,2]

BiOD

$\tilde{A}\,{}_1A'$[a] C_s
$T_0 = 22815$ gas LF[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	BiO stretch	266	gas	LF	2

$A_0 - 1/2(B_0 + C_0) = 12.68(2)$ LF[2]

$\tilde{a}\,{}_1A'$[a] C_s
$T_0 = 11294(50)$ gas LF[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	BiO stretch	520(70)	gas	LF	2

$\tilde{X}\,{}_3A'$[a] C_s
$T_0 = 6179.3(2)$ gas CL[1,2]
$A_0 - (B_0 + C_0) = 12.37(2)$ LF[2]

$\tilde{X}\,{}_2A''$[a] C_s
$T_0 = 6168.1$ gas CL[1] $\tilde{X}_2A'' - \tilde{X}_1A'$ 1582–1665 nm
$A_0 - 1/2(B_0 + C_0) = 12.0$ CL[1]

$\tilde{X}\,{}_1A'$[a] C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2662(50)	gas	LF	2
	3	BiO stretch	492.6(5)	gas	CL,LF	1,2

$A_0 - 1/2(B_0 + C_0) = 12.49(2)$ CL[1]LF[2]

[a]Fine structure component of electronic state.

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HPCl

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

$T_0 = 21305(6)$ gas EM[1] $\tilde{A}-\tilde{X}$ 420–590 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	622(4)	gas	EM	1
	3	PCl stretch	529(8)	gas	EM	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	868(2)	gas	EM	1

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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

$T_0 = 7029.688$ gas AB[9,15]EM[10,16,19,20,35,41] $\tilde{A}-\tilde{X}$ 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[16,20,41]

$\tilde{X}\,^2A''$ 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
			3412.5 s[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
			1388.5 vs[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
			1101.1 s[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
			2529.5 m[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
			1019.9 s[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
			1122.9 vw[a]	Ar	IR	7

$A_0 = 11.194$; $B_0 = 1.056$;
$C_0 = 0.961$ MW[14,27,34,42]EM[21,42]LMR[22,23,34]ESR[23]

[a]Refined value from unpublished Fourier transform spectra.

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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[5,8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SH stretch	2463T 2460T	Ar	IR	7
	2	Bend	904(8)	gas	CL	4
			903T	Ar	IR	7
	3	SS stretch	595(4)	gas	CL	4

$A_0 = 9.906$; $B_0 = 0.267$; $C_0 = 0.259$ MW[5,8]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[5,8]

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HO_2^-

Threshold for electron detachment from ground-state HO_2^- is 8790(50).[1,2]

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

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

DO_2^-

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

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

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

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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	1,2,11,14,18
			2647	Ar	IR	3
	2	Bend	909.63	gas	IR,DL	1,11,14,17
			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[6,8,10,11] to HOBr.

In the gas phase, an absorption maximum near 350 nm (28600) has been assigned[6,8,10,11] to HOBr.

In the gas phase, a relatively weak absorption maximum and a maximum in the production of OH near 457 nm (21900) is believed to arise from excitation of HOBr to a dissociative triplet state.[9–11]

$\tilde{X}$ 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	2668.79	gas	IR	12
			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^3IR^{12}

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HOI

In the gas phase, broad absorption maxima at 29380 (340 nm) and 24610 (406 nm) have been assigned[4] to 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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$NeHF^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NeH stretch	292.4T	Ne	IR	1
Σ^+	3	HF stretch	2218.4	Ne	IR	1

$NeDF^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	DF stretch	1663.0	Ne	IR	1

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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[ab]	Ar	IR	1–3,7,9,10
			252.8[b]	Kr	IR	7,9
			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	1–3,7,9,10
			662.8	Kr	IR	7,9,10
			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[ab]	Ar	IR	1–3,9
			255.3[b]	Kr	IR	7
Σ_u^+	3	Asym. stretch	496.2	Ne	IR	8
			489.3			
			463[a]	Ar	IR	1–3,10
			437.7	Kr	IR	7,10

[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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HArF

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	HAr stretch	2020.8[a]	Ar	IR	1,2
			2016.3[a]			
			1969.5			
Π	2	Bend	697.0[a]	Ar	IR	1,2
			693.5[a]			
			687.0			
Σ^+	3	ArF stretch	435.7	Ar	IR	1

DArF

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	DAr stretch	1497.1[a]	Ar	IR	1,2
			1493.8[a]			
			1466.3			
Π	2	Bend	513.0	Ar	IR	1
Σ^+	3	ArF stretch	435.3	Ar	IR	1

[a]Relatively great thermal stability.[2]

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HKrCl

In a krypton matrix, a maximum in the photodecomposition cross section of HKrCl has been observed[2] near 35700 (280 nm).

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

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

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HXeCl

In a xenon matrix, an unstructured absorption maximum at 40650 (246 nm) has been assigned[3] to HXeCl.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	HXe stretch	1611.8	Ne	IR	2
			1664	Kr	IR	1
			1649	Xe	IR	1,3

DXeCl

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	DXe stretch	1172.1	Ne	IR	2
			1198	Xe	IR	1

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[3] J. Ahokas, K. Vaskonen, J. Eloranta, and H. Kunttu, J. Phys. Chem. A **104**, 9506 (2000).

HXeBr

In a xenon matrix, an unstructured absorption maximum at 38170 (262 nm) has been assigned[4] to HXeBr.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	HXe stretch	1452.5	Ne	IR	2,3
			1524	Kr	IR	1
			1504vs	Xe	IR	1,4
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	1064.1	Ne	IR	3
			1100s	Xe	IR	1

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HXeI

In a xenon matrix, an unstructure absorption maximum at 31750 (315 nm) has been assigned[4] to 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	1–4
Π	2	Bend	450w	Xe	IR	1,3
Σ^+	3	XeI stretch	146T	Xe	IR	3

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	1–3

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[1] M. Pettersson, J. Lundell, and M. Räsänen, J. Chem. Phys. **102**, 6423 (1995).
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[4] J. Ahokas, K. Vaskonen, J. Eloranta, and H. Kunttu, J. Phys. Chem. A **104**, 9506 (2000).

HAr_2^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	237[a]	Ar	IR	5
Σ_u^+	3	Asym. stretch	903.4wm[b]	Ar	IR	1,2,4–6

DAr_2^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	644s[b]	Ar	IR	1–5,7

[a] $(\nu_1+\nu_3)-\nu_3$.
[b] Assigned in Ref. 1 to vibration of uncharged H (or D) atoms trapped in the Ar lattice. Reassigned by Ref. 2 to the cation. Peak at 644 cm^{-1} was prominent in deuteron radiolysis experiments.[3] Reference 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^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	155[a]	Kr	IR	4,7,8
Σ_u^+	3	Asym. stretch	885.3T[b]	Ar	IR	5,6
			853.2m[c]	Kr	IR	1–4,7,8

DKr_2^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	165[a]	Kr	IR	4,8
Σ_u^+	3	Asym. stretch	625T	Ar	IR	5
			606m[c]	Kr	IR	1,4,8

[a] $(\nu_1+\nu_3)-\nu_3$.
[b] Reassignment proposed by Ref. 6.
[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. Reference 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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[1] V. E. Bondybey and G. C. Pimentel, J. Chem. Phys. **56**, 3832 (1972).
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HXe_2^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	124.4T[ab]	Ar	IR	2,3
			118.6T[ab]	Kr	IR	2,3
			111.9[b]	Xe	IR	1,4
Σ_u^+	3	Asym. stretch	828.1T[a]	Ar	IR	2,3
			781.7T[a]	Kr	IR	2,3
			729.9	Xe	IR	1,4

DXe_2^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	118.0[b]	Xe	IR	1,4
Σ_u^+	3	Asym. stretch	538.1T	Kr	IR	2
			516.7	Xe	IR	1,4

[a]Reassignment proposed by Ref. 3.
[b]$(\nu_1+\nu_3)-\nu_3$.

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[4] T. D. Fridgen, X. K. Zhang, J. M. Parnis, and R. E. March, J. Phys. Chem. A **104**, 3487 (2000).

Kr_2H[a]

$\tilde{A}$
$T_0=64500$ Kr AB[4,6]
In a Kr matrix, unstructured emission with maximum at 49600 (202 nm)[1–4]
τ=48 ns Kr EM[2]

Kr_2D

$\tilde{A}$
$T_0=64800$ Kr AB[4,6]
In an Ar matrix, unstructured emission with maximum at 50750 (197 nm)[5]
In a Kr matrix, unstructured emission with maximum at 49700 (201 nm)[2,4]
τ=58 ns Ar EM[5]
46 ns Kr EM[2]

[a]Excimer. Extensive delocalization of positive charge in Kr and Xe matrices.

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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
$T_0=14575.5$ gas MPI[2,3,5,6]DR[7,8] $\tilde{A}-\tilde{X}$ 660–706 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	261.4	gas	MPI	6
	2		112.6	gas	MPI	6

$B=0.57$ MPI[4]. $A_{ps}=0.738$; $B_{ps}=0.398$; $C_{ps}=0.255$ DR[7]

$\tilde{X}\,^2E'$ 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]. $A_{ps}=0.705$; $B_{ps}=0.468$; $C_{ps}=0.278$ DR[7]

[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	MPIPF	8

Extensive vibronic structure has been tentatively assigned[8] to energy levels derived from excitation of $\nu_2(e')$, perturbed by dynamic Jahn–Teller interaction.
$\tau_0 = 7(3)$ ns gas MPI[7]
$\tau_{frag} = 1.12$ 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]
$T_0 = 16124.46$ gas MPI[1–6,17,20–24]DPI[12]TPE[18]DR[28] $\tilde{B}–\tilde{X}$ 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]

$2 \, ^4E'$ D_{3h}
$T_0 = 15791.39 + x$ He LF[27,30] $2 \, ^4E' – 1 \, ^4A_2'$ 616–649 nm

e'	2	Asym. stretch	88.2	He	LF	27

$\tilde{A} \, ^2E''(^2A_2)$ $D_{3h}(C_{2v})^a$ Structure: MPI[15,16]
$T_0 = 14894.769(4)$ gas MPI[1,2,4–6,11,13,15,16,26] DPI[12]DR[28] $\tilde{A}–\tilde{X}$ 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.
$\tau_0 = 60(10)$ 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}
$T_0 = 13200$U gas DPI[12,29]

$1 \, ^4A_2'$ D_{3h}
$T_0 = x$ He LF[27,30] $2 \, ^4E' – 1 \, ^4A_2'$ 616–649 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	40T	He	LF	30
e'	2	Asym. stretch	40T	He	LF	30

$\tilde{X} \, ^2E'(^2B_2)$ $D_{3h}(C_{2v})^a$ 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

$A_0 = 0.179$; $B_0 = 0.085$; $C_0 = 0.057$ MPI[15,16,22]DR[28]

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

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K_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Sym. stretch	81.5	Kr	Ra	1
		Deformation	61.0	Kr	Ra	1

Reference

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Rb_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Sym. stretch	53.9	Ar	Ra	1
		Deformation	38.3	Ar	Ra	1

Reference

[1] A. Kornath, A. Zoermer, and R. Ludwig, Inorg. Chem. **38**, 4696 (1999).

Cs_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Sym. stretch	39.5	Ar	Ra	1
		Deformation	24.4	Ar	Ra	1

Reference

[1] A. Kornath, A. Zoermer, and R. Ludwig, Inorg. Chem. **38**, 4696 (1999).

Hf_3

In an argon matrix, overlapping absorption maxima are observed[1] at 16500, 16390, 16260, and 16150 (606, 610, 615, and 619 nm, respectively).

$\tilde{E}$ D_{3h}
$T_0 = 785.4(2)$ Ar Ra[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	150.3	Ar	Ra	1
e'	2	Deformation	108.7	Ar	Ra	1

$\tilde{D}$ D_{3h}
$T_0 = 642.8(5)$ Ar Ra[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	149.5(9)	Ar	Ra	1
e'	2	Deformation	108.4(9)	Ar	Ra	1

$\tilde{C}$
$T_0 = 609.6(5)$ Ar Ra[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			116.7(1.3)	Ar	Ra	1

$\tilde{B}$
$T_0 = 413.4(6)$ Ar Ra[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	141.7(1.1)	Ar	Ra	1

$\tilde{A}$ D_{3h}
$T_0 = 319.0(3)$ Ar Ra[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	152.3(4)	Ar	Ra	1
e'	2	Deformation	102.7(1.9)	Ar	Ra	1

$\tilde{X}\,E'$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	142.5	Ar	Ra	1

Reference

[1] H. Wang, Z. Hu, H. Haouari, R. Craig, Y. Liu, J. R. Lombardi, and D. M. Lindsay, J. Chem. Phys. **106**, 8339 (1997).

Ta_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	251.2	Ar	Ra	1

Reference

[1] L. Fang, X. Shen, X. Chen, and J. R. Lombardi, Chem. Phys. Lett. **332**, 299 (2000).

Cr_3

In an argon matrix, an absorption maximum at 20960 (477 nm) behaves appropriately for assignment to Cr_3.[1,2] The corresponding maximum appears in a krypton matrix at 20880 (479 nm).[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	400	Ar	Ra	2
e'	2	Deformation	302	Ar	Ra	2

References

[1] W. E. Klotzbücher and G. A. Ozin, J. Am. Chem. Soc. **100**, 2262 (1978).
[2] L. Fang, B. Davis, H. Lu, and J. R. Lombardi, J. Phys. Chem. A **105**, 9375 (2001).

Fe_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Sym. stretch	249T	Ar	Ra	1

Reference

[1] T. L. Haslett, K. A. Bosnick, S. Fedrigo, and M. Moskovits, J. Chem. Phys. **111**, 6456 (1999).

Ru_3

$T_0 = 581.5$ Ar Ra[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	303.4	Ar	Ra	1

Reference

[1] L. Fang, X. Shen, X. Chen, and J. R. Lombardi, Chem. Phys. Lett. **332**, 299 (2000).

Rh_3

$T_0 = 400$ Ar Ra[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	321.9(5)	Ar	Ra	1
	2	Bend	247.9(8)	Ar	Ra	1
b_2	3	Asym. stretch	259	Ar	Ra	1

Reference

[1] L. Fang, X. Shen, X. Chen, and J. R. Lombardi, J. Chem. Phys. **113**, 7178 (2000).

Ag_3

In an argon matrix study with mass selection,[8,12] an absorption maximum at 31150 (321 nm) behaves appropriately for assignment to Ag_3, as does an emission maximum at 26700 (374 nm). Irradiation of the deposit at 388 nm results in the replacement of this absorption maximum by peaks at 28570 (350 nm) and 27550 (363 nm) and by growth in the same fluorescence emission.[12] The new absorption maxima are attributed to Ag_3 trapped in more stable sites.

In a krypton matrix study,[6] the corresponding absorption maximum lies at 30200 (331 nm), and there is an emission maximum at 26200 (381 nm). In mass-selection observations,[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

$\tau < 80$ 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. In an argon-matrix study of mass-selected Ag_3,[12] the maximum at 23870 (419 nm) was replaced by one at 23470 (426 nm) on 388-nm irradiation of the deposit.

$^2A_1'$? 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. A subsequent study[12] of mass-selected Ag_3 isolated in an argon matrix suggested that an absorption maximum at 19880 (503 nm) and an emission maximum at 16450 (608 nm) are associated with a less stable site. That study also suggested the existence of a third site with absorption and emission maxima at 20490 (488 nm) and 16180 (618 nm), respectively. 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
			119	Ar	Ra	11
			120T	Kr	Ra	1
e'	2	Deformation	99	gas	LF	7,9

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

References

[1] W. Schulze, H. U. Becker, R. Minkwitz, and K. Manzel, Chem. Phys. Lett. **55**, 59 (1978).
[2] W. Schulze, H. U. Becker, and H. Abe, Chem. Phys. **35**, 177 (1978).
[3] G. A. Ozin, H. Huber, and S. A. Mitchell, Inorg. Chem. **18**, 2932 (1979).
[4] P. Y. Cheng and M. A. Duncan, Chem. Phys. Lett. **152**, 341 (1988); Chem. Phys. Lett. **156**, 420 (1989).
[5] K. LaiHing, P. Y. Cheng, and M. A. Duncan, Z. Phys. D **13**, 161 (1989).
[6] W. Harbich, S. Fedrigo, F. Meyer, D. M. Lindsay, J. Lignieres, J. C. Rivoal, and D. Kreisle, J. Chem. Phys. **93**, 8535 (1990).
[7] A. M. Ellis, E. S. J. Robles, and T. A. Miller, Chem. Phys. Lett. **201**, 132 (1993).

[8] S. Fedrigo, W. Harbich, and J. Buttet, J. Chem. Phys. **99**, 5712 (1993).
[9] E. E. Wedum, E. R. Grant, P. Y. Cheng, K. F. Willey, and M. A. Duncan, J. Chem. Phys. **100**, 6312 (1994).
[10] T. Okazaki, Y. Saito, A. Kasuya, and Y. Nishina, J. Chem. Phys. **104**, 812 (1996).
[11] T. L. Haslett, K. A. Bosnick, S. Fedrigo, and M. Moskovits, J. Chem. Phys. **111**, 6456 (1999).
[12] I. Rabin, W. Schulze, G. Ertl, C. Felix, C. Sieber, W. Harbich, and J. Buttet, Chem. Phys. Lett. **320**, 59 (2000).

Hg_3

In the gas phase, an excitation maximum at 44135 has been tentatively attributed[2] to Hg_3.

In an argon matrix, a weak, broad absorption and an excitation maximum at 39800 have been attributed[1] to Hg_3.

In the gas phase, fluorescence maxima at 24745, 22930, and 20000 have been tentatively attributed[2] to Hg_3.

In an argon matrix, a fluorescence maximum at 19800 has been attributed[1] to Hg_3.

References

[1] C. Crépin and A. Tramer, J. Chem. Phys. **100**, 5475 (1994).
[2] J. Koperski, J. B. Atkinson, and L. Krause, J. Mol. Spectrosc. **187**, 181 (1998).

LiOLi

$^1B_1$ C_{2v}

$T_0 = 21331$ gas MPI[5]LF[6] $^1B_1 - \tilde{X}$ 433–645 nm

$\tilde{X}\ ^1\Sigma^+$ $D_{\infty h}$ Structure: MPI[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	784(6) (ω)	gas	LF	6
Π_u	2	Bend	122(4) (ω)	gas	LF	6
			112	Kr	IR	2
Σ_u^+	3	Asym. stretch	964(7)H	gas	LF	6
			997.3	Ar	IR	4
			986.5	Kr	IR	1,2
			945.6	N_2	IR	3

$B_0 = 0.466(4)$ MPI[5]

References

[1] D. White, K. S. Seshadri, D. F. Dever, D. E. Mann, and M. J. Linevsky, J. Chem. Phys. **39**, 2463 (1963).
[2] K. S. Seshadri, D. White, and D. E. Mann, J. Chem. Phys. **45**, 4697 (1966).
[3] R. C. Spiker, Jr., and L. Andrews, J. Chem. Phys. **58**, 702 (1973).
[4] L. Andrews, W. Saffell, and J. T. Yustein, Chem. Phys. **189**, 343 (1994).
[5] D. Bellert and W. H. Breckenridge, J. Chem. Phys. **114**, 2871 (2001).
[6] D. Bellert, D. K. Winn, and W. H. Breckenridge, Chem. Phys. Lett. **348**, 39 (2001).

cyc-Co_2N

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CoN s-stretch	746.8	Ar	IR	1
			745.4	N_2	IR	1

Reference

[1] L. Andrews, A. Citra, G. V. Chertihin, W. D. Bare, and M. Neurock, J. Phys. Chem. A **102**, 2561 (1998).

CoCoN

$\tilde{X}$ C_5

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CoN stretch	1016.6T	N_2	IR	1

Reference

[1] L. Andrews, A. Citra, G. V. Chertihin, W. D. Bare, and M. Neurock, J. Phys. Chem. A **102**, 2561 (1998).

cyc-RhRhN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	728.0	Ar	IR	1
			738.9	N_2	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **103**, 3410 (1999).

RhRhN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	RhN stretch	975.6	Ar	IR	1
			971.5	N_2	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **103**, 3410 (1999).

NiNiN

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NiN stretch	1003.2	Ar	IR	1
			996.0	N_2	IR	1

Reference

[1] L. Andrews, A. Citra, G. V. Chertihin, W. D. Bare, and M. Neurock, J. Phys. Chem. A **102**, 2561 (1998).

Pt_2N

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			732.1	N_2	IR	1

Reference

[1] A. Citra, X. Wang, W. D. Bare, and L. Andrews, J. Phys. Chem. A **105**, 7799 (2001).

PtPtN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1095.2	N_2	IR	1

Reference

[1] A. Citra, X. Wang, W. D. Bare, and L. Andrews, J. Phys. Chem. A **105**, 7799 (2001).

Pr_2N

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	PrN stretch	475.7	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **102**, 10238 (1998).

Nd_2N

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NdN stretch	477.4	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **102**, 10238 (1998).

Eu_2N

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	EuN stretch	451.3	N_2	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **102**, 10238 (1998).

Gd_2N

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	GdN stretch	494.4	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **102**, 10238 (1998).

Tb_2N

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	TbN stretch	502.7	Ar	IR	1
			468.6	N_2	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 1311 (1999).

Dy_2N

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	DyN stretch	505.3	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 1311 (1999).

Ho_2N

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	HoN stretch	509.4	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 1311 (1999).

Lu_2N

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	LuN stretch	522.0	Ar	IR	1
			513.3	N_2	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 1311 (1999).

ScOSc

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	892.9	Ar	IR	1

Reference

[1] G. V. Chertihin, L. Andrews, M. Rosi, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **101**, 9085 (1997).

CrOCr

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Antisym. stretch	804T	Ar	IR	1

Reference

[1] G. V. Chertihin, W. D. Bare, and L. Andrews, J. Chem. Phys. **107**, 2798 (1997).

MnOMn

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Asym. stretch	808.3	Ar	IR	1
			806.0	N_2	IR	1

Reference

[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. A **101**, 8547 (1997).

cyc-Ir_2O

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	673.3	Ar	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **103**, 4182 (1999).

AgOAg

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Stretch	443.3T	Ar	IR	1,2

References

[1] D. E. Tevault, R. R. Smardzewski, M. W. Urban, and K. Nakamoto, J. Chem. Phys. **77**, 577 (1982).
[2] A. Citra and L. Andrews, J. Mol. Struct. **489**, 95 (1999).

cyc-B_2C

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	B–B stretch	1392.8	Ar	IR	1

Reference

[1] C. W. Larson and J. D. Presilla-Márquez, J. Chem. Phys. **111**, 1988 (1999).

ScCC

$\tilde{B}$
$T_0 = 8880(240)$ gas PE[1]
$\tilde{A}$
$T_0 = 2340(240)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ScC stretch	550(60)	gas	PE	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		ScC_2 s-stretch	670(40)	gas	PE	1

Reference

[1] X. Li and L.-S. Wang, J. Chem. Phys. **111**, 8389 (1999).

TiCC

$\tilde{D}$
$T_0 = 9410(500)$ gas PE[1]
$\tilde{C}$
$T_0 = 7240(290)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			720(50)	gas	PE	1

$\tilde{B}$
$T_0 = 4620(260)$ gas PE[1]
$\tilde{A}$
$T_0 = 3730(230)$ gas PE[1]
$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			560(50)	gas	PE	1

Reference

[1] X.-B. Wang, C.-F. Ding, and L.-S. Wang, J. Phys. Chem. A **101**, 7699 (1997).

VCC

$\tilde{C}$
$T_0 = 13800(160)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		VC stretch	370(40)	gas	PE	1

$\tilde{B}$
$T_0 = 12020(160)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		VC stretch	480(40)	gas	PE	1

$\tilde{A}$
$T_0 = 3870(160)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		VC stretch	520(50)	gas	PE	1

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		VC stretch	550(40)	gas	PE	1

Reference

[1] X. Li and L.-S. Wang, J. Chem. Phys. **111**, 8389 (1999).

NbCC

$\tilde{A}\,^4A_2$ C_{2v}
$T^a = 9400(280)$ gas PE[1]

$\tilde{c}\,^2A_1$ C_{2v}
$T^a = 8350(280)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		560(50)	gas	PE	1

$\tilde{b}\,^2a_2$ C_{2v}
$T^a = 6250(280)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		540(50)	gas	PE	1

$\tilde{a}\,^2B_1$ C_{2v}
$T^a = 3510(260)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		550(40)	gas	PE	1

$\tilde{X}\,^4B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		530(30)	gas	PE	1

[a] From vertical electron detachment energy.

Reference

[1] H.-J. Zhai, S.-R. Liu, X. Li, and L.-S. Wang, J. Chem. Phys. **115**, 5170 (2001).

CrCC

$\tilde{G}$
$T_0 = 14280(160)$ gas PE[1]

$\tilde{F}$
$T_0 = 11130(160)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CrC stretch	550(60)	gas	PE	1

$\tilde{E}$
$T_0 = 10080(160)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CrC stretch	540(60)	gas	PE	1

$\tilde{D}$
$T_0 = 8470(160)$ gas PE[1]

$\tilde{C}$
$T_0 = 6780(160)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CrC stretch	480(60)	gas	PE	1

$\tilde{B}$
$T_0 = 5650(160)$ gas PE[1]

$\tilde{A}$
$T_0 = 3150(80)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CrC stretch	540(30)	gas	PE	1

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CrC stretch	510(30)	gas	PE	1

Reference

[1] X. Li and L.-S. Wang, J. Chem. Phys. **111**, 8389 (1999).

MnCC

$\tilde{B}$
$T_0 = 7580(160)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		MnC stretch	330(40)	gas	PE	1

$\tilde{A}$
$T_0 = 5970(80)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		MnC stretch	450(40)	gas	PE	1

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		MnC stretch	520(30)	gas	PE	1

Reference

[1] X. Li and L.-S. Wang, J. Chem. Phys. **111**, 8389 (1999).

FeCC

$\tilde{B}$
$T_0 = 9520(160)$ gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		FeC stretch	420(60)	gas	PE	2

$\tilde{A}$
$T_0 = 8070(160)$ gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		FeC stretch	480(50)	gas	PE	2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		FeC_2 s-stretch	560(30)	gas	PE	2

References

[1] J. Fan and L.-S. Wang, J. Phys. Chem. **98**, 11814 (1994).
[2] X. Li and L.-S. Wang, J. Chem. Phys. **111**, 8389 (1999).

CoCC

$\tilde{A}$
$T_0 = 7420(480)$ gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CoC stretch	540(60)	gas	PE	1

Reference

[1] X. Li and L.-S. Wang, J. Chem. Phys. **111**, 8389 (1999).

LiOSi

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SiO stretch	998.5vs	Ar	IR	1
	2	Bend	249w	Ar	IR	1
	3	LiO stretch	668.4wm	Ar	IR	1

Reference

[1] B. Tremblay, M. E. Alikhani, and L. Manceron, Chem. Phys. **218**, 37 (1997).

$ScCC^-$

Threshold for electron detachment from ground-state $ScCC^- = 13310(240)$ gas PE[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ScC_2 s-stretch	500T	gas	PE	1

Reference

[1] X. Li and L.-S. Wang, J. Chem. Phys. **111**, 8389 (1999).

$TiCC^-$

Threshold for electron detachment from ground-state $TiCC^- = 12440(160)$ gas PE[1]

Reference

[1] X.-B. Wang, C.-F. Ding, and L.-S. Wang, J. Phys. Chem. A **101**, 7699 (1997).

VCC^-

Threshold for electron detachment from ground-state $VCC^- = 11460(160)$ gas PE[1]

Reference

[1] X. Li and L.-S. Wang, J. Chem. Phys. **111**, 8389 (1999).

$NbCC^-$

Threshold for electron detachment from ground-state $NbCC^- = 11130(200)$ gas PE[1]

Reference

[1] H.-J. Zhai, S.-R. Liu, X. Li, and L.-S. Wang, J. Chem. Phys. **115**, 5170 (2001).

$CrCC^-$

Threshold for electron detachment from ground-state $CrCC^- = 13150(80)$ gas PE[1]

Reference

[1] X. Li and L.-S. Wang, J. Chem. Phys. **111**, 8389 (1999).

$MnCC^-$

Threshold for electron detachment from ground-state $MnCC^- = 17100(80)$ gas PE[1]

Reference

[1] X. Li and L.-S. Wang, J. Chem. Phys. **111**, 8389 (1999).

$FeCC^-$

Threshold for electron detachment from ground-state $FeCC^- = 15980(80)$ gas PE[1,2]

References

[1] J. Fan and L.-S. Wang, J. Phys. Chem. **98**, 11814 (1994).
[2] X. Li and L.-S. Wang, J. Chem. Phys. **111**, 8389 (1999).

$CoCC^-$

Threshold for electron detachment from ground-state $CoCC^- = 13720(565)$ gas PE[1]

Reference

[1] X. Li and L.-S. Wang, J. Chem. Phys. **111**, 8389 (1999).

BeCN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CN stretch	2183.1	Ar	IR	1
	3	BeC stretch	805.8	Ar	IR	1

Reference

[1] D. V. Lanzisera and L. Andrews, J. Am. Chem. Soc. **119**, 6392 (1997).

BeNC

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NC stretch	2088.7	Ar	IR	1
	3	BeN stretch	938.4	Ar	IR	1

Reference

[1] D. V. Lanzisera and L. Andrews, J. Am. Chem. Soc. **119**, 6392 (1997).

MgNC

$\tilde{A}\,^2\Pi$ $C_{\infty v}$
$T_0 = 26084.01$ gas LF[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend (ω)	193	gas	LF	6
		($\kappa\,^2\Sigma$)	206.6	gas	LF	6
Σ^+	3	MgN stretch	581.7	gas	LF	6

$A = 36.93$ gas LF[6]
$B_0 = 0.204$ LF[6]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NC stretch	2076.1	Ar	IR	4
Π	2	Bend	86T	gas	MW	3
Σ^+	3	MgN stretch	513.7	Ar	IR	4

$B_0 = 0.199$ MW[1,5]LF[6]

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).
[4] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **101**, 9666 (1997).
[5] K. A. Walker and M. C. L. Gerry, J. Mol. Spectrosc. **189**, 40 (1998).
[6] R. R. Wright and T. A. Miller, J. Mol. Spectrosc. **194**, 219 (1999).
[7] E. Kagi and K. Kawaguchi, J. Mol. Spectrosc. **199**, 309 (2000).

CaNC

$\tilde{D}\,^2A'$ C_s
$T_0 = 31515$ gas LF[11] $\tilde{D}-\tilde{X}$ 298–317 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	175	gas	LF	11
	3	CaN stretch	480	gas	LF	11

$\tilde{C}\,^2\Pi$ $C_{\infty v}$
Unstructured absorption gas LF[1] $\tilde{C}-\tilde{X}$ 385–418 nm
$\tau = 165(38)$ 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
$\tau(607\text{ nm}) = 40.8(1.5)$ 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]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NC stretch	2058.4	Ar	IR	10
Σ^+	3	CaN stretch	403	Ar	IR	10

$B_0 = 0.135$ 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); J. Chem. Phys. **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).
[10] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **101**, 9666 (1997).
[11] G. M. Greetham and A. M. Ellis, J. Chem. Phys. **113**, 8945 (2000).

SrNC[a]

$\tilde{E}\,^2A'$ C_s
$T_0 = 32768$ gas LF[4] $\tilde{E}-\tilde{X}$ 294–305 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	179	gas	LF	4

$\tilde{D}\,^2A'$ C_s
$T_0 = 29114$ gas LF[4] $\tilde{D}-\tilde{X}$ 322–345 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Bend	170	gas	LF	4

$\tilde{C}$ C_s
$T_0 = 21580$ gas LF[1,5]MPI[5] $\tilde{C}-\tilde{X}$ 395–463 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	SrN stretch	337	gas	LF,MPI	5

$\tau = 104.4(6.3)$ ns gas LF[1,5]

$\tilde{A},\tilde{B}\,^2\Pi,^2\Sigma^+$ $C_{\infty v}$
Unassigned structure gas LF[1,2] $\tilde{A},\tilde{B}-\tilde{X}$ 645–725 nm
$\tau = 51.2(6.2)$ ns gas LF[1]
$A(\tilde{A}) = 301$ gas LF[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NC stretch	2052.3	Ar	IR	3
Π	2	Bend	70T	gas	LF	5
Σ^+	3	SrN stretch	338(2)	Ar	IR	3

[a]Originally assigned to the SrCN structure.

References

[1]L. Pasternack and P. J. Dagdigian, J. Chem. Phys. **65**, 1320 (1976).
[2]M. Douay and P. F. Bernath, Chem. Phys. Lett. **174**, 230 (1990).
[3]D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **101**, 9666 (1997).
[4]G. M. Greetham and A. M. Ellis, J. Chem. Phys. **113**, 8945 (2000).
[5]G. M. Greetham and A. M. Ellis, Chem. Phys. Lett. **332**, 303 (2000).

BaNC[a]

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

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

$\tau=229(13)$ ns gas LF[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NC stretch	2048.9	Ar	IR	2

[a]Electronic spectrum originally assigned to the BaCN structure.

References

[1]L. Pasternack and P. J. Dagdigian, J. Chem. Phys. **65**, 1320 (1976).
[2]D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **101**, 9666 (1997).

FeNC

$T_0=27235.7(2)$ gas LF[1] 350–370 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	FeN stretch	523	gas	LF	1

$B_0=0.151$ LF[1]

$\tilde{X}\,^6\Delta$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	FeN stretch	468(15)	gas	LF	1

$B_0=0.144$ LF[1]

Reference

[1]J. Lie and P. J. Dagdigian, J. Chem. Phys. **114**, 2137 (2001).

CuCN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	CuC stretch	480(30)	gas	PE	1

Reference

[1]A. I. Boldyrev, X. Li, and L.-S. Wang, J. Chem. Phys. **112**, 3627 (2000).

AgCN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	AgC stretch	390(30)	gas	PE	1

Reference

[1]A. I. Boldyrev, X. Li, and L.-S. Wang, J. Chem. Phys. **112**, 3627 (2000).

$ScCO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1962.4	Ne	IR	1
			1923.5	Ar	IR	1

Reference

[1]M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 2964 (1999).

YCO^+

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1903.6	Ar	IR	1

Reference

[1]M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 2964 (1999).

$TiCO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	2041.3	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 5259 (1999).

$ReCO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	2102.1	Ne	IR	1

Reference

[1] L. Andrews, M. Zhou, X. Wang, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **104**, 8887 (2000).

$FeCO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	2123.0	Ne	IR	2
			2081.5	Ar	IR	1

References

[1] M. Zhou, G. V. Chertihin, and L. Andrews, J. Chem. Phys. **109**, 10893 (1998).
[2] M. Zhou, and L. Andrews, J. Chem. Phys. **110**, 10370 (1999).

$RuCO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	2134.9	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 6956 (1999).

$OsCO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	2106.0	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 6956 (1999).

$CoCO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	2165.5	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7773 (1999).

$RhCO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	2174.1	Ne	IR	1,2

References

[1] M. Zhou and L. Andrews, J. Am. Chem. Soc. **121**, 9171 (1999).
[2] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7773 (1999).

$IrCO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	2156.5	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7773 (1999).

$NiCO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	2206.5	Ne	IR	1
			2176.3	Ar	IR	1

Reference

[1] B. Liang, M. Zhou, and L. Andrews, J. Phys. Chem. A **104**, 3905 (2000).

$PdCO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	2206.4	Ne	IR	1

Reference

[1] B. Liang, M. Zhou, and L. Andrews, J. Phys. Chem. A **104**, 3905 (2000).

$PtCO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	2204.7	Ne	IR	1

Reference

[1] B. Liang, M. Zhou, and L. Andrews, J. Phys. Chem. A **104**, 3905 (2000).

$CuCO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	2234.4	Ne	IR	1
			2174.4T	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Chem. Phys. **111**, 4548 (1999).

$AgCO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	2233.1	Ne	IR	1

Reference

[1] B. Liang and L. Andrews, J. Phys. Chem. A **104**, 9156 (2000).

$AuCO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	2236.8	Ne	IR	1

Reference

[1] B. Liang and L. Andrews, J. Phys. Chem. A **104**, 9156 (2000).

cyc-BCC

$T_0 = 11745(3)$ Ne AB^3

$T_0 = 6296$ Ne AB^3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CBC s-stretch	1196.8(1.0)	Ne	IR	3
			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).
[3] M. Wyss, M. Grutter, and J. P. Maier, J. Phys. Chem. A **102**, 9106 (1998).

BNB

$\bar{A}\,^2\Sigma_g^+$ $D_{\infty h}$
$T_0 = 6330(40)$ gas PE[5,6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1174(40)	gas	PE	5,6
Σ_u^+	3	Asym. stretch	2492(40)	gas	PE	5,6

In the argon-matrix study,[2] the $\nu_1+\nu_3$ combination band at 1998.3, originally assigned to the cyclic isomer, and other bands between 3250 and 6150 are moderately intense, suggesting strong vibronic coupling to a low-lying excited electronic state. These bands are also seen in the gas-phase photoelectron spectrum,[6] confirming that ground-state bands involving odd numbers of quanta of ν_3 are strongly coupled to the $\bar{A}$ state.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1143(40)	gas	PE	5,6
			1116[a]	Ar	IR	2
Σ_u^+	3	Asym. stretch	855(40)	gas	PE	5,6
			882.3s	Ar	IR	2–4
			910.4	N_2	IR	1
			890.3			

[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).
[5] K. R. Asmis, T. R. Taylor, and D. M. Neumark, Eur. Phys. J. D **9**, 257 (1999).
[6] K. R. Asmis, T. R. Taylor, and D. M. Neumark, J. Chem. Phys. **111**, 8838 (1999).

AlNAl

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	544.9T	N_2	IR	1
Σ_u^+	3	Asym. stretch	981.3	Ar	IR	1
			974.8			
			956.7	N_2	IR	1

Reference

[1] L. Andrews, M. Zhou, G. V. Chertihin, W. D. Bare, and Y. Hannachi, J. Phys. Chem. A **104**, 1656 (2000).

GaNGa

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	757.4T	N_2	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 1648 (2000).

InNIn

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	666.5	N_2	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 1648 (2000).

AlCC

$\tilde{A}$
$T_0 = 7910(320)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		AlC stretch	590(50)	gas	PE	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		AlC_2 s-stretch	590(40)	gas	PE	1

Reference

[1] A. I. Boldyrev, J. Simons, X. Li, and L.-S. Wang, J. Am. Chem. Soc. **121**, 10193 (1999).

AlCSi

$\tilde{A}$
$T_0 = 4200(640)$ gas PE[1]

Reference

[1] A. I. Boldyrev, J. Simons, X. Li, and L.-S. Wang, J. Am. Chem. Soc. **121**, 10193 (1999).

Al_2P

$\tilde{B}\,^2B_1$ C_{2v}
$T^a = 3770(260)$ gas PE[1]

$\tilde{A}\,^2A_1$ C_{2v}
$T^a = 2560(260)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	421(15)	gas	PE	1

$\tilde{X}\,^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	70T	gas	PE	1

[a] From vertical ionization potential.

Reference

[1] H. Gómez, T. R. Taylor, and D. M. Neumark, J. Phys. Chem. A **105**, 6886 (2001).

Ga_2P

$\tilde{B}$
$T^a = 3230T$ gas PE[3]

$\tilde{A}$ C_{2v}
$T_0 = 2160(200)$ gas PE[2,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	311	gas	PE	2,3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	64	gas	PE	2
b_2	3	Asym. stretch	281.2	Ar	IR	1

[a] From vertical photodetachment energy with respect to the neutral ground state.

References

[1] S. Li, R. J. Van Zee, and W. Weltner, Jr., J. Phys. Chem. **97**, 11393 (1993).
[2] T. R. Taylor, K. R. Asmis, H. Gomez, and D. M. Neumark, Eur. Phys. J. D **9**, 317 (1999).
[3] T. R. Taylor, H. Gómez, K. R. Asmis, and D. M. Neumark, J. Chem. Phys. **115**, 4620 (2001).

In_2P

$\tilde{A}$
$T_0 = 1860T$ gas PE[2,3]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	204(2)	gas	TPE	3
	2	Bend	47.0(3)	gas	TPE	3
b_2	3	Asym. stretch	249.3	Ar	IR	1

References

[1] S. Li, R. J. Van Zee, and W. Weltner, Jr., J. Phys. Chem. **98**, 2275 (1994).
[2] C. Xu, E. de Beer, D. W. Arnold, C. C. Arnold, and D. M. Neumark, J. Chem. Phys. **101**, 5406 (1994).
[3] C. C. Arnold and D. M. Neumark, Can. J. Phys. **72**, 1322 (1994).

Ga_2As

$\tilde{B}$
$T_0 = 2260T$ gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1		279	gas	PE	2

$\tilde{A}$
$T_0 = 1690(320)$ gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1		200	gas	PE	2

$\tilde{X}$ 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

References

[1] S. Li, R. J. Van Zee, and W. Weltner, Jr., J. Phys. Chem. **97**, 11393 (1993).
[2] T. R. Taylor, H. Gómez, K. R. Asmis, and D. M. Neumark, J. Chem. Phys. **115**, 4620 (2001).

$PdCN^-$

Threshold for electron detachment from ground-state $PdCN^- = 20520(60)$ gas PE[1]

Reference

[1] S. A. Klopcic, V. D. Moravec, and C. C. Jarrold, J. Chem. Phys. **110**, 8986 (1999).

$CuCN^-$

Threshold for electron detachment from ground-state $CuCN^- = 11830(80)$ gas PE[1,2]

References

[1] A. I. Boldyrev, X. Li, and L.-S. Wang, J. Chem. Phys. **112**, 3627 (2000).
[2] Y. Negishi, T. Yasuike, F. Hayakawa, M. Kizawa, S. Yabushita, A. Nakajima, and K. Kaya, J. Chem. Phys. **113**, 1725 (2000).

$CuNC^-$

Threshold for electron detachment from ground-state $CuNC^- = 13150(1200)$ gas PE[1]

Reference

[1] Y. Negishi, T. Yasuike, F. Hayakawa, M. Kizawa, S. Yabushita, A. Nakajima, and K. Kaya, J. Chem. Phys. **113**, 1725 (2000).

$AgCN^-$

Threshold for electron detachment from ground-state $AgCN^- = 12810(80)$ gas PE[1]

Reference

[1] A. I. Boldyrev, X. Li, and L.-S. Wang, J. Chem. Phys. **112**, 3627 (2000).

ScCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1851.4	Ne	IR	1
			1834.2	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 2964 (1999).

YCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1874.1	Ar	IR	1
			1869.0			

Reference

[1]M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 2964 (1999).

TiCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1920.0	Ne	IR	2
			1887.8	Ar	IR	1,2

References

[1]G. V. Chertihin and L. Andrews, J. Am. Chem. Soc. **117**, 1595 (1995).
[2]M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 5259 (1999).

ZrCO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1899.5	Ne	IR	1

Reference

[1]M. Zhou and L. Andrews, J. Am. Chem. Soc. **122**, 1531 (2000).

HfCO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1868.6	Ne	IR	1

Reference

[1]M. Zhou and L. Andrews, J. Am. Chem. Soc. **122**, 1531 (2000).

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	1930.6	Ne	IR	3
			1904.7	Ar	IR	1,3
			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).
[3]M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 5259 (1999).

CNbO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NbO stretch	919.8	Ne	IR	1
		NbC stretch	783.7	Ne	IR	1

Reference

[1]M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7785 (1999).

NbCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1932.0	Ne	IR	1

Reference

[1]M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7785 (1999).

TaCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1865.2	Ne	IR	2
			1862.7			
			1831T	Ar	IR	1
			1819T			

References

[1]R. L. DeKock, Inorg. Chem. **10**, 1205 (1971).
[2]M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7785 (1999).

CrCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1975.3	Ar	IR	1,2

References

[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).
[2] P. F. Souter and L. Andrews, J. Am. Chem. Soc. **119**, 7350 (1997).

MoCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1862.6	Ar	IR	1

Reference

[1] P. F. Souter and L. Andrews, J. Am. Chem. Soc. **119**, 7350 (1997).

WCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1848.8	Ar	IR	1

Reference

[1] P. F. Souter and L. Andrews, J. Am. Chem. Soc. **119**, 7350 (1997).

MnCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1950.7	Ne	IR	1
			1933.6	Ar	IR	1

Reference

[1] L. Andrews, M. Zhou, X. Wang, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **104**, 8887 (2000).

ReCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1884.0	Ar	IR	1

Reference

[1] L. Andrews, M. Zhou, X. Wang, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **104**, 8887 (2000).

FeCO

$\tilde{a}\,^5\Sigma^-$ $C_{\infty v}$
$T_0 = 1135(25)$ gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1990(15)	gas	PE	2
Π	2	Bend	180(60)	gas	PE	2
Σ^+	3	FeC stretch	460(15)	gas	PE	2

$\tilde{X}\,^3\Sigma^-$ $C_{\infty v}$ Structure: $MW^{3,5}DL^4$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1946.47	gas	PE,DL	1,2,4
			1933.7	Ne	IR	8
			1922.0T[a]	Ar	IR	7
Π	2	Bend	330(50)	gas	PE	2
Σ^+	3	FeC stretch	530(10)	gas	PE	2

$B_0 = 0.146$ $MW^{3,5,6}DL^4$

[a] As discussed in Ref. 8, isotopic shift disparities suggest that this peak may be contributed by an ArFeCO species or by FeCO in the low-lying $^3\Delta$ state, which may lie below the $^3\Sigma^-$ state for FeCO isolated in solid argon.

References

[1] R. J. Ryther and E. Weitz, J. Phys. Chem. **95**, 9841 (1991).
[2] P. W. Villalta and D. G. Leopold, J. Chem. Phys. **98**, 7730 (1993).
[3] Y. Kasai, K. Obi, Y. Ohshima, Y. Endo, and K. Kawaguchi, J. Chem. Phys. **103**, 90 (1995).
[4] K. Tanaka, K. Sakaguchi, and T. Tanaka, J. Chem. Phys. **106**, 2118 (1997).
[5] K. Tanaka, M. Shirasaka, and T. Tanaka, J. Chem. Phys. **106**, 6821 (1997).
[6] E. Kagi, Y. Kasai, H. Ungerechts, and K. Kawaguchi, Astrophys. J. **488**, 776 (1997).
[7] M. Zhou, G. V. Chertihin, and L. Andrews, J. Chem. Phys. **109**, 10893 (1998).
[8] M. Zhou and L. Andrews, J. Chem. Phys. **110**, 10370 (1999).

RuCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1935.6	Ne	IR	1
			1917.7	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 6956 (1999).

OsCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1972.6	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 6956 (1999).

CoCO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1973.9	Ne	IR	3
			1960.7	Ar	IR	1,2,4
			1957.3vs			
			1952	Kr	IR	1
			1944			
			1947	Xe	IR	1
			1941			
Π	2	Bend	424.9w	Ar	IR	4
Σ^+	3	CoC stretch	579.2vw	Ar	IR	4

References

[1] L. A. Hanlan, H. Huber, E. P. Kündig, B. R. McGarvey, and G. A. Ozin, J. Am. Chem. Soc. **97**, 7054 (1975).
[2] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 10250 (1998).
[3] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7773 (1999).
[4] B. Tremblay, M. E. Alikhani, and L. Manceron, J. Phys. Chem. A **105**, 11388 (2001).

RhCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	2022.5	Ne	IR	2,3
			2008.0	Ar	IR	1,3

References

[1] G. A. Ozin and A. J. L. Hanlan, Inorg. Chem. **18**, 2091 (1979).
[2] M. Zhou and L. Andrews, J. Am. Chem. Soc. **121**, 9171 (1999).
[3] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7773 (1999).

IrCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	2024.5	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7773 (1999).

NiCO

$T_0 = 11050(240)$ gas PE[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1940(80)	gas	PE	2
			2006.6	Ne	IR	5
			1994.5vs	Ar	IR	1,3,4
Π	2	Bend	409.1vw	Ar	IR	3
Σ^+	3	NiC stretch	591.1vw	Ar	IR	3

References

[1] R. L. DeKock, Inorg. Chem. **10**, 1205 (1971).
[2] A. E. Stevens, C. S. Feigerle, and W. C. Lineberger, J. Am. Chem. Soc. **104**, 5026 (1982).
[3] H. A. Joly and L. Manceron, Chem. Phys. **226**, 61 (1998).
[4] M. Zhou and L. Andrews, J. Am. Chem. Soc. **120**, 11499 (1998).
[5] B. Liang, M. Zhou, and L. Andrews, J. Phys. Chem. A **104**, 3905 (2000).

PdCO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	2140(60)	gas	PE	3
			2056.4	Ne	IR	5
			2044.2vs	Ar	IR	1,2,4
			2045	Kr	IR	2
Π	2	Bend	615.7vw	Ar	IR	4
Σ^+	3	PdC stretch	350(40)	gas	PE	3
			472.0w	Ar	IR	4

References

[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. 1079 (1973).
[3] S. A. Klopcic, V. D. Moravec, and C. C. Jarrold, J. Chem. Phys. **110**, 8986 (1999).
[4] B. Tremblay and L. Manceron, Chem. Phys. **250**, 187 (1999).
[5] B. Liang, M. Zhou, and L. Andrews, J. Phys. Chem. A **104**, 3905 (2000).

PtCO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	2065.5	Ne	IR	3
			2051.9	Ar	IR	1,2
Π	2	Bend	916.8	Ar	IR	2
Σ^+	3	PtC stretch	580.8	Ar	IR	2

$B_0 = 0.111$ MW[4]

References

[1] E. P. Kündig, D. McIntosh, M. Moskovits, and G. A. Ozin, J. Am. Chem. Soc. **95**, 7234 (1973).
[2] L. Manceron, B. Tremblay, and M. E. Alikhani, J. Phys. Chem. A **104**, 3750 (2000).
[3] B. Liang, M. Zhou, and L. Andrews, J. Phys. Chem. A **104**, 3905 (2000).
[4] C. J. Evans and M. C. L. Gerry, J. Phys. Chem. A **105**, 9659 (2001).

CuCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	CO stretch	2029.7	Ne	IR	4
			2010.4	Ar	IR	1–4
			2029.5	N_2	IR	2
	2	Bend	207.5	Ar	IR	3
	3	CuC stretch	322.7	Ar	IR	3

References

[1] H. Huber, E. P. Kündig, M. Moskovits, and G. A. Ozin, J. Am. Chem. Soc. **97**, 2097 (1975).
[2] S. Dobos and S. Nunziante Cesaro, High Temp. Mater. Sci. **37**, 81 (1997).
[3] B. Tremblay and L. Manceron, Chem. Phys. **242**, 235 (1999).
[4] M. Zhou and L. Andrews, J. Chem. Phys. **111**, 4548 (1999).

AuCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	2053.2	Ne	IR	1

Reference

[1] B. Liang and L. Andrews, J. Phys. Chem. A **104**, 9156 (2000).

ThCO

In a neon matrix, rearranges to CThO when the sample is exposed to radiation in the 470–580 nm spectral region.[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1817.5	Ne	IR	1,2

References

[1] M. Zhou, L. Andrews, J. Li, and B. E. Bursten, J. Am. Chem. Soc. **121**, 12188 (1999).
[2] J. Li, B. E. Bursten, M. Zhou, and L. Andrews, Inorg. Chem. **40**, 5448 (2001).

CThO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	ThO stretch	812.2	Ne	IR	1,2
	3	ThC stretch	617.7	Ne	IR	1,2

References

[1] M. Zhou, L. Andrews, J. Li, and B. E. Bursten, J. Am. Chem. Soc. **121**, 12188 (1999).
[2] J. Li, B. E. Bursten, M. Zhou, and L. Andrews, Inorg. Chem. **40**, 5448 (2001).

CUO

$\tilde{a}\,^3\Phi$ $C_{\infty v}$

When CUO is isolated in an argon matrix, a new absorption pattern results, attributed to a sufficiently large shift in the energy of this very low-lying excited state to place it below the $\tilde{X}\,^1\Sigma^+$ state of the free molecule.[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Mixed	852.5	Ar	IR	2
	3	Mixed	804.3	Ar	IR	2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	UC stretch	1047.3	Ne	IR	1
	3	UO stretch	872.2	Ne	IR	1

References

[1] M. Zhou, L. Andrews, J. Li, and B. E. Bursten, J. Am. Chem. Soc. **121**, 9712 (1999).
[2] L. Andrews, B. Liang, J. Li, and B. E. Bursten, Angew. Chem. Int. Ed. **39**, 4565 (2000).

UCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1917.8	Ne	IR	3
			1893	Ar	IR	1–3

References

[1] J. L. Slater, R. K. Sheline, K. C. Lin, and W. Weltner, Jr., J. Chem. Phys. **55**, 5129 (1971).
[2] T. J. Tague, Jr., L. Andrews, and R. D. Hunt, J. Phys. Chem. **97**, 10920 (1993).
[3] M. Zhou, L. Andrews, J. Li, and B. E. Bursten, J. Am. Chem. Soc. **121**, 9712 (1999).

ScNN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NN stretch	1902.0	Ar	IR	1

Reference

[1] G. V. Chertihin, L. Andrews, and C. W. Bauschlicher, Jr., J. Am. Chem. Soc. **120**, 3205 (1998).

cyc-ScNN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NN stretch	1714.0T	Ar	IR	1

Reference

[1] G. V. Chertihin, L. Andrews, and C. W. Bauschlicher, Jr., J. Am. Chem. Soc. **120**, 3205 (1998).

cyc-YNN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NN stretch	1763.4	Ar	IR	1

Reference

[1] G. V. Chertihin, W. D. Bare, and L. Andrews, J. Phys. Chem. A **102**, 3697 (1998).

cyc-LaNN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NN stretch	1770.7	Ar	IR	1

Reference

[1] G. V. Chertihin, W. D. Bare, and L. Andrews, J. Phys. Chem. A **102**, 3697 (1998).

TiNN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NN stretch	1847.1	Ar	IR	1,2

References

[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. **98**, 5891 (1994).
[2] G. P. Kushto, P. F. Souter, G. V. Chertihin, and L. Andrews, J. Chem. Phys. **110**, 9020 (1999).

cyc-TiNN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NN stretch	1125.9	Ar	IR	1

Reference

[1] G. P. Kushto, P. F. Souter, G. V. Chertihin, and L. Andrews, J. Chem. Phys. **110**, 9020 (1999).

NTiN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		TiN_2 a-stretch	867.3	Ar	IR	1

Reference

[1] G. P. Kushto, P. F. Souter, G. V. Chertihin, and L. Andrews, J. Chem. Phys. **110**, 9020 (1999).

ZrNN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NN stretch	1797.5	Ar	IR	1

Reference

[1] G. P. Kushto, P. F. Souter, G. V. Chertihin, and L. Andrews, J. Chem. Phys. **110**, 9020 (1999).

cyc-ZrNN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NN stretch	1022.8	Ar	IR	1

Reference

[1] G. P. Kushto, P. F. Souter, G. V. Chertihin, and L. Andrews, J. Chem. Phys. **110**, 9020 (1999).

NZrN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ZrN stretch	706.3	Ar	IR	1

Reference

[1] G. P. Kushto, P. F. Souter, G. V. Chertihin, and L. Andrews, J. Chem. Phys. **110**, 9020 (1999).

HfNN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NN stretch	1793.8	Ar	IR	1

Reference

[1] G. P. Kushto, P. F. Souter, G. V. Chertihin, and L. Andrews, J. Chem. Phys. **110**, 9020 (1999).

NHfN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		HfN stretch	708.1	Ar	IR	1

Reference

[1] G. P. Kushto, P. F. Souter, G. V. Chertihin, and L. Andrews, J. Chem. Phys. **110**, 9020 (1999).

NVN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			820.1	N_2	IR	1

Reference

[1] L. Andrews, W. D. Bare, and G. V. Chertihin, J. Phys. Chem. A **101**, 8417 (1997).

VNN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NN stretch	1945.0	Ar	IR	1

Reference

[1] L. Andrews, W. D. Bare, and G. V. Chertihin, J. Phys. Chem. A **101**, 8417 (1997).

cyc-VNN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NN stretch	1709.1	Ar	IR	1

Reference

[1] L. Andrews, W. D. Bare, and G. V. Chertihin, J. Phys. Chem. A **101**, 8417 (1997).

NbNN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NN stretch	1914.5	Ar	IR	1
			1965.2T	N_2	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 9061 (1998).

cyc-NbN_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NN stretch	1888.7	Ar	IR	1
			1815.6	N_2	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 9061 (1998).

NNbN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NbN_2 s-stretch	918.6	Ar	IR	1
			914.9			
b_2	3	NbN_2 a-stretch	685.4	Ar	IR	1
			680.8			

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 9061 (1998).

TaNN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NN stretch	1952.8	Ar	IR	1
			1947.6T	N_2	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 9061 (1998).

cyc-TaN_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NN stretch	1762.6	N_2	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 9061 (1998).

NTaN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	TaN_2 s-stretch	922.7	Ar	IR	1
b_2	3	TaN_2 a-stretch	740.3	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 9061 (1998).

NCrN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	956.1	N_2	IR	1
b_2	3	Asym. stretch	875.7	N_2	IR	1

Reference

[1] L. Andrews, W. D. Bare, and G. V. Chertihin, J. Phys. Chem. A **101**, 8417 (1997).

NMoN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	MoN s-stretch	975.1	N_2	IR	1
b_2	3	MoN a-stretch	877.1	Ar	IR	1
			861.6	N_2	IR	1
			860.6			

Reference

[1] L. Andrews, P. F. Souter, W. D. Bare, and B. Liang, J. Phys. Chem. A **103**, 4649 (1999).

MoNN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NN stretch	1938.7T	Ar	IR	1

Reference

[1] L. Andrews, P. F. Souter, W. D. Bare, and B. Liang, J. Phys. Chem. A **103**, 4649 (1999).

NWN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	WN a-stretch	878.3	Ar	IR	1
			870.3	N_2	IR	1
			865.1			

Reference

[1] L. Andrews, P. F. Souter, W. D. Bare, and B. Liang, J. Phys. Chem. A **103**, 4649 (1999).

WNN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NN stretch	1894.3T	Ar	IR	1

Reference

[1] L. Andrews, P. F. Souter, W. D. Bare, and B. Liang, J. Phys. Chem. A **103**, 4649 (1999).

NMnN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	858.7	N_2	IR	1

Reference

[1] L. Andrews, W. D. Bare, and G. V. Chertihin, J. Phys. Chem. A **101**, 8417 (1997).

cyc-MnNN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NN stretch	1819.3	Ar	IR	1

Reference

[1] L. Andrews, W. D. Bare, and G. V. Chertihin, J. Phys. Chem. A **101**, 8417 (1997).

ReNN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NN stretch	1940.1	Ar	IR	1
			1944.7T	N_2	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 9061 (1998).

cyc-ReN_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NN stretch	1894.7T	N_2	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 9061 (1998).

NRuN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	831.9	Ar	IR	1,2
			831.5	N_2	IR	2

References

[1] A. Citra and L. Andrews, J. Am. Chem. Soc. **121**, 11567 (1999).
[2] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 1152 (2000).

NOsN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	900.4	Ar	IR	1,2
			901.1	N_2	IR	1,2

References

[1] A. Citra and L. Andrews, J. Am. Chem. Soc. **121**, 11567 (1999).
[2] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 1152 (2000).

CoNN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NN stretch	2100.9	Ar	IR	1,2
			2109	N_2	IR	2

References

[1] G. A. Ozin and A. Vander Voet, Can. J. Chem. **51**, 637 (1973).
[2] L. Andrews, A. Citra, G. V. Chertihin, W. D. Bare, and M. Neurock, J. Phys. Chem. A **102**, 2561 (1998).

cyc-CoNN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NN stretch	1873.5	N_2	IR	1

Reference

[1] L. Andrews, A. Citra, G. V. Chertihin, W. D. Bare, and M. Neurock, J. Phys. Chem. A **102**, 2561 (1998).

RhNN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NN stretch	2153.3	Ar	IR	1,2

References

[1] G. A. Ozin and A. Vander Voet, Can. J. Chem. **51**, 3332 (1973).
[2] A. Citra and L. Andrews, J. Phys. Chem. A **103**, 3410 (1999).

NRhN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	RhN_2 a-stretch	823.2	Ar	IR	1
			830.9	N_2	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **103**, 3410 (1999).

NINN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NN stretch	2089.2vs	Ar	IR, Ra	1–4
Π	2	Bend	357.0w	Ar	IR	4
Σ^+	3	NiN stretch	563.7wm	Ar	IR	3,4

References

[1] H. Huber, E. P. Kündig, M. Moskovits, and G. A. Ozin, J. Am. Chem. Soc. **95**, 332 (1973).
[2] W. Klotzbücher and G. A. Ozin, J. Am. Chem. Soc. **97**, 2672 (1975).
[3] L. Andrews, A. Citra, G. V. Chertihin, W. D. Bare, and M. Neurock, J. Phys. Chem. A **102**, 2561 (1998).
[4] L. Manceron, M. E. Alikhani, and H. A. Joly, Chem. Phys. **228**, 73 (1998).

cyc-NiNN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NN stretch	1879.3	Ar	IR	1
			1902.7T	N_2	IR	1
			1870.6T	N_2	IR	1

Reference

[1] L. Andrews, A. Citra, G. V. Chertihin, W. D. Bare, and M. Neurock, J. Phys. Chem. A **102**, 2561 (1998).

PdNN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NN stretch	2215	Ar	IR,Ra	1,2
		PdN stretch	378	Ar	IR	2

References

[1] H. Huber, E. P. Kündig, M. Moskovits, and G. A. Ozin, J. Am. Chem. Soc. **95**, 332 (1973).
[2] W. Klotzbücher and G. A. Ozin, J. Am. Chem. Soc. **97**, 2672 (1975).

PtNN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NN stretch	2169.5	Ne	IR	4
			2168.5	Ar	IR	1–4
			2170.7	Kr	IR	2
			2168.8			
			2173.0	N_2	IR	4
Σ^+	3	PtN stretch	499.6	Ar	IR	4

References

[1] E. P. Kündig, M. Moskovits, and G. A. Ozin, Can. J. Chem. **51**, 2710 (1973).
[2] D. W. Green, J. Thomas, and D. M. Gruen, J. Chem. Phys. **58**, 5453 (1973).
[3] W. Klotzbücher and G. A. Ozin, J. Am. Chem. Soc. **97**, 2672 (1975).
[4] A. Citra, X. Wang, W. D. Bare, and L. Andrews, J. Phys. Chem. A **105**, 7799 (2001).

NCeN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	790.9	Ar	IR	1
			756.4	N_2	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **102**, 10238 (1998).

CeNN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NN stretch	1569.1	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **102**, 10238 (1998).

NPrN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	809.6	N_2	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **102**, 10238 (1998).

NNdN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	778.4	N_2	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **102**, 10238 (1998).

NSmN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	738.1	N_2	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **102**, 10238 (1998).

SmNN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NN stretch	1576.8	N_2	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **102**, 10238 (1998).

cyc-SmNN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NN stretch	1744.9	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **102**, 10238 (1998).

cyc-EuNN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NN stretch	1787.5	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **102**, 10238 (1998).

cyc-GdNN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NN stretch	1876.9	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **102**, 10238 (1998).

GdNN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NN stretch	1558.2	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **102**, 10238 (1998).

cyc-TbNN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NN stretch	1859.5	Ar	IR	1
			1846.1			

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 1311 (1999).

cyc-DyNN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NN stretch	1809.2	Ar	IR	1
			1799.8			
			1794.8			
			1759.4	N_2	IR	1
			1755.5			
			1744.7			

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 1311 (1999).

cyc-HoNN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NN stretch	1798.3	Ar	IR	1
			1754.7	N_2	IR	1
			1749.3			

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 1311 (1999).

cyc-ErNN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NN stretch	1802	Ar	IR	1
			1769.7	N_2	IR	1
			1753.4			
			1748.5			

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 1311 (1999).

cyc-TmNN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NN stretch	1799.5	Ar	IR	1
			1752.3	N_2	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 1311 (1999).

cyc-YbNN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NN stretch	1744.1	N_2	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 1311 (1999).

cyc-LuNN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NN stretch	1845.3	Ar	IR	1
			1840.2			
			1836.0			
			1824.3			
			1852.0	N_2	IR	1
			1848.9			
			1846.0			
			1844.2			
			1839.5			

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 1311 (1999).

NThN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	756.6	Ar	IR	1

Reference

[1] G. P. Kushto, P. F. Souter, and L. Andrews, J. Chem. Phys. **108**, 7121 (1998).

ThNN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NN stretch	1673.9	Ar	IR	1

Reference

[1] G. P. Kushto, P. F. Souter, and L. Andrews, J. Chem. Phys. **108**, 7121 (1998).

NUN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1008.3[a]	Ar	IR	2
Σ_u^+	3	Asym. stretch	1076.6	Ne	IR	4
			1051.0	Ar	IR	1,2,5
			996T	N_2	IR	2,3,5

[a]Calculated from position of $^{14}NU^{15}N$ absorption.

References

[1] D. W. Green and G. T. Reedy, J. Chem. Phys. **65**, 2921 (1976).
[2] R. D. Hunt, J. T. Yustein, and L. Andrews, J. Chem. Phys. **98**, 6070 (1993).
[3] K. Sankaran, K. Sundararajan, and K. S. Viswanathan, Bull. Mater. Sci. **22**, 785 (1999).
[4] M. Zhou and L. Andrews, J. Chem. Phys. **111**, 11044 (1999).
[5] K. Sankaran, K. Sundararajan, and K. S. Viswanathan, J. Phys. Chem. A **105**, 3995 (2001).

cyc-$ScNO^+$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1159.8	Ne	IR	2
			1117.0	Ar	IR	1

References

[1] G. P. Kushto, M. Zhou, L. Andrews, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **103**, 1115 (1999).
[2] L. Andrews and X. Wang, J. Phys. Chem. A **106**, 1196 (2002).

cyc-VNO^+

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO stretch	1146.5	Ne	IR	1
			1143.7			
			1139.5	Ar	IR	1
			1137.0			

Reference

[1] L. Andrews and X. Wang, J. Phys. Chem. A **106**, 1196 (2002).

NVO^+

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1020.5	Ne	IR	1

Reference

[1] L. Andrews and X. Wang, J. Phys. Chem. A **106**, 1196 (2002).

$FeNO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO stretch	1897.3	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 3915 (2000).

$RuNO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO stretch	1918.0	Ne	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 8689 (2000).

$OsNO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO stretch	1921.8	Ne	IR	1
			1901.5	Ar	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 8689 (2000).

$CoNO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO stretch	1957.5	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 3915 (2000).

$RhNO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO stretch	1957.5	Ne	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 11897 (2000).

$IrNO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO stretch	1990.0	Ne	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 11897 (2000).

$NiNO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO stretch	2001.9	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 3915 (2000).

$PdNO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO stretch	1921.8	Ne	IR	1
			1921.6	Ar	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 8160 (2000).

$PtNO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO stretch	2019.6	Ne	IR	1
			2010.4	Ar	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 8160 (2000).

$CuNO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO stretch	1907.9	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 2618 (2000).

$AgNO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO stretch	1910.9	Ne	IR	1
			1904.3	Ar	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **105**, 3042 (2001).

NUO^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	UN stretch	1118.6	Ne	IR	1
	3	UO stretch	969.8	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Chem. Phys. **111**, 11044 (1999).

BCC^-

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

$T_0 = 23131(11)$ Ne AB[1] $\tilde{A}-\tilde{X}$ 361–432 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1		1535(11)	Ne	AB	1
	3		1081(11)	Ne	AB	1,2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CC stretch	1936	Ne	IR	1

References

[1] M. Wyss, M. Grutter, and J. P. Maier, J. Phys. Chem. A **102**, 9106 (1998).
[2] C. Léonard, D. Panten, P. Rosmus, M. Wyss, and J. P. Maier, Chem. Phys. **264**, 267 (2001).

BNB^-

Threshold for electron detachment from ground-state $BNB^- = 25000(40)$ gas PE[3,4]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1130(40)	gas	PE	4
Σ_u^+	3	Asym. stretch	1728(40)	gas	PE	4
			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).
[3] K. R. Asmis, T. R. Taylor, and D. M. Neumark, Eur. Phys. J. D **9**, 257 (1999).
[4] K. R. Asmis, T. R. Taylor, and D. M. Neumark, J. Chem. Phys. **111**, 8838 (1999).

BCN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CN stretch	2170.8	Ar	IR	1
	3	BC stretch	800.0	Ar	IR	1

Reference

[1] D. V. Lanzisera, L. Andrews, and P. R. Taylor, J. Phys. Chem. A **101**, 7134 (1997).

BNC

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NC stretch	2055.2	Ar	IR	1
	3	BN stretch	984.3	Ar	IR	1

Reference

[1] D. V. Lanzisera, L. Andrews, and P. R. Taylor, J. Phys. Chem. A **101**, 7134 (1997).

$AlCC^-$

Threshold for electron detachment from ground-state $AlCC^- = 21380(240)$ gas PE[1]

Reference

[1] A. I. Boldyrev, J. Simons, X. Li, and L.-S. Wang, J. Am. Chem. Soc. **121**, 10193 (1999).

$AlCSi^-$

Threshold for electron detachment from ground-state $AlCSi^- = 20170(480)$ gas PE[1]

Reference

[1] A. I. Boldyrev, J. Simons, X. Li, and L.-S. Wang, J. Am. Chem. Soc. **121**, 10193 (1999).

AlCN

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

$T_0 = 28755.3(3)$ gas LF[2,3] $\tilde{A}-\tilde{X}$ 325–405 nm

$B_0 = 0.181(4)$ LF[3]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CN stretch	1974.5(1.5)	gas	LF	2,3
			2143.7	Ar	IR	1
Π	2	Bend	131.9(1.3)	gas	LF	2,3
Σ^+	3	AlC stretch	523.5(0.7)	gas	LF	2,3

$B_0 = 0.168$ LF^3MW^4

References

[1] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **101**, 9660 (1997).
[2] M. Fukushima, Chem. Phys. Lett. **283**, 337 (1998).
[3] I. Gerasimov, X. Yang, and P. J. Dagdigian, J. Chem. Phys. **110**, 220 (1999).
[4] K. A. Walker and M. C. L. Gerry, Chem. Phys. Lett. **301**, 200 (1999).

AlNC

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

$T_0 = 36389.1(2)$ gas LF^3 $\tilde{A}-\tilde{X}$ 265–279 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend (ω)	238	gas	LF	3
		($\kappa\,^1\Sigma^+$)	371	gas	LF	3
Σ^+	3	NC stretch	598	gas	LF	3

$\epsilon = +0.53$ LF^3

$B_0 = 0.210$ LF^3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NC stretch	2069(21)	gas	LF	3
			2051.4	Ar	IR	2
Π	2	Bend	100(6)	gas	LF	3
Σ^+	3	AlN stretch	557	gas	LF	3

$B_0 = 0.200$ MW^1

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[1] J. S. Robinson, A. J. Apponi, and L. M. Ziurys, Chem. Phys. Lett. **278**, 1 (1997).
[2] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **101**, 9660 (1997).
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GaCN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CN stretch	2137.8	Ar	IR	1

Reference

[1] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **101**, 9660 (1997).

GaNC

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NC stretch	2046.4	Ar	IR	1

Reference

[1] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **101**, 9660 (1997).

InCN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CN stretch	2132.4	Ar	IR	1

Reference

[1] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **101**, 9660 (1997).

InNC

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NC stretch	2051.1	Ar	IR	1

Reference

[1] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **101**, 9660 (1997).

BNSi

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BN stretch	1528.0	N_2	IR	1

Reference

[1] G. Meloni, S. Nunziante Cesaro, and N. Sanna, Chem. Phys. Lett. **343**, 113 (2001).

Al_2P^-

Threshold for electron detachment from ground-state $Al_2P^- = 20280(160)$ gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	450(20)	gas	PE	1

Reference

[1] H. Gómez, T. R. Taylor, and D. M. Neumark, J. Phys. Chem. A **105**, 6886 (2001).

Ga_2P^-

Threshold for electron detachment from ground-state $Ga_2P^- = 20020(120)$ 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	375(25)	gas	PE	1,2

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[1] T. R. Taylor, K. R. Asmis, H. Gomez, and D. M. Neumark, Eur. Phys. J. D **9**, 317 (1999).
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In_2P^-

Threshold for electron detachment from ground-state $In_2P^- = 19360(8)$ gas PE[1,3]TPE[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	295T	gas	TPE	2
	2	Bend	100T	gas	TPE	2
b_2	3	Asym. stretch	223T	gas	TPE	2

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[1] C. Xu, E. de Beer, D. W. Arnold, C. C. Arnold, and D. M. Neumark, J. Chem. Phys. **101**, 5406 (1994).
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[3] K. R. Asmis, T. R. Taylor, and D. M. Neumark, Chem. Phys. Lett. **308**, 347 (1999).

Ga_2As^-

Threshold for electron detachment from ground-state $Ga_2As^- = 19820(120)$ gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1		245	gas	PE	1

Reference

[1] T. R. Taylor, H. Gómez, K. R. Asmis, and D. M. Neumark, J. Chem. Phys. **115**, 4620 (2001).

TlCN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CN stretch	2125.7	Ar	IR	1

Reference

[1] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **101**, 9660 (1997).

TlNC

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NC stretch	2047.7	Ar	IR	1

Reference

[1] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **101**, 9660 (1997).

Ga_2O

$\tilde{C}$

$T_0 = 36939(15)$ Ar AB[6] $\tilde{C}-\tilde{X}$ 265–271 nm
$36226(15)$ Kr AB[6] $\tilde{C}-\tilde{X}$ 270–276 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	GaO s-stretch	527	Ar	AB	6
	2	Bend	182	Ar	AB	6
			218	Kr	AB	6

$\tilde{B}$

$T_0 = 28328(15)$ Kr EM[6] $\tilde{B}-\tilde{X}$ 353–403 nm

$\tilde{A}$

$T_0 = 20600(15)$ Kr EM[6]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	822.3	Ar	IR	2,4,5,7
			809.4	N_2	IR	1,3–5

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[1] A. J. Hinchcliffe and J. S. Ogden, Chem. Commun. 1053 (1969).
[2] D. M. Makowiecki, D. A. Lynch, Jr., and K. D. Carlson, J. Phys. Chem. **75**, 1963 (1971).
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In_2O

$\tilde{C}$

$T_0 = 32699(15)$ Ar AB[6] $\tilde{C}-\tilde{X}$ 300–306 nm
31854(15) Kr AB[6] $\tilde{C}-\tilde{X}$ 306–314 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	576	Ar	AB	6
	2	Bend	139	Kr	AB	6

$\tilde{B}_2$ C_{2v}

$T_0 = 26524.53$ gas LF[8] $\tilde{B}_2-\tilde{X}$ 373–377 nm
$\tau = 1.350(25)$ μs gas LF[8]

$\tilde{B}_1$ C_{2v}

$T_0 = 25815$ gas LF[8] $\tilde{B}_1-\tilde{X}$ 380–388 nm
25644(15) Kr AB[6]
25535(15) Kr EM[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	InO s-stretch	219.2	gas	AB	8
	2	Bend	94T	gas	AB	8

$\tau = 1.74(4)$ μs gas LF[8]

$\tilde{A}$

$T_0 = 19260(15)$ Kr EM[6]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	InO s-stretch	222	gas	LF	8
Π_u	2	Bend	52H	gas	LF	8
Σ_u^+	3	InO a-stretch	745.4	Ne	IR	2
			735.2	Ar	IR	2,4,5,7
			728.2	Kr	IR	2
			722.4	N_2	IR	1–5

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[1] A. J. Hinchcliffe and J. S. Ogden, Chem. Commun. 1053 (1969).
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[6] M. A. Douglas, R. H. Hauge, and J. L. Margrave, High Temp. Sci. **16**, 35 (1983).
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Tl_2O

$\tilde{X}$

Vib.	No.	Approximate	cm^{-1}	Med.	Type	Refs.
	3	Asym. stretch	643.6	Ar	IR	2,4
			634.6	Kr	IR	2
			625.3	N_2	IR	1–3

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C_3

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

$T_0 = 52826(30)$ Ar AB[15] 170–190 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1080(30)	Ar	AB	15
Π_u	2	Bend	300(30)H	Ar	AB	15
Σ_u^+	3	Asym. stretch	780(30)H[a]	Ar	AB	15

$\tilde{B}\,^1\Delta_u$ $D_{\infty h}$

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. These same bands, as well as bands at somewhat lower energies (possibly below the ionization threshold) and bands arising from a $\Sigma_u^+-\Pi_g$ vibronic transition, have also been studied using LF measurements on cooled beams.[23,47] The average B' values for the Σ and Π vibronic levels are 0.395(14) and 0.398(17), respectively.[47] In a neon matrix,[8,39] 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.
Σ_g^+	1	Sym. stretch	940(60)	gas	LF	47
Π_u	2	Bend	222(20)H	Ne	AB	39
			195H	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[17,23,33,35,36,42,43,46] $\tilde{A}-\tilde{X}$ 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[11,45] $\tilde{A}-\tilde{X}$ 352–624 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	36,46

$\tau_0 = 200(10)$ ns gas LF[12,13]
In a neon or argon matrix,[11,45] efficient intersystem crossing into the $\tilde{a}\,^3\Pi_u$ state occurs, and $\tau \lesssim 10$ 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
17080 Ne EM[5]LF[11] $\tilde{a}-\tilde{X}$ 585–631 nm
IR32 $\tilde{b}-\tilde{a}$ 1250–1538 nm
16930 Ar EM[5,34]LF[45] $\tilde{a}-\tilde{X}$ 590–857 nm
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]
$\cong 0.01$ s Ar LF[45]
$A = 15.16(4)$ 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
			1216.4(6)	Ar	IR,EM,LF	19,34,45
			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
			73.0(3)H	Ar	LF	45
Σ_u^+	3	Asym. stretch	2040.02	gas	IR,DL,LF	16,18,23
			2042	Ne	IR	4
			2038.9s	Ar	IR	4,10,45
			2033.3	Kr	IR	41
			2036.0	H_2	IR	40,44
			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,[11,45] a second site was observed with $T_0 = 24408$.
[c] ω. Large Renner splitting, with $\epsilon = 0.537$.[6] Detailed comparisons of gas-phase with neon- and argon-matrix band positions are given in Refs. 8 and 14. Reference 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 $2\nu_3 = 1680$. Reference 46 reports a barrier of 284.3 in the double-minimum potential for the antisymmetric stretching fundamental of $C_3\,\tilde{A}\,^1\Pi_u$.
[e] Sum of values for $\tilde{a}-\tilde{X}$ and $\tilde{b}-\tilde{a}$ transitions.
[f] ω. Large Renner splitting, with $\epsilon = 0.447$.[37]
[g] $(\nu_1+\nu_3)-\nu_3$.
[h] ω. Large Renner splitting, with $\epsilon = 0.566$.[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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Si_3

$\tilde{G}$ 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

$\tilde{F}$ 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

$\tilde{E}$ C_{2v}
$T_0 = 17250(6)$ Ne AB[1,6] $\tilde{E}-X$ 530–580 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	250T	Ne	AB	6

$\tilde{C}\,{}^1A_1^a$ C_{2v}
$T_0 = 14200(160)$ gas PE[2,7]
12839(3) Ne AB[6] $\tilde{C}-\tilde{X}$ 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

$\tilde{B}\,{}^1B_1^b$ C_{2v}
$T_0 = 11549(160)$ gas PE[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	480(20)	gas	PE	7
	2	Bend	260(20)	gas	PE	7

$\tilde{c}\,{}^3B_1^c$ C_{2v}
$T_0 = 8880(80)$ gas PE[2,7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	480(20)	gas	PE	7
	2	Bend	260(20)	gas	PE	7

$\tilde{b}\,{}^3A_1^d$ C_{2v}
$T_0 = 7180(80)$ gas PE[2,7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	500(20)	gas	PE	7

$\tilde{A}\,{}^1B_2$ C_{2v}
$T_0 = 3630(80)$ gas PE[2,7]EM[3]

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

[a]Photoelectron band E (Ref. 7).
[b]Photoelectron band D (Ref. 7).
[c]Photoelectron band C (Ref. 7).
[d]Photoelectron band B (Ref. 7).

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. **100**, 1797 (1994).
[5] S. Li, R. J. Van Zee, W. Weltner, Jr., and K. Raghavachari, Chem. Phys. Lett. **243**, 275 (1995).
[6] J. Fulara, P. Freivogel, M. Grutter, and J. P. Maier, J. Phys. Chem. **100**, 18042 (1996).
[7] C. Xu, T. R. Taylor, G. R. Burton, and D. M. Neumark, J. Chem. Phys. **108**, 1395 (1998).

Sn_3

$\tilde{D}$
$T_0 = 5890(800)$ gas PE[1]

$\tilde{C}$
$T_0 = 5400(80)$ gas PE[1]

$\tilde{B}$
$T_0 = 2980(160)$ gas PE[1]

$\tilde{A}$
$T_0 = 890(110)$ gas PE[1]

Reference

[1] V. D. Moravec, S. A. Klopcic, and C. C. Jarrold, J. Chem. Phys. **110**, 5079 (1999).

CCN^+

$\tilde{A}\,^1\Pi$ $C_{\infty v}$
$T_0 = 21637(10)$ Ne AB[1] $\tilde{A}-\tilde{X}$ 427–462 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	"Asym." stretch	1725(20)	Ne	AB	1
Σ^+	3	"Sym." stretch	1223(20)	Ne	AB	1

Reference

[1] M. Wyss, E. Riaplov, J. P. Maier, M. Hochlaf, and P. Rosmus, Helv. Chim. Acta **84**, 1432 (2001).

CNC^+

$\tilde{A}\,^1\Pi_u$ $D_{\infty h}$
$T_0 = 30694(20)$ Ne AB[2] $\tilde{A}-\tilde{X}$ 301–326 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1100T	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_u^+	3	Asym. stretch	1974.07	gas	DL	1
			1972.9	Ne	IR	2,3

$B_0 = 0.461$ DL[1]

References

[1] M. Fehér, C. Salud, and J. P. Maier, J. Chem. Phys. **94**, 5377 (1991).
[2] M. Wyss, E. Riaplov, J. P. Maier, M. Hochlaf, and P. Rosmus, Helv. Chim. Acta **84**, 1432 (2001).
[3] A. M. Smith-Gicklhorn, M. Lorenz, R. Kołos, and V. E. Bondybey, J. Chem. Phys. **115**, 7534 (2001).

$ScCO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1732.0	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 2964 (1999).

$TiCO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1789.9	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 5259 (1999).

VCO^-

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1806.7	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 5259 (1999).

$CNbO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NbO stretch	877.8	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7785 (1999).

$CTaO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		TaO stretch	902.0	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7785 (1999).

$TaCO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1700.9T	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7785 (1999).

$MnCO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1807.5	Ne	IR	1
			1789.4	Ar	IR	1

Reference

[1] L. Andrews, M. Zhou, X. Wang, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **104**, 8887 (2000).

$ReCO^-$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1728.0	Ne	IR	1
			1704.2	Ar	IR	1

Reference

[1] L. Andrews, M. Zhou, X. Wang, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **104**, 8887 (2000).

$FeCO^-$

Threshold for electron detachment from ground-state $FeCO^- = 9335(40)$ gas PE[1,2]

$\tilde{X}\,^4\Sigma^-$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1980(100)T	gas	PE	1
			1782.0	Ne	IR	4
			1770.3	Ar	IR	3
Π	2	Bend	230(40)	gas	PE	2
Σ^+	3	FeC stretch	465(10)	gas	PE	2

References

[1] P. C. Engelking and W. C. Lineberger, J. Am. Chem. Soc. **101**, 5569 (1979).
[2] P. W. Villalta and D. G. Leopold, J. Chem. Phys. **98**, 7730 (1993).
[3] M. Zhou, G. V. Chertihin, and L. Andrews, J. Chem. Phys. **109**, 10893 (1998).
[4] M. Zhou and L. Andrews, J. Chem. Phys. **110**, 10370 (1999).

$RuCO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1792.8	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 6956 (1999).

$OsCO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1785.5	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 6956 (1999).

$CoCO^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1820.2	Ne	IR	2
			1804.0	Ar	IR	1

References

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 10250 (1998).
[2] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7773 (1999).

$RhCO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1828.6	Ne	IR	1,2
			1813.7	Ar	IR	2

References

[1] M. Zhou and L. Andrews, J. Am. Chem. Soc. **121**, 9171 (1999).
[2] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7773 (1999).

$IrCO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1842.6	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7773 (1999).

$NiCO^-$

Threshold for electron detachment from ground-state $NiCO^- = 6490(100)$ gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1860.6	Ne	IR	3
			1850.1	Ar	IR	2
			1847.0			

References

[1] A. E. Stevens, C. S. Feigerle, and W. C. Lineberger, J. Am. Chem. Soc. **104**, 5026 (1982).
[2] M. Zhou and L. Andrews, J. Am. Chem. Soc. **120**, 11499 (1998).
[3] B. Liang, M. Zhou, and L. Andrews, J. Phys. Chem. A **104**, 3905 (2000).

$PdCO^-$

Threshold for electron detachment from ground-state $PdCO^- = 4870(80)$ gas PE[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1909.0	Ne	IR	2

References

[1] S. A. Klopcic, V. D. Moravec, and C. C. Jarrold, J. Chem. Phys. **110**, 8986 (1999).
[2] B. Liang, M. Zhou, and L. Andrews, J. Phys. Chem. A **104**, 3905 (2000).

$PtCO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1896.3	Ne	IR	1

Reference

[1] B. Liang, M. Zhou, and L. Andrews, J. Phys. Chem. A **104**, 3905 (2000).

$CuCO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1746.2	Ne	IR	1
			1733.4	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Chem. Phys. **111**, 4548 (1999).

$CThO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ThO stretch	761.7	Ne	IR	1

Reference

[1] J. Li, B. E. Bursten, M. Zhou, and L. Andrews, Inorg. Chem. **40**, 5448 (2001).

CUO^-

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	UC stretch	929.3	Ne	IR	1
	3	UO stretch	803.3	Ne	IR	1

Reference

[1] M. Zhou, L. Andrews, J. Li, and B. E. Bursten, J. Am. Chem. Soc. **121**, 9712 (1999).

UCO^-

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1689.2	Ne	IR	1

Reference

[1] M. Zhou, L. Andrews, J. Li, and B. E. Bursten, J. Am. Chem. Soc. **121**, 9712 (1999).

$PtNN^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NN stretch	2054.1	Ne	IR	1
			2045.8	Ar	IR	1
			2048.9	N_2	IR	1

Reference

[1] A. Citra, X. Wang, W. D. Bare, and L. Andrews, J. Phys. Chem. A **105**, 7799 (2001).

BeNO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BeNO s-stretch	913.8	Ar	IR	1

Reference

[1] G. P. Kushto, F. Ding, B. Liang, X. Wang, A. Citra, and L. Andrews, Chem. Phys. **257**, 223 (2000).

MgNO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO stretch	1461.3	Ar	IR	1

Reference

[1] G. P. Kushto, F. Ding, B. Liang, X. Wang, A. Citra, and L. Andrews, Chem. Phys. **257**, 223 (2000).

NScO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	ScO stretch	931.1	Ne	IR	2
			909.5	Ar	IR	1
	3	ScN stretch	480.8	Ne	IR	2
			471.1	Ar	IR	1

References

[1] G. P. Kushto, M. Zhou, L. Andrews, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **103**, 1115 (1999).
[2] L. Andrews and X. Wang, J. Phys. Chem. A **106**, 1196 (2002).

ScNO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO stretch	1589.4	Ne	IR	2
			1563.3	Ar	IR	1

References

[1] G. P. Kushto, M. Zhou, L. Andrews, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **103**, 1115 (1999).
[2] L. Andrews and X. Wang, J. Phys. Chem. A **106**, 1196 (2002).

cyc-ScNO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			860.8	Ne	IR	2
			865.5	Ar	IR	1
			644.4	Ne	IR	2
			644.1	Ar	IR	1

References

[1] G. P. Kushto, M. Zhou, L. Andrews, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **103**, 1115 (1999).
[2] L. Andrews and X. Wang, J. Phys. Chem. A **106**, 1196 (2002).

NTiO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	TiO stretch	915.0	Ne	IR	3
			900.7s	Ar	IR	1,2
	2	Bend	248.2wm	Ar	IR	2
	3	TiN stretch	732.0	Ne	IR	3
			718.3s	Ar	IR	1,2

References

[1] G. P. Kushto, M. Zhou, L. Andrews, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **103**, 1115 (1999).
[2] L. Krim, C. Prot, E. M. Alikhani, and L. Manceron, Chem. Phys. **254**, 267 (2000).
[3] L. Andrews and X. Wang, J. Phys. Chem. A **106**, 1196 (2002).

TiNO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO stretch	1614.7	Ar	IR	1

Reference

[1] G. P. Kushto, M. Zhou, L. Andrews, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **103**, 1115 (1999).

NZrO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ZrO stretch	861.3	Ne	IR	2
			844.2	Ar	IR	1
	3	ZrN stretch	687.9	Ne	IR	2
			673.3	Ar	IR	1

References

[1] G. P. Kushto and L. Andrews, J. Phys. Chem. A **103**, 4836 (1999).
[2] L. Andrews and X. Wang, J. Phys. Chem. A **106**, 1196 (2002).

NHfO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	HfO stretch	855.2	Ar	IR	1
	3	HfN stretch	685.3	Ar	IR	1

Reference

[1] G. P. Kushto and L. Andrews, J. Phys. Chem. A **103**, 4836 (1999).

NVO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	VN stretch	1007.0	Ne	IR	2
			998.1	Ar	IR	1
	3	VO stretch	912.0	Ne	IR	2
			906.4	Ar	IR	1

References

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 478 (1999).
[2] L. Andrews and X. Wang, J. Phys. Chem. A **106**, 1196 (2002).

VNO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NO stretch	1606.0	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 478 (1999).

cyc-VNO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO stretch	1069.8	Ne	IR	2
			1075.7	Ar	IR	1

References

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 478 (1999).
[2] L. Andrews and X. Wang, J. Phys. Chem. A **106**, 1196 (2002).

NNbO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NbN stretch	977.3 975.3	Ar	IR	1
	3	NbO stretch	852.6 850.6	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 10025 (1998).

NTaO

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	TaN stretch	967.6 965.9	Ar	IR	1
	3	TaO stretch	857.9 855.8	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 10025 (1998).

NCrO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CrN stretch	969.7	Ne	IR	2
			976.1	Ar	IR	1
	3	CrO stretch	869.1	Ne	IR	2
			866.2	Ar	IR	1

References

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 7452 (1998).
[2] L. Andrews and X. Wang, J. Phys. Chem. A **106**, 1196 (2002).

CrNO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NO stretch	1637.5	Ne	IR	2
			1609.1	Ar	IR	1
	3	CrN stretch	533.3	Ar	IR	1

References

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 7452 (1998).
[2] L. Andrews and X. Wang, J. Phys. Chem. A **106**, 1196 (2002).

cyc-CrNO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO stretch	1123.9	Ne	IR	2
			1108.8	Ar	IR	1
	2	CrN stretch	528.2vw	Ar	IR	1
	3	CrO stretch	478.0vw	Ar	IR	1

References

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 7452 (1998).
[2] L. Andrews and X. Wang, J. Phys. Chem. A **106**, 1196 (2002).

NMoO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	MoN stretch	999.1	Ar	IR	1
	3	MoO stretch	846.5	Ar	IR	1

Reference

[1] L. Andrews and M. Zhou, J. Phys. Chem. A. **103**, 4167 (1999).

MoNO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO stretch	1620.6	Ar	IR	1

Reference

[1] L. Andrews and M. Zhou, J. Phys. Chem. A. **103**, 4167 (1999).

NWO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	WN stretch	1016.3	Ar	IR	1
	3	WO stretch	907.3	Ar	IR	1

Reference

[1] L. Andrews and M. Zhou, J. Phys. Chem. A. **103**, 4167 (1999).

NMnO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	MnN stretch	922.6	Ne	IR	2
			932.3	Ar	IR	1
	3	MnO stretch	872.7	Ne	IR	2
			874.0	Ar	IR	1

References

[1] L. Andrews, M. Zhou, and D. W. Ball, J. Phys. Chem. A **102**, 10041 (1998).
[2] L. Andrews and X. Wang, J. Phys. Chem. A **106**, 1196 (2002).

MnNO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO stretch	1754.5	Ne	IR	2
			1748.6T	Ar	IR	1

References

[1] L. Andrews, M. Zhou, and D. W. Ball, J. Phys. Chem. A **102**, 10041 (1998).
[2] L. Andrews and X. Wang, J. Phys. Chem. A **106**, 1196 (2002).

cyc-MnNO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO stretch	1235.7	Ne	IR	2
			1236.8	Ar	IR	1
			1232.4			

References

[1] L. Andrews, M. Zhou, and D. W. Ball, J. Phys. Chem. A **102**, 10041 (1998).
[2] L. Andrews and X. Wang, J. Phys. Chem. A **106**, 1196 (2002).

NReO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ReN stretch	1052.9	Ar	IR	1
	3	ReO stretch	901.2	Ar	IR	1

Reference

[1] L. Andrews, M. Zhou, and D. W. Ball, J. Phys. Chem. A **102**, 10041 (1998).

cyc-ReNO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO stretch	1137.2	Ar	IR	1

Reference

[1] L. Andrews, M. Zhou, and D. W. Ball, J. Phys. Chem. A **102**, 10041 (1998).

FeNO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO stretch	1766.0	Ne	IR	3
			1748.7	Ar	IR	1,3
			1746.8	N_2	IR	2
			1731.0			

References

[1] D. W. Ball and J. A. Chiarelli, J. Mol. Struct. **372**, 113 (1995).
[2] L. Andrews, G. V. Chertihin, A. Citra, and M. Neurock, J. Phys. Chem. **100**, 11235 (1996).
[3] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 3915 (2000).

cyc-FeNO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	NO stretch	1342.2	Ne	IR	1
			1343.8	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 3915 (2000).

RuNO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO stretch	1785.8	Ne	IR	1
			1765.9	Ar	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 8689 (2000).

NRuO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	RuN stretch	991.5	Ne	IR	1
			991.8	Ar	IR	1
	3	RuO stretch	800.4	Ne	IR	1
			803.0	Ar	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 8689 (2000).

OsNO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO stretch	1809.4	Ne	IR	1
			1789.1	Ar	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 8689 (2000).

NOsO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	OsN stretch	1057.6	Ne	IR	1
			1052.0	Ar	IR	1
	3	OsO stretch	892.0	Ne	IR	1
			886.9	Ar	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 8689 (2000).

cyc-OsNO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	NO stretch	1168.0	Ne	IR	1
			1132.6	Ar	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 8689 (2000).

CoNO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NO stretch	1794.2	Ne	IR	3
			1761.0	Ar	IR	1,3
			1771.4	N_2	IR	2
	3	CoN stretch	620.1	Ar	IR	3

References

[1] G. K. Ruschel, T. M. Nemetz, and D. W. Ball, J. Mol. Struct. **384**, 101 (1996).
[2] G. V. Chertihin, A. Citra, L. Andrews, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **101**, 8793 (1997).
[3] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 3915 (2000).

cyc-CoNO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	NO stretch	1317.4	Ne	IR	1
			1284.2	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 3915 (2000).

RhNO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO stretch	1806.4	Ne	IR	2
			1775.1	Ar	IR	1
			1765.9	N_2	IR	1

References

[1] A. Citra and L. Andrews, J. Phys. Chem. A **103**, 3410 (1999).
[2] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 11897 (2000).

NRhO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	RhN stretch	967.8	Ne	IR	1
			964.2	Ar	IR	1
	3	RhO stretch	813.7	Ar	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 11897 (2000).

IrNO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO stretch	1851.1	Ne	IR	1
			1833.7	Ar	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 11897 (2000).

NIrO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	IrN stretch	994.6	Ne	IR	1
			977.3	Ar	IR	1
	3	IrO stretch	868.9	Ne	IR	1
			850.6	Ar	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 11897 (2000).

NiNO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO stretch	1680.1	Ne	IR	3
			1677.1	Ar	IR	1–3
	3	NiN stretch	608.4	Ar	IR	2,3

References

[1] G. K. Ruschel, T. M. Nemetz, and D. W. Ball, J. Mol. Struct. **384**, 101 (1996).
[2] L. Krim, L. Manceron, and M. E. Alikhani, J. Phys. Chem. A **103**, 2592 (1999).
[3] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 3915 (2000).

cyc-NiNO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO stretch	1292.6	Ne	IR	2
			1293.9	Ar	IR	1,2
	2		540.5	Ar	IR	1
	3		464.4	Ar	IR	1

References

[1] L. Krim, L. Manceron, and M. E. Alikhani, J. Phys. Chem. A **103**, 2592 (1999).
[2] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 3915 (2000).

PdNO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO stretch	1676.4	Ne	IR	1
			1661.3s	Ar	IR	1,2
	2	Bend	229.8vw	Ar	IR	2
	3	PdN stretch	522.1w	Ar	IR	2

References

[1] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 8160 (2000).
[2] L. Krim, E. M. Alikhani, and L. Manceron, J. Phys. Chem. A **105**, 7812 (2001).

PtNO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO stretch	1712.6	Ne	IR	1
			1677.0	Ar	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 8160 (2000).

CuNO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO stretch	1602.2	Ne	IR	1
			1587.1	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 2618 (2000).

AgNO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO stretch	1711.8	Ne	IR	1
			1707.3			
			1680.3	Ar	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **105**, 3042 (2001).

NCeO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CeO stretch	757.2s	Ar	IR	1
Σ^+	3	CeN stretch	690.3w	Ar	IR	1

Reference

[1] S. P. Willson, L. Andrews, and M. Neurock, J. Phys. Chem. A **104**, 3446 (2000).

CeNO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO stretch	1341.1	Ar	IR	1

Reference

[1] S. P. Willson, L. Andrews, and M. Neurock, J. Phys. Chem. A **104**, 3446 (2000).

NPrO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	PrN stretch	900.8s	Ar	IR	1
Σ^+	3	PrO stretch	742.0m	Ar	IR	1

Reference

[1] S. P. Willson, L. Andrews, and M. Neurock, J. Phys. Chem. A **104**, 3446 (2000).

PrNO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO stretch	1359.3	Ar	IR	1

Reference

[1] S. P. Willson, L. Andrews, and M. Neurock, J. Phys. Chem. A **104**, 3446 (2000).

NNdO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Mixed	768.7s	Ar	IR	1
Σ^+	3	Mixed	661.4w	Ar	IR	1

Reference

[1] S. P. Willson, L. Andrews, and M. Neurock, J. Phys. Chem. A **104**, 3446 (2000).

NSmO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Mixed	736.9	Ar	IR	1

Reference

[1] S. P. Willson, L. Andrews, and M. Neurock, J. Phys. Chem. A **104**, 3446 (2000).

NEuO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		EuO stretch	657.8	Ar	IR	1

Reference

[1] S. P. Willson, L. Andrews, and M. Neurock, J. Phys. Chem. A **104**, 3446 (2000).

cyc-EuNO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			963.8	Ar	IR	1

Reference

[1] S. P. Willson, L. Andrews, and M. Neurock, J. Phys. Chem. A **104**, 3446 (2000).

NGdO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		GdO stretch	769.8	Ar	IR	1

Reference

[1] S. P. Willson, L. Andrews, and M. Neurock, J. Phys. Chem. A **104**, 3446 (2000).

cyc-GdNO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			997.6	Ar	IR	1

Reference

[1] S. P. Willson, L. Andrews, and M. Neurock, J. Phys. Chem. A **104**, 3446 (2000).

NTbO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Mixed	770.6	Ar	IR	1
Σ^+	3	Mixed	674.2	Ar	IR	1

Reference

[1] S. P. Willson, L. Andrews, and M. Neurock, J. Phys. Chem. A **104**, 3446 (2000).

cyc-TbNO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1111.4	Ar	IR	1

Reference

[1] S. P. Willson, L. Andrews, and M. Neurock, J. Phys. Chem. A **104**, 3446 (2000).

NDyO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		DyO stretch	784.9	Ar	IR	1

Reference

[1] S. P. Willson, L. Andrews, and M. Neurock, J. Phys. Chem. A **104**, 3446 (2000).

cyc-DyNO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			771.4	Ar	IR	1
			641.1	Ar	IR	1

Reference

[1] S. P. Willson, L. Andrews, and M. Neurock, J. Phys. Chem. A **104**, 3446 (2000).

NHoO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		HoO stretch	724.5	Ar	IR	1

Reference

[1] S. P. Willson, L. Andrews, and M. Neurock, J. Phys. Chem. A **104**, 3446 (2000).

cyc-HoNO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			764.7	Ar	IR	1

Reference

[1] S. P. Willson, L. Andrews, and M. Neurock, J. Phys. Chem. A **104**, 3446 (2000).

NErO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ErO stretch	790.3	Ar	IR	1

Reference

[1] S. P. Willson, L. Andrews, and M. Neurock, J. Phys. Chem. A **104**, 3446 (2000).

cyc-ErNO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			760.1	Ar	IR	1

Reference

[1] S. P. Willson, L. Andrews, and M. Neurock, J. Phys. Chem. A **104**, 3446 (2000).

NTmO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		TmO stretch	795.0	Ar	IR	1

Reference

[1] S. P. Willson, L. Andrews, and M. Neurock, J. Phys. Chem. A **104**, 3446 (2000).

NYbO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		YbO stretch	782.0	Ar	IR	1

Reference

[1] S. P. Willson, L. Andrews, and M. Neurock, J. Phys. Chem. A **104**, 3446 (2000).

NLuO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	LuO stretch	797.2	Ar	IR	1
	3	LuN stretch	425.6	Ar	IR	1

Reference

[1] S. P. Willson, L. Andrews, and M. Neurock, J. Phys. Chem. A **104**, 3446 (2000).

NThO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ThO stretch	784.2	Ne	IR	2
			760.3	Ar	IR	1
	3	ThN stretch	709.8	Ne	IR	2
			697.3	Ar	IR	1

References

[1] G. P. Kushto and L. Andrews, J. Phys. Chem. A **103**, 4836 (1999).
[2] M. Zhou and L. Andrews, J. Chem. Phys. **111**, 11044 (1999).

NUO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	UN stretch	1004.9	Ne	IR	4
			983.6	Ar	IR	1,2
			938	N_2	IR	3
	3	UO stretch	833.5	Ne	IR	4
			818.9	Ar	IR	2
			795	N_2	IR	3

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).
[3] K. Sankaran, K. Sundararajan, and K. S. Viswanathan, Bull. Mater. Sci. **22**, 785 (1999).
[4] M. Zhou and L. Andrews, J. Chem. Phys. **111**, 11044 (1999).

cyc-ScO_2^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	OO stretch	892.9	Ar	IR	1
	2	OScO s-stretch	641.1	Ar	IR	1
b_2	3	OScO a-stretch	624.8	Ar	IR	1

Reference

[1] C. W. Bauschlicher, Jr., M. Zhou, L. Andrews, J. R. Tobias Johnson, I. Panas, A. Snis, and B. O. Roos, J. Phys. Chem. A **103**, 5463 (1999).

cyc-YO_2^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	OO stretch	816.3	Ar	IR	1
	2	OYO s-stretch	595.3	Ar	IR	1
b_2	3	OYO a-stretch	587.5	Ar	IR	1

Reference

[1] L. Andrews, M. Zhou, G. V. Chertihin, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **103**, 6525 (1999).

cyc-LaO_2^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	OO stretch	804.0	Ar	IR	1

Reference

[1] L. Andrews, M. Zhou, G. V. Chertihin, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **103**, 6525 (1999).

$OLaO^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^-	3	Asym. stretch	689.3	Ar	IR	1

Reference

[1] L. Andrews, M. Zhou, G. V. Chertihin, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **103**, 6525 (1999).

$ONbO^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	989.7 988.0	Ar	IR	1
b_2	3	Asym. stretch	938.4 937.1	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 8251 (1998).

$OTaO^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	993.1 991.5	Ar	IR	1,2
b_2	3	Asym. stretch	938.8 937.4	Ar	IR	1,2

References

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 8251 (1998).
[2] M. Chen, X. Wang, L. Zhang, M. Yu, and Q. Qin, Chem. Phys. **242**, 81 (1999).

$OPrO^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	939.8	Ne	IR	1
			914.1	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 3171 (1999).

$ONdO^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	894.5	Ne	IR	1
			869.5	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 3171 (1999).

OUO^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	980.1	Ne	IR	1
			952.3	Ar	IR	1

Reference

[1] M. Zhou, L. Andrews, N, Ismail, and C. Marsden, J. Phys. Chem. A **104**, 5495 (2000).

NAlN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	656.9	N_2	IR	1

Reference

[1] L. Andrews, M. Zhou, G. V. Chertihin, W. D. Bare, and Y. Hannachi, J. Phys. Chem. A **104**, 1656 (2000).

NGaN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	586.4	N_2	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 1648 (2000).

NInN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	479.5	N_2	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 1648 (2000).

GaCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1875.6 1866.5	Ar	IR	1

Reference

[1] H.-J. Himmel, A. J. Downs, J. C. Green, and T. M. Greene, J. Phys. Chem. A **104**, 3642 (2000).

InCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1920.8	Ar	IR	1

Reference

[1] H.-J. Himmel, A. J. Downs, J. C. Green, and T. M. Greene, J. Phys. Chem. A **104**, 3642 (2000).

AlOSi

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	''Sym.'' stretch	524.2	CH_4	Ra	1
	3	''Asym.'' stretch	1012.7	Ar	IR	1
			1007.7	CH_4	IR	1

Reference

[1] M. Junker, M. Friesen, and H. Schnöckel, J. Chem. Phys. **112**, 1444 (2000).

cyc-AlP_2

$\tilde{A}\,^2A_1$ C_{2v}
$T^a = 5780(210)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Sym. stretch	425(10)	gas	PE	1

$\tilde{X}\,^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Sym. stretch	306(10)	gas	PE	1

[a]From vertical ionization potential.

Reference

[1] H. Gómez, T. R. Taylor, and D. M. Neumark, J. Phys. Chem. A **105**, 6886 (2001).

cyc-GaP_2

$\tilde{B}\,^2B_1$ C_{2v}
$T_0 = 21000(400)$ gas PE[2,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	P–P stretch	500	gas	PE	2,3
	2	GaP_2 s-stretch	234	gas	PE	2,3

$\tilde{A}\,^2A_1$ C_{2v}
$T_0 = 8420(800)$ gas PE[2,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	GaP_2 s-stretch	328	gas	PE	2,3

$\tilde{X}\,^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	P–P stretch	322T	Kr	IR	1
	2	GaP_2 s-stretch	222	gas	PE	2,3
			220.9	Ar	IR	1

References

[1] S. Li, R. J. Van Zee, and W. Weltner, Jr., J. Phys. Chem. **97**, 11393 (1993).
[2] T. R. Taylor, K. R. Asmis, H. Gomez, and D. M. Neumark, Eur. Phys. J. D **9**, 317 (1999).
[3] T. R. Taylor, H. Gómez, K. R. Asmis, and D. M. Neumark, J. Chem. Phys. **115**, 4620 (2001).

cyc-InP_2

$\tilde{A}\,^2A_1$ C_{2v}
$T_0 = 10330(8)$ gas PE[1]TPE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	PInP s-stretch	287	gas	TPE	2

$\tilde{X}\,^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	P=P stretch	479	gas	TPE	2
	2	PInP s-stretch	190.0(2)	gas	TPE	2

References

[1] C. Xu, E. de Beer, D. W. Arnold, C. C. Arnold, and D. M. Neumark, J. Chem. Phys. **101**, 5406 (1994).
[2] C. C. Arnold and D. M. Neumark, Can. J. Phys. **72**, 1322 (1994).

cyc-$GaAs_2$

$\tilde{A}\,^2A_1$ C_{2v}
$T_0 = 5600(620)$ gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		235	gas	PE	2

$\tilde{X}\,^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1		231.0T	Ar	IR	1
	2		176	gas	PE	2
			174.1	Ar	IR	1

References

[1] S. Li, R. J. Van Zee, and W. Weltner, Jr., J. Phys. Chem. **97**, 11393 (1993).
[2] T. R. Taylor, H. Gómez, K. R. Asmis, and D. M. Neumark, J. Chem. Phys. **115**, 4620 (2001).

C_3^-

$\tilde{E}$

$T_0 = 32003(3)$ gas PD[7] $\tilde{E}-\tilde{X}$ 308–313 nm

$\tilde{D}$

$T_0 = 29885(3)$ gas PD[7] $\tilde{D}-\tilde{X}$ 327–335 nm
29833(20) Ne AB[7] $\tilde{D}-\tilde{X}$ 329–336 nm

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

$T_0 = 28507(3)$ gas 20PD[6,7] $\tilde{C}-\tilde{X}$ 337–351 nm
28660(7) Ne AB[6,7] $\tilde{C}-\tilde{X}$ 335–349 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1140(6)	gas	PD	7
			1180(14)	Ne	AB	6
Π_u	2	Bend	445H	gas	PD	7

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

$T_0 = 25948(3)$ gas PD[6] $\tilde{B}-\tilde{X}$ 355–386 nm
25968(7) Ne AB[6] $\tilde{B}-\tilde{X}$ 370–385 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1072(6)	gas	PD	6
			1062(14)	Ne	AB	6
Π_u	2	Bend (ω)	407	gas	PD	6

$B_0 = 0.416$ PD[6]

$\tilde{A}\,^2\Delta_u$ $D_{\infty h}$

$T_0 = 24743(3)$ gas PD[6] $\tilde{A}-\tilde{X}$ 386–405 nm
24810(7) Ne AB[6] $\tilde{A}-\tilde{X}$ 385–403 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1140(6)	gas	PD	6
			1110(14)	Ne	AB	6
Π_u	2	Bend (ω)	410	gas	PD	6

$B_0 = 0.418$ PD[6]

$\tilde{b}\,^4\Pi_u$ $D_{\infty h}$

$T_0 = 22342(3)$ gas PD[6] $\tilde{b}-\tilde{X}$ 429–448 nm
22306(7) Ne AB[6] $\tilde{b}-\tilde{X}$ 412–448 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	959(4)	gas	PD	6
			953(10)	Ne	AB	6

Threshold for electron detachment from ground-state $C_3^- = 15980(160)$ gas PE[1–3]

$\tilde{X}\,^2\Sigma_g^+$ $D_{\infty h}$ Structure: IR[5]

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	1721.8	Ar	IR	4,5

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).
[5] J. Szczepanski, C. Wehlburg, and M. Vala, J. Phys. Chem. A **101**, 7039 (1997).
[6] M. Tulej, J. Fulara, A. Sobolewski, M. Jungen, and J. P. Maier, J. Chem. Phys. **112**, 3747 (2000).
[7] N. M. Lakin, F. Güthe, M. Tulej, M. Pachkov, and J. P. Maier, Faraday Discuss. **115**, 383 (2000).

Sn_3^-

Threshold for electron detachment from ground-state $Sn_3^- = 18070(80)$ gas PE[1]

Reference

[1] V. D. Moravec, S. A. Klopcic, and C. C. Jarrold, J. Chem. Phys. **110**, 5079 (1999).

CCN

$\tilde{D}\,^2\Pi$ $C_{\infty v}$

$T_0 = 27322(15)$ Ne AB[16]

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

$T_0 = 26661.80$ gas AB^1LF[14] $\tilde{C}-\tilde{X}$ 310–375 nm
26645(15) Ne AB[16]

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) (ω)	gas	LF	14

$B_0 = 0.413$ AB^1LF[14]

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

$T_0 = 22413.25$ gas AB^1 $\tilde{B}-\tilde{X}$ 442–446 nm
22430(10) Ne AB[16]
22180 Ar AB[3]

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

$B_0 = 0.405$ AB^1

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

$T_0 = 21259.203$ gas $AB^1LF^4EM^9$ $\tilde{A}-\tilde{X}$ 376–471 nm
21248(10) Ne AB^{16}
21377 Ar LF^2AB^3 $\tilde{A}-\tilde{X}$ 373–550 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Stretch	1770.77	gas	AB	1
			1732(2)	Ar	LF	2
Π	2	Bend	457.1 (ω)	gas	AB,LF	1,6,14
Σ^+	3	Stretch	1241.64	gas	AB	1
			1225(2)	Ar	LF	2

$\tau = 170$ ns Ar LF^2
$A_{eff} = -0.807$ gas $AB^1LF^{4,6}$
$B_0 = 0.414$ $AB^1LF^{4,6}DR^7$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Stretch	1923.25	gas	LF,EM, LMR,DL	5,8,9,12, 10,11
			1717	Ar	LF	2
Π	2	Bend	319.78 (ω)	gas	AB,LF,LMR	1,8,15
			179.60 ($\mu^2\Sigma^-$)	gas	LF,LMR	14,15
Σ^+	3	Stretch	1050.76	gas	LF,EM	5,8,9
			1066	Ar	LF	2

$A_0 = 42.539$, $\epsilon\omega_2 = 133.63$ gas $LF^8DL^{10,11}LMR^{12,15}$
$B_0 = 0.398$ $AB^1LF^{4,6}DL^{10,11}LMR^{12,15}MW^{13}$

References

[1] A. J. Merer and D. N. Travis, Can. J. Phys. **43**, 1795 (1965).
[2] V. E. Bondybey and J. H. English, J. Mol. Spectrosc. **70**, 236 (1978).
[3] M. E. Jacox, J. Mol. Spectrosc. **71**, 369 (1978).
[4] M. Kakimoto and T. Kasuya, J. Mol. Spectrosc. **94**, 380 (1982).
[5] K. Hakuta and H. Uehara, J. Chem. Phys. **78**, 6484 (1983).
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[7] T. Suzuki, S. Saito, and E. Hirota, J. Chem. Phys. **83**, 6154 (1985).
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[11] M. Fehér, C. Salud, J. P. Maier, and A. J. Merer, J. Mol. Spectrosc. **150**, 280 (1991).
[12] D. A. Gillett and J. M. Brown, Can. J. Phys. **72**, 2002 (1994).
[13] Y. Ohshima and Y. Endo, J. Mol. Spectrosc. **172**, 225 (1995).
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[16] M. Wyss, E. Riaplov, J. P. Maier, M. Hochlaf, and P. Rosmus, Helv. Chim. Acta **84**, 1432 (2001).

SiCN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CN stretch	2077.3m	Ar	IR	1
	3	SiC stretch	584.6vs	Ar	IR	1

$A_{eff} = 70.8$ gas MW^3
$B_0 = 0.185$ $MW^{2,3}$

References

[1] G. Maier, H. P. Reisenauer, H. Egenolf, and J. Glatthaar, Eur. J. Org. Chem. **1998**, 1307.
[2] A. J. Apponi, M. C. McCarthy, C. A. Gottlieb, and P. Thaddeus, Astrophys. J. **536**, L55 (2000).
[3] M. C. McCarthy, A. J. Apponi, C. A. Gottlieb, and P. Thaddeus, J. Chem. Phys. **115**, 870 (2001).

CNC

$\tilde{B}\,^2\Sigma_u^-$ $D_{\infty h}$ Structure: AB^1

$T_0 = 34802.33$ gas AB^1 $\tilde{B}-\tilde{X}$ 283–288 nm
34652(20) gas AB^3
34602(20) Ar[a] AB^2 $\tilde{B}-\tilde{X}$ 276–292 nm
34305(20)

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

$B_0 = 0.443$ AB^1

$\tilde{A}\,^2\Delta_u$ $D_{\infty h}$ Structure: AB^1

$T_0 = 30338.53$ gas AB^1 $\tilde{A}-\tilde{X}$ 325–332 nm
30294(20) Ne AB^3
30048(20) Ar AB^2 $\tilde{A}-\tilde{X}$ 324–333 nm

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

$A = 0.33$ gas AB^1
$B_0 = 0.450$ AB^1

$\tilde{X}\,^2\Pi_g$ $D_{\infty h}$ Structure: AB^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	321[b]	gas	AB	1
Σ_u^+	3	Asym. stretch	1452.4	Ne	IR	3
			1453s	Ar	IR	2

$A = 26.41$; $\epsilon = 0.549$ AB^1
$B_0 = 0.454$ AB^1

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

References

[1] A. J. Merer and D. N. Travis, Can. J. Phys. **44**, 353 (1966).
[2] M. E. Jacox, J. Mol. Spectrosc. **71**, 369 (1978).
[3] M. Wyss, E. Riaplov, J. P. Maier, M. Hochlaf, and P. Rosmus, Helv. Chim. Acta **84**, 1432 (2001).

SiNC

In an argon matrix,[1] irradiation at 366 nm results in photoisomerization to SiCN.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NC stretch	1945.2vs	Ar	IR	1
	3	SiN stretch	629.1m	Ar	IR	1

$A_{eff}=58.8$ gas MW[3]
$B_0=0.213$ MW[2]

References

[1] G. Maier, H. P. Reisenauer, H. Egenolf, and J. Glatthaar, Eur. J. Org. Chem. **1998**, 1307.
[2] A. J. Apponi, M. C. McCarthy, C. A. Gottlieb, and P. Thaddeus, Astrophys. J. **536**, L55 (2000).
[3] M. C. McCarthy, A. J. Apponi, C. A. Gottlieb, and P. Thaddeus, J. Chem. Phys. **115**, 870 (2001).

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]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	904.0	Ar	IR	2
			910.0	N_2	IR	2

$B_0=0.112$ MPI[1]

References

[1] D. J. Brugh and M. D. Morse, Chem. Phys. Lett. **267**, 370 (1997).
[2] G. Meloni, S. Nunziante Cesaro, and N. Sanna, Chem. Phys. Lett. **343**, 113 (2001).

SnCN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	SnC stretch	380(10)	gas	PE	1

$A=2300(65)$ gas PE[1]

Reference

[1] V. D. Moravec and C. C. Jarrold, J. Chem. Phys. **113**, 1035 (2000).

$NTiO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		TiO stretch	791.4	Ne	IR	2
			784.3	Ar	IR	1

References

[1] G. P. Kushto, M. Zhou, L. Andrews, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **103**, 1115 (1999).
[2] L. Andrews and X. Wang, J. Phys. Chem. A **106**, 1196 (2002).

$NTaO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		TaO stretch	819.1T	Ar	IR	1
			814.1T			

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 10025 (1998).

$CrNO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO stretch	1519.9	Ne	IR	2
			1511.5	Ar	IR	1

References

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 7452 (1998).
[2] L. Andrews and X. Wang, J. Phys. Chem. A **106**, 1196 (2002).

$NReO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	ReN stretch	1038.0T	Ar	IR	1
	3	ReO stretch	860.9T	Ar	IR	1

Reference

[1] L. Andrews, M. Zhou, and D. W. Ball, J. Phys. Chem. A **102**, 10041 (1998).

$CoNO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO stretch	1585.7	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 3915 (2000).

$NiNO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO stretch	1454.7	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 3915 (2000).

$PdNO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO stretch	1487.6	Ne	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 8160 (2000).

$PtNO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO stretch	1462.1	Ne	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 8160 (2000).

$AgNO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO stretch	1399.2	Ne	IR	1
			1392.3	Ar	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **105**, 3042 (2001).

$NCeO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CeO stretch	624.8	Ar	IR	1

Reference

[1] S. P. Willson, L. Andrews, and M. Neurock, J. Phys. Chem. A **104**, 3446 (2000).

$NPrO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	PrN stretch	718.2	Ar	IR	1
	3	PrO stretch	612.3	Ar	IR	1

Reference

[1] S. P. Willson, L. Andrews, and M. Neurock, J. Phys. Chem. A **104**, 3446 (2000).

GaNO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NO stretch	1578.5	Ar	IR	1

Reference

[1] L. Andrews, M. Zhou, and X. Wang, J. Phys. Chem. A **104**, 8475 (2000).

InNO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NO stretch	1524.9	Ar	IR	1

Reference

[1] L. Andrews, M. Zhou, and X. Wang, J. Phys. Chem. A **104**, 8475 (2000).

TINO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO stretch	1454.6	Ar	IR	1

Reference

[1] L. Andrews, M. Zhou, and X. Wang, J. Phys. Chem. A **104**, 8475 (2000).

OScO

$\tilde{C}$
$T_0 = 10330(800)$ gas PE[1]
$\tilde{B}$
$T_0 = 3870T$ gas PE[1]
$\tilde{A}$
$T_0 = 3070T$ gas PE[1]
$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	740(80)	gas	PE	1

Reference

[1] H. Wu and L.-S. Wang, J. Phys. Chem. A **102**, 9129 (1998).

OYO

$\tilde{C}$
$T_0 = 10330(540)$ gas PE[1]
$\tilde{B}$
$T_0 = 6050(470)$ gas PE[1]
$\tilde{A}$
$T_0 = 3710(765)$ 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	640(80)	gas	PE	1
			708.2	Ar	IR	2

References

[1] H. Wu and L.-S. Wang, J. Phys. Chem. A **102**, 9129 (1998).
[2] L. Andrews, M. Zhou, G. V. Chertihin, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **103**, 6525 (1999).

OLaO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	569.8	Ar	IR	1

Reference

[1] L. Andrews, M. Zhou, G. V. Chertihin, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **103**, 6525 (1999).

OTiO

$\tilde{A}\,^1B_2$ $D_{\infty h}$
$T_0 = 19360(1600)$ gas PE[3]
18880 Ne EM[1] 529–621 nm

$\tilde{a}\,^3B_2$
$T_0 = 15800(800)$ gas PE[4]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	965T	gas	IR,PE	2,4
			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).
[4] H. Wu and L.-S. Wang, J. Chem. Phys. **107**, 8221 (1997).

OZrO

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

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

$A_0 = 0.663$; $B_0 = 0.257$; $C_0 = 0.185$ MW[2]

References

[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. **99**, 6356 (1995).
[2] D. J. Brugh, R. D. Suenram, and W. J. Stevens, J. Chem. Phys. **111**, 3526 (1999).

OVO

$\tilde{C}\,^2A_2$ C_{2v}
$T_0 = 21000(800)$ gas PE[2]

$\tilde{B}\,^2B_2$ C_{2v}
$T_0 = 16140(800)$ gas PE[2]

$\tilde{A}\,^2B_1$ C_{2v}
$T_0 = 4840(800)$ gas PE[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	970(40)	gas	PE	2
			946.3w	Ar	IR	1
b_2	3	Asym. stretch	935.9s	Ar	IR	1

References

[1] G. V. Chertihin, W. D. Bare, and L. Andrews, J. Phys. Chem. A **101**, 5090 (1997).
[2] H. Wu and L.-S. Wang, J. Chem. Phys. **108**, 5310 (1998).

ONbO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	933.5	Ar	IR	1
b_2	3	Asym. stretch	875.9	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 8251 (1998).

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	965.3	Ar	IR	1–3
b_2	3	Asym. stretch	912.2	Ar	IR	1–3

References

[1] W. Weltner, Jr. and D. McLeod, Jr., J. Chem. Phys. **42**, 882 (1965).
[2] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 8251 (1998).
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OCrO

$\tilde{B}$
$T^a = 14680(430)$ gas PE[10]

$\tilde{A}$
$T^a = 7910(430)$ gas PE[10]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	895(20)	gas	PE	6,10
			920.8	Ne	IR	9
			914.4	Ar	IR	7,8
	2	Bend	220(20)	gas	PE	6,10
b_2	3	Asym. stretch	974.9	Ne	IR	9
			965.4	Ar	IR	1–5,7,8

[a]From vertical electron detachment energies.

References

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[2] M. Poliakoff, K. P. Smith, J. J. Turner, and A. J. Wilkinson, J. Chem. Soc., Dalton Trans. 651 (1982).
[3] M. J. Almond, A. J. Downs, and R. N. Perutz, Inorg. Chem. **24**, 275 (1985).
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[5] M. J. Almond and M. Hahne, J. Chem. Soc., Dalton Trans. 2255 (1988).
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[9] M. Zhou and L. Andrews, J. Chem. Phys. **111**, 4230 (1999).
[10] G. L. Gutsev, P. Jena, H.-J. Zhai, and L.-S. Wang, J. Chem. Phys. **115**, 7935 (2001).

OMoO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	950.7	Ne	IR	1,4
			939.3	Ar	IR	1–3
b_2	3	Asym. stretch	901.3	Ne	IR	1,4
			885.5	Ar	IR	1–3

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).
[3] W. D. Bare, P. F. Souter, and L. Andrews, J. Phys. Chem. A **102**, 8279 (1998).
[4] M. Zhou and L. Andrews, J. Chem. Phys. **111**, 4230 (1999).

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

$^3A_1$? C_{2v}
$T_0 \geqslant 8010(100)$ gas PE[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	945(25)	gas	PE	4
	2	Bend	340(20)	gas	PE	4

$^1B_1$? C_{2v}
$T_0 \geqslant 6260(100)$ gas PE[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	970(15)	gas	PE	4

$\tilde{a}\,^3B_1$ C_{2v}
$T_0 \geqslant 2640(100)$ gas PE[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	995(25)	gas	PE	4
	2	Bend	320(15)	gas	PE	4

OMnO

$\tilde{X}\,^4B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	816.4	Ar	IR	2
b_2	3	Asym. stretch	948.0s	Ar	IR	1,2
			969.6	N_2	IR	2
			962.4			

References

[1] L. V. Serebrennikov and A. A. Maltsev, Vestn. Mosk. Univ., Ser. 2, Khim. **2**, 148 (1980).
[2] G. V. Chertihin and L. Andrews, J. Phys. Chem. A **101**, 8547 (1997).

cyc-MnO_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	OO stretch	1108.2	Ar	IR	1,2
			1108.4	N_2	IR	2
	2	OMnO s-stretch	686.4s	Ar	IR	1,2
			686.6	N_2	IR	2

References

[1] L. V. Serebrennikov and A. A. Maltsev, Vestn. Mosk. Univ., Ser. 2, Khim. **2**, 148 (1980).
[2] G. V. Chertihin and L. Andrews, J. Phys. Chem. A **101**, 8547 (1997).

MnOO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	1224.5T	Ar	IR	1

Reference

[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. A **101**, 8547 (1997).

OReO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	989.2	Ne	IR	1
			981.9	Ar	IR	1
b_2	3	Asym. stretch	941.0	Ne	IR	1
			931.7	Ar	IR	1

Reference

[1] M. Zhou, A. Citra, B. Liang, and L. Andrews, J. Phys. Chem. A **104**, 3457 (2000).

ORuO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	911.9	Ne	IR	2
			902.1	Ar	IR	1,2

References

[1] J. G. Kay, D. W. Green, K. Duca, and G. L. Zimmerman, J. Mol. Spectrosc. **138**, 49 (1989).
[2] M. Zhou, A. Citra, B. Liang, and L. Andrews, J. Phys. Chem. A **104**, 3457 (2000).

OOsO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	957.3	Ne	IR	1
			949.9	Ar	IR	1

Reference

[1] M. Zhou, A. Citra, B. Liang, and L. Andrews, J. Phys. Chem. A **104**, 3457 (2000).

OCoO

$\tilde{X}$ $D_{\infty h}$ Structure: ESR[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	790(60)	gas	PD	3
Σ_u^+	3	Asym. stretch	945.4	Ar	IR	2
			978.6	N_2	IR	2

References

[1] R. J. Van Zee, Y. M. Hamrick, S. Li, and W. Weltner, Jr., J. Phys. Chem. **96**, 7247 (1992).
[2] G. V. Chertihin, A. Citra, L. Andrews, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **101**, 8793 (1997).
[3] L.-S. Wang, cited by Ref. 2.

CoOO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	1286.8	Ar	IR	1
			1284	N_2	IR	1

Reference

[1] G. V. Chertihin, A. Citra, L. Andrews, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **101**, 8793 (1997).

cyc-CoOO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	OO stretch	984.9	Ar	IR	1
			1018.8	N_2	IR	1

Reference

[1] G. V. Chertihin, A. Citra, L. Andrews, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **101**, 8793 (1997).

ORhO

$\tilde{X}$ $D_{\infty h}$ Structure: ESR[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	845T	Ar	IR	2
Σ_u^+	3	Asym. stretch	900.1	Ar	IR	2

References

[1] R. J. Van Zee, Y. M. Hamrick, S. Li, and W. Weltner, Jr., J. Phys. Chem. **96**, 7247 (1992).
[2] A. Citra and L. Andrews, J. Phys. Chem. A **103**, 4845 (1999).

OIrO

$\tilde{X}$ $D_{\infty h}$ Structure: ESR[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	960T	Ar	IR	2
Σ_u^+	3	Asym. stretch	929.0	Ar	IR	2

References

[1] R. J. Van Zee, Y. M. Hamrick, S. Li, and W. Weltner, Jr., J. Phys. Chem. **96**, 7247 (1992).
[2] A. Citra and L. Andrews, J. Phys. Chem. A **103**, 4182 (1999).

cyc-IrOO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	OO stretch	1022.7	Ar	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A. **103**, 4182 (1999).

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
Π_u	2	Bend	125.0	Ar	IR	3
Σ_u^+	3	Asym. stretch	954.9	Ar	IR	1,3
			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).
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cyc-NiO_2

$\tilde{A}$

$T_0 = 8000$T 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	967.1s	Ar	IR	1,2,4
			970.1	N_2	IR	2
	2	ONiO s-stretch	538.3w	Ar	IR	2,4
b_2	3	ONiO a-stretch	511.7m	Ar	IR	2,4

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).
[4] D. Danset, L. Manceron, and L. Andrews, J. Phys. Chem. A **105**, 7205 (2001).

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	1030.1	Ne	IR	3
			1023.0	Ar	IR	1,2
			997.7	N_2	IR	2
	2	OPdO 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).
[2] W. D. Bare, A. Citra, G. V. Chertihin, and L. Andrews, J. Phys. Chem. A **103**, 5456 (1999).
[3] X. Wang and L. Andrews, J. Phys. Chem. A **105**, 5812 (2001).

OPtO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	900T	Ar	IR	1
Σ_u^+	3	Asym. stretch	958.7	Ne	IR	2
			961.8	Ar	IR	1,3
			953.3			

References

[1] W. D. Bare, A. Citra, G. V. Chertihin, and L. Andrews, J. Phys. Chem. A **103**, 5456 (1999).
[2] X. Wang and L. Andrews, J. Phys. Chem. A **105**, 5812 (2001).
[3] D. Danset, L. Manceron, and L. Andrews, J. Phys. Chem. A **105**, 7205 (2001).

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	930.0	Ne	IR	3
			928.0s	Ar	IR	1,2,4
	2	OPtO s-stretch	512.3w	Ar	IR	4
b_2	3	OPtO a-stretch	551.2wm	Ar	IR	4

References

[1] H. Huber, W. Klotzbücher, G. A. Ozin, and A. Vander Voet, Can. J. Chem. **51**, 2722 (1973).
[2] W. D. Bare, A. Citra, G. V. Chertihin, and L. Andrews, J. Phys. Chem. A **103**, 5456 (1999).
[3] X. Wang and L. Andrews, J. Phys. Chem. A **105**, 5812 (2001).
[4] D. Danset, L. Manceron, and L. Andrews, J. Phys. Chem. A **105**, 7205 (2001).

OCuO

$T_0 = 20699$ Ne $LF^{3,7}$ 432–540 nm
20486.5 Ar $LF^{1,3,7}$
20064 Kr LF^7
19686.9 Xe UV^2LF^7 440–586 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	CuO s-stretch	611.5	Ne	LF	3,7
			627.5	Ar	LF	7
			625.9			
			608.1			
			618.9	Xe	AB,LF	2,7
			614.1	N_2	LF	7
Π_u	2	Bend	135.6	Ne	LF	3,7
			118	Xe	LF	7
Σ_u^+	3	Asym. stretch	628	Xe	LF	7

$\tilde{E}'$

$T_0 = 13640(160)$ gas PE[5]

$\tilde{D}$

$T_0 = 11309.5$ Ne LF^7
11268.5 Xe LF^7

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	636.8	Ne	LF	7
Π_u	2	Bend	234	Ne	LF	7

$\tilde{C}$

$T_0 = 11110.5$ Ne LF^7
11060 Xe LF^7

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	640.8	Ne	LF	7

$\tilde{C}'$
$T_0 = 9680(160)$ gas PE[5]

$\tilde{C}''$
$T_0 = 6540(160)$ gas PE[4,5]

$\tilde{B}$
$T_0 = 6683.4$ Xe LF[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	569.7	Xe	LF	7

$\tilde{B}'$
$T_0 = 5080(160)$ gas PE[4,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			640(80)	gas	PE	4,5

$\tilde{A}$
$T_0 = 3850T$ Ne LF[3,7]
3387.3 Xe LF[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	590	Ne	LF	3
			597.5	Xe	LF	7
Π_u	2	Bend	113	Xe	LF	7

$\tilde{A}'$
$T_0 = 2580(160)$ 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	3,7
			668	Ar	LF	1
			664.2	Xe	EM,LF	2,7
Π_u	2	Bend	193.4	Ne	LF	3,7
			161.5	Xe	LF	7
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. Garćia-Prieto, J. Am. Chem. Soc. **105**, 6399 (1983).
[3] V. E. Bondybey and J. H. English, J. Phys. Chem. **88**, 2247 (1984).
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[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).
[7] N. Caspary, E. V. Savchenko, A. Thoma, A. Lammers, and V. E. Bondybey, Low Temp. Phys. **26**, 744 (2000).

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	1102.5	Ne	IR	3
			1075.7	Ar	IR	1,2

References

[1] D. E. Tevault, R. R. Smardzewski, M. W. Urban, and K. Nakamoto, J. Chem. Phys. **77**, 577 (1982).
[2] A. Citra and L. Andrews, J. Mol. Struct. **489**, 95 (1999).
[3] X. Wang and L. Andrews, J. Phys. Chem. A **105**, 5812 (2001).

AuOO

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 AuO_2.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OO stretch	1213.6	Ne	IR	3
			1093.8	Ar	IR	1,2

References

[1] D. McIntosh and G. A. Ozin, Inorg. Chem. **15**, 2869 (1976).
[2] A. Citra and L. Andrews, J. Mol. Struct. **489**, 95 (1999).
[3] X. Wang and L. Andrews, J. Phys. Chem. A **105**, 5812 (2001).

OAuO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	824.2	Ne	IR	2
			817.9	Ar	IR	1

References

[1] A. Citra and L. Andrews, J. Mol. Struct. **489**, 95 (1999).
[2] X. Wang and L. Andrews, J. Phys. Chem. A **105**, 5812 (2001).

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
			757.3w	Ar	IR,EM	1–3
			714	N_2	IR,EM	1
b_2	3	Asym. stretch	759s	Ne	IR	1
			736.7s	Ar	IR	1–3
			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).
[3]S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 3171 (1999).

cyc-CeO_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	OO stretch	823.7	Ar	IR	1

Reference

[1]S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 3171 (1999).

OPrO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	711.7T	Ne	IR	3
			696.0T	Ar	IR	3
Σ_u^+	3	Asym. stretch	752.5	Ne	IR	3
			730.1	Ar	IR	1–3

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).
[3]S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 3171 (1999).

cyc-PrO_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	OO stretch	827T	Ar	IR	1

Reference

[1]S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 3171 (1999).

ONdO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	661.8T	Ar	IR	1
Σ_u^+	3	Asym. stretch	737.6	Ne	IR	1
			716.9	Ar	IR	1

Reference

[1]S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 3171 (1999).

OSmO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	602.5T	Ar	IR	1
Σ_u^+	3	Asym. stretch	643.2	Ar	IR	1

Reference

[1]S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 3171 (1999).

OEuO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	622.8	Ar	IR	1

Reference

[1]S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 3171 (1999).

OGdO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	635.5	Ar	IR	1

Reference

[1]S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 3171 (1999).

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	2,3
b_2	3	Asym. stretch	718.8	Ar	IR	1–3

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).
[3] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 6972 (1999).

ODyO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	612.2T	Ar	IR	1
Σ_u^+	3	Asym. stretch	599.2	Ne	IR	1
			580.5	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 6972 (1999).

OHoO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	668.2	Ne	IR	1
			649.2	Ar	IR	1
b_2	3	Asym. stretch	548.8	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 6972 (1999).

OTmO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	706.6	Ar	IR	1
b_2	3	Asym. stretch	615.7	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 6972 (1999).

OYbO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	632.1T	Ar	IR	1
Σ_u^+	3	Asym. stretch	627.7	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 6972 (1999).

OThO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	808.4	Ne	IR	3
			787.3	Ar	IR	1,2
b_2	3	Asym. stretch	756.7	Ne	IR	3
			735.0	Ar	IR	1,2

References

[1] S. D. Gabelnick, G. T. Reedy, and M. G. Chasanov, J. Chem. Phys. **60**, 1167 (1974).
[2] G. P. Kushto and L. Andrews, J. Phys. Chem. A **103**, 4836 (1999).
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OUO

^3H_g? $D_{\infty h}$

When OUO is isolated in an argon or heavier rare-gas matrix, an absorption pattern which differs from that characteristic of a neon matrix results. This is attributed[4] to a sufficiently large shift in this very low-lying excited state to place it below the ground state of the free molecule.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	776.1	Ar	IR	1–4
			768.0	Kr	IR	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	914.8	Ne	IR	4

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[1] S. D. Gabelnick, G. T. Reedy, and M. G. Chasanov, J. Chem. Phys. **58**, 4468 (1973).
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$AlCO^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1682.3	Ar	IR	1

Reference

[1] L. Zhang, J. Dong, M. Zhou, and Q. Qin, J. Chem. Phys. **113**, 10169 (2000).

NAlO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	AlO stretch	1079.5	Ar	IR	1

Reference

[1] L. Andrews, M. Zhou, and W. D. Bare, J. Phys. Chem. A **102**, 5019 (1998).

AlNO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO stretch	1644.3	Ar	IR	1
	3	AlN stretch	510.2	Ar	IR	1

Reference

[1] L. Andrews, M. Zhou, and W. D. Bare, J. Phys. Chem. A **102**, 5019 (1998).

AlON

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	ON stretch	1282.1	Ar	IR	1,2
	3	AlO stretch	566.7	Ar	IR	2

References

[1] G. K. Ruschel and D. W. Ball, High Temp. Mater. Sci. **37**, 63 (1997).
[2] L. Andrews, M. Zhou, and W. D. Bare, J. Phys. Chem. A **102**, 5019 (1998).

cyc-AlP_2^-

Threshold for electron detachment from ground-state *cyc*-AlP_2^- = 15600(56) gas PE[1]

Reference

[1] H. Gómez, T. R. Taylor, and D. M. Neumark, J. Phys. Chem. A **105**, 6886 (2001).

cyc-InP_2^-

Threshold for electron detachment from ground-state InP_2^- = 13050(8) gas PE[1]TPE[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	PInP s-stretch	227T	gas	TPE	2

References

[1] C. Xu, E. de Beer, D. W. Arnold, C. C. Arnold, and D. M. Neumark, J. Chem. Phys. **101**, 5406 (1994).
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cyc-$GaAs_2^-$

Threshold for electron detachment from ground-state *cyc*-$GaAs_2^-$ = 15280(270) gas PE[1]

Reference

[1] T. R. Taylor, H. Gómez, K. R. Asmis, and D. M. Neumark, J. Chem. Phys. **115**, 4620 (2001).

CCO

$\tilde{c}\,{}^1\Pi$ $C_{\infty v}$
T_0 = 22390(160) gas PF,PE[17]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	CC stretch	1234(140)	gas	PE	17

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[10–12,14,20] $\tilde{A}$–$\tilde{X}$ 500–860 nm
11650(3) Ne AB[18]
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
			2045(3)	Ne	AB	18
Π	2	Bend	594.75[a]	gas	AB,DL	3,12
Σ^+	3	CC stretch	1283.60	gas	AB,DL	3,14
			1279(3)	Ne	AB	18

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, sug-

gesting perturbation by the $\tilde{b}\,^1\Sigma^+$ and $\tilde{a}\,^1\Delta$ states, as well as by high ground-state vibrational levels.
$A=-35.36$; $\epsilon=-0.172$ gas AB^3DL[10]
$B_0=0.407$ AB^3DL[10]

$\tilde{b}\,^1\Sigma^+$ $C_{\infty v}$
$T_0=8190(145)$ gas PE[15,17]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1920(160)	gas	PE	15,17

$\tilde{a}\,^1\Delta$ $C_{\infty v}$
$T_0=5270(140)$ gas PE[15,17]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1942.85	gas	PE,DL	15,17,19

$B_0=0.383$ DL[19]

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

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SiCO

$\tilde{A}\,^3\Pi$? $C_{\infty v}$
$T_0=24056(10)$ Ar AB^1 $\tilde{A}-\tilde{X}$ 365–416 nm

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

$\tilde{X}\,^3\Sigma^-$?

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1898.1	Ar	IR	1,2

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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	2,3
			1908	Kr	IR	1
			1921.3	N_2	IR	2
			1924.0	CO	IR	2

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SnCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1941.1	Ar	IR	2
			1921	Kr	IR	1

References

[1] A. Bos, J. Chem. Soc., Chem. Commun. 26 (1972).
[2] L. Zhang, J. Dong, and M. Zhou, J. Chem. Phys. **113**, 8700 (2000).

CCS

$\tilde{A}\,^3\Pi$ $C_{\infty v}$
$T_0 < 14663$ gas LF[4] $\tilde{A}-\tilde{X}$ 600–690 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CC stretch	1760T	gas	LF	4

$\tau \cong 4\ \mu s$ gas LF[4]
$A = -122.4$ LF[4]
$B = 0.213$ LF[4]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CC stretch	1671(3)	gas	LF	4
Π	2	Bend	267(3)	gas	LF	4
Σ^+	3	CS stretch	858(3)	gas	LF	4

$B_0 = 0.216$ MW[1–3]

References

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NCN

$\tilde{d}\,^1\Delta_u$ $D_{\infty h}$
$T_0 = 43530(80)$ gas AB[6]PF[14] $\tilde{d}-\tilde{a}$ 250–290 nm
In the gas phase,[14] this state photodissociates into $N_2(X\,^1\Sigma_g^+) + C(^1\Delta)$.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1020T	gas	PF	14

$\tilde{c}\,^1\Pi_u$ $D_{\infty h}$ Structure: AB[5]
$T_0 = 38200(80)$ gas AB[5]PF[14] $\tilde{c}-\tilde{a}$ 330–334 nm
In the gas phase,[14] this state photodissociates into $N_2(X\,^1\Sigma_g^+) + C(^3P)$.

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

$\epsilon\omega_2 = -84.2$ gas AB[5]
$B_0 = 0.395$ AB[5]

$\tilde{B}\,^3\Sigma_u^-$ $D_{\infty h}$
$T_0 = 33488$ gas AB[6]PF[14] $\tilde{B}-\tilde{X}$ 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, the bands are diffuse,[6] and photodissociation into $N_2(X\,^1\Sigma_g^+) + C(^3P)$ predominates.[14] The threshold for photodecomposition into $C + N_2$ is 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	1050T	gas	AB,PF	6,14
			1050(10)	Ar,N_2	AB	2
Π_u	2	Bend	540(20)	gas	PF	14

$\tilde{A}\,^3\Pi_u$ $D_{\infty h}$ Structure: AB[1]LF[10]
$T_0 = 30383.967$ gas AB[1]LF[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

$A = -37.57$; $\epsilon\omega_2 = -91.12$ gas AB[1]LF[12]
$\tau_0 = 183(6)$ ns gas LF[8]
$B_0 = 0.397$ AB[1]LF[10,12]

$\tilde{b}\,^1\Sigma_g^+$ $D_{\infty h}$
$T_0 = 13140(80)$ gas PE[13]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1120(50)	gas	PE	13

$\tilde{a}\,^1\Delta_g$ $D_{\infty h}$ Structure: AB[5]
$T_0 = 8150(80)$ gas AB[5]PE[13] $\tilde{c}-\tilde{a}$ 330–334 nm
$B_0 = 0.399$ AB[5]

$\tilde{X}\,^3\Sigma_g^-$ $D_{\infty h}$ Structure: AB[1]LF[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[1]LF[9,10]IR[9]

[a]Frequency deduced from weak combination with ν_3 which appears at 2672.

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CNN

An absorption which appears in a nitrogen matrix at 51070 when a high concentration of CNN is present has been tentatively attributed to this species.[10]

$\tilde{C}\,^3\Pi$? $C_{\infty v}$
$T_0 = 48540(50)$ Ar AB[10] $\tilde{C}-\tilde{X}$ 206 nm
49100(50) N_2 AB[10] $\tilde{C}-\tilde{X}$ 203.7 nm

$\tilde{B}\,^3\Sigma^-$? $C_{\infty v}$
$T_0 \leqslant 40985$ gas PF[14]
39950 Ar AB[10] $\tilde{B}-\tilde{X}$ 210–251 nm
39850 N_2 AB[10] $\tilde{B}-\tilde{X}$ 210–251 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	"Sym." stretch	1000T	gas	PF	14
			990(40)	Ar,N_2	AB	10
	3	"Asym." stretch	1455	gas	PF	14
			1450(40)	Ar,N_2	AB	10

$\tilde{A}\,^3\Pi$? $C_{\infty v}$
$T_0 = 23850$[a] gas AB[6]LF[11]PF[14] $\tilde{A}-\tilde{X}$ 395–420 nm
23750 Ne AB[5] $\tilde{A}-\tilde{X}$ 397–420 nm
23830
23597 Ar AB[2,3]LF[8,9] $\tilde{A}-\tilde{X}$ 401–424 nm
23865 N_2 AB[2,3] $\tilde{A}-\tilde{X}$ 396–419 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	"Sym." stretch	1386	gas	PF	14
			1325(10)	Ne	AB	5
			1322(2)	Ar	AB,LF	2,3,8,9
			1335(10)	N_2	AB	2,3
Π	2	Bend	525(2)	Ar	LF	8
Σ^+	3	"Asym." stretch	1807(2)	Ar	LF	8

$\tau_0 = 250(30)$ ns Ar LF[8,9]
$A = -26.5$[b] gas LF[11]
$A = 9$; $\varepsilon = -0.07$ Ar LF[8]
$B_0 = 0.425(10)$[a] LF[11]

$\tilde{b}\,^1\Sigma^+$ $C_{\infty v}$
$T_0 = 10690(120)$ gas PE[13]

$\tilde{a}\,^1\Delta$ $C_{\infty v}$
$T_0 = 6830(120)$ gas PE[13]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	"Asym." stretch	1600(120)	gas	PE	13

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	"Sym." stretch	1230(120)	gas	PE	13
			1235	Ne	EM	5
			1235	Ar	LF	8,12
			1241 N_2	Ar	IR	3
			1252	N_2	IR	3,4,7
Π	2	Bend	390(120)	gas	PE	13
			396	Ar	LF	8,12
			393 N_2	Ar	IR	3
			394	N_2	IR	4,7
Σ^+	3	"Asym." stretch	1425(120)	gas	PE	13
			1419[b]	Ar	LF	12

$B_0 = 0.414(10)$[b] LF[11]

[a] Approximate value, used in simulation.
[b] For many years, a prominent infrared absorption of CNN which appeared at 2847 in an argon matrix was assigned as the highest frequency fundamental, with approximate C≡N stretching character. Recently, a fluorescence signal corresponding to approximately half that value has been detected.[12] Associated CASSCF calculations indicate that the infrared absorption intensity of $2\nu_3$ of CNN should be greater than that of the fundamental.

SiNN

$\tilde{B}\,^3\Sigma^-$? $C_{\infty v}$
$T_0 = 32162(10)$ Ar AB[1] $\tilde{B}-\tilde{X}$ 295–311 nm
31892(25) Kr AB[2] $\tilde{B}-\tilde{X}$ 297–314 nm

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

References

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[10] M. E. Jacox, J. Mol. Spectrosc. **72**, 26 (1978).
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[12] B. E. Wurfel, A. Thoma, R. Schlachta, and V. E. Bondybey, Chem. Phys. Lett. **190**, 119 (1992).
[13] E. P. Clifford, P. G. Wenthold, W. C. Lineberger, G. A. Petersson, K. M. Broadus, S. R. Kass, S. Kato, C. H. DePuy, V. M. Bierbaum, and G. B. Ellison, J. Phys. Chem. A **102**, 7100 (1998).
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$\tilde{A}\,^3\Pi$? $C_{\infty v}$

$T_0 \leqslant 27170(20)$ Ar AB[1] $\tilde{A}-\tilde{X}$ 331–368 nm

Kr AB[2] $\tilde{A}-\tilde{X}$ 333–360 nm

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

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NN stretch	1731.6vs	Ar	IR	1,3
			1754.7vs	N_2	IR	3
	3	SiN stretch	484.3vw	Ar	IR	1,3
			461.6vw	N_2	IR	3

References

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

[2] M. A. Douglas, R. H. Hauge, and J. L. Margrave, High Temp. Sci. **22**, 47 (1986).

[3] G. Maier, H. P. Reisenauer, and J. Glatthaar, Organomet. **19**, 4775 (2000).

cyc-SiN_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NN stretch	1475.6	N_2	IR	1
	2	SiN s-stretch	716.0	N_2	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, and J. Glatthaar, Organomet. **19**, 4775 (2000).

$SnCN^-$

Threshold for electron detachment from ground-state $SnCN^-$ = 15510(50) gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	SnC stretch	330(20)	gas	PE	1

Reference

[1] V. D. Moravec and C. C. Jarrold, J. Chem. Phys. **113**, 1035 (2000).

ClLiCl

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

T^a = 2140(450) gas PE[1]

A = 810 gas PE[1]

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

A = 565(450) gas PE[1]

[a]From vertical detachment energies. First VDE($ClLiCl^-$) = 47760(320), or 5.92(4) eV gas PE[1].

Reference

[1] X.-B. Wang, C.-F. Ding, L.-S. Wang, A. I. Boldyrev, and J. Simons, J. Chem. Phys. **110**, 4763 (1999).

ClNaCl

$\tilde{C}\,^2\Sigma_g^+$ $D_{\infty h}$

T^a = 3790(540) gas PE[1]

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

T^a = 1370(580) gas PE[1]

[a]From vertical detachment energies. Because of relatively large uncertainties in $\tilde{X}$ and $\tilde{A}$ state assignments, measured from first VDE. First VDE($ClNaCl^-$) = 47280(480), or 5.86(6) eV gas PE[1].

Reference

[1] X.-B. Wang, C.-F. Ding, L.-S. Wang, A. I. Boldyrev, and J. Simons, J. Chem. Phys. **110**, 4763 (1999).

BrLiBr

$\tilde{C}\,^2\Sigma_g^+$ $D_{\infty h}$

T^a = 6780(340) gas PE[1]

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

T^a = 6210(340) gas PE[1]

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

T^a = 2820(540) gas PE[1]

A = 1780(540) gas PE[1]

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

A = 1940(540) gas PE[1]

[a]From vertical detachment energies. Measured from first VDE. First VDE($BrLiBr^-$) = 43730(240), or 5.42(3) eV.

Reference

[1] X.-B. Wang, C.-F. Ding, L.-S. Wang, A. I. Boldyrev, and J. Simons, J. Chem. Phys. **110**, 4763 (1999).

BrNaBr

$\tilde{C}\,^2\Sigma_g^+$ $D_{\infty h}$
$T^a = 5890(580)$ gas PE[1]

$\tilde{B}\,^2\Sigma_u^+$ $D_{\infty h}$
$T^a = 3870(540)$ gas PE[1]

$\tilde{A}\,^2\Pi_u$ $D_{\infty h}$
$T^a = 730(580)$ gas PE[1]
$A = 1290(400)$ gas PE[1]

$\tilde{X}\,^2\Pi_g$ $D_{\infty h}$
$A = 1940(680)$ gas PE[1]

[a]From vertical detachment energies. First VDE($BrNaBr^-$) = 43250(480), or 5.36(6) eV gas PE[1].

Reference

[1] X.-B. Wang, C.-F. Ding, L.-S. Wang, A. I. Boldyrev, and J. Simons, J. Chem. Phys. **110**, 4763 (1999).

ILiI

$\tilde{C}\,^2\Sigma_g^+$ $D_{\infty h}$
$T^a = 9200(630)$ gas PE[1]

$\tilde{B}\,^2\Sigma_u^+$ $D_{\infty h}$
$T^a = 8470(630)$ gas PE[1]

$\tilde{A}\,^2\Pi_u$ $D_{\infty h}$
$T^a = 1290(640)$ gas PE[1]
$A = 1860(340)$ gas PE[1]

$\tilde{X}\,^2\Pi_g$ $D_{\infty h}$
$A = 2900(540)$ gas PE[1]

[a]From vertical detachment energies. First VDE($ILiI^-$) = 39370(240), or 4.88(3) eV gas PE[1].

Reference

[1] X.-B. Wang, C.-F. Ding, L.-S. Wang, A. I. Boldyrev, and J. Simons, J. Chem. Phys. **110**, 4763 (1999).

INaI

$\tilde{C}\,^2\Sigma_g^+$ $D_{\infty h}$
$T^a = 9600(760)$ gas PE[1]

$\tilde{B}\,^2\Sigma_u^+$ $D_{\infty h}$
$T^a = 7660(730)$ gas PE[1]

$\tilde{A}\,^2\Pi_u$ $D_{\infty h}$
$T^a = 1210(790)$ gas PE[1]
$A = 1780(400)$ gas PE[1]

$\tilde{X}\,^2\Pi_g$ $D_{\infty h}$
$A = 2100(680)$ gas PE[1]

[a]From vertical detachment energies. First VDE($INaI^-$) = 39050(480), or 4.84(6) eV gas PE[1].

Reference

[1] X.-B. Wang, C.-F. Ding, L.-S. Wang, A. I. Boldyrev, and J. Simons, J. Chem. Phys. **110**, 4763 (1999).

$OScO^-$

Threshold for electron detachment from ground-state $OScO^-$ = 18720(160) gas PE[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type. meas.	Refs.
b_2	3	ScO_2 a-stretch	722.5	Ar	IR	1,3
			705.4	N_2	IR	1,3

References

[1] G. V. Chertihin, L. Andrews, M. Rosi, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **101**, 9085 (1997).
[2] H. Wu and L.-S. Wang, J. Phys. Chem. A **102**, 9129 (1998).
[3] C. W. Bauschlicher, Jr., M. Zhou, L. Andrews, J. R. Tobias Johnson, I. Panas, A. Snis, and B. O. Roos, J. Phys. Chem. A **103**, 5463 (1999).

OYO^-

Threshold for electron detachment from ground-state OYO^- = 16140(240) 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	702.0	Ar	IR	2
b_2	3	Asym. stretch	618.6	Ar	IR	2

References

[1] H. Wu and L.-S. Wang, J. Phys. Chem. A **102**, 9129 (1998).
[2] L. Andrews, M. Zhou, G. V. Chertihin, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **103**, 6525 (1999).

$OLaO^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type. meas.	Refs.
a_1	1	Sym. stretch	656.6	Ar	IR	1
b_2	3	Asym. stretch	559.2	Ar	IR	1

Reference

[1] L. Andrews, M. Zhou, G. V. Chertihin, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **103**, 6525 (1999).

$OZrO^-$

Threshold for electron detachment from ground-state $OZrO^- = 14520(3200)$ gas PE[2]

$\tilde{X}$ 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

References

[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. **99**, 6356 (1995).
[2] O. C. Thomas, S. Xu, T. P. Lippa, and K. H. Bowen, J. Cluster Sci. **10**, 525 (1999).

OVO^-

Threshold for electron detachment from ground-state $OVO^- = 16380(80)$ gas PE[2]

$\tilde{X}$ C_{2v}
$T_0 = 2500(80)$T gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type. meas.	Refs.
b_2	3	Asym. stretch	896.9 894.3	Ar	IR	1

References

[1] G. V. Chertihin, W. D. Bare, and L. Andrews, J. Phys. Chem. A **101**, 5090 (1997).
[2] H. Wu and L.-S. Wang, J. Chem. Phys. **108**, 5310 (1998).

$ONbO^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type. meas.	Refs.
b_2	3	Asym. stretch	854.1	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 8251 (1998).

$OTaO^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type. meas.	Refs.
b_2	3	Asym. stretch	817.1	Ar	IR	1,2

References

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 8251 (1998).
[2] M. Chen, X. Wang, L. Zhang, M. Yu, and Q. Qin, Chem. Phys. **242**, 81 (1999).

$OCrO^-$

Threshold for electron detachment from ground-state $OCrO^- = 19470(65)$ gas EB[1]PE[2,4]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type. meas.	Refs.
a_1	1	Sym. stretch	847.1	Ne	IR	3
b_2	3	Asym. stretch	918.7	Ne	IR	3

References

[1] G. D. Flesch, R. M. White, and H. J. Svec, Int. J. Mass Spectrom. Ion Phys. **3**, 339 (1969).
[2] P. G. Wenthold, K.-L. Jonas, and W. C. Lineberger, J. Chem. Phys. **106**, 9961 (1997).
[3] M. Zhou and L. Andrews, J. Chem. Phys. **111**, 4230 (1999).
[4] G. L. Gutsev, P. Jena, H.-J. Zhai, and L.-S. Wang, J. Chem. Phys. **115**, 7935 (2001).

$OMoO^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type. meas.	Refs.
a_1	1	Sym. stretch	883.1	Ne	IR	1
b_2	3	Asym. stretch	837.3	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Chem. Phys. **111**, 4230 (1999).

OWO^-

Threshold for electron detachment from ground-state $OWO^- \leqslant 16120(80)$ 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	952.3	Ne	IR	2
			946.3	Ar	IR	2
b_2	3	Asym. stretch	887.8	Ne	IR	2
			880.0	Ar	IR	2

References

[1] G. E. Davico, R. L. Schwartz, T. M. Ramond, and W. C. Lineberger, J. Phys. Chem. A **103**, 6167 (1999).
[2] M. Zhou and L. Andrews, J. Chem. Phys. **111**, 4230 (1999).

$OMnO^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type. meas.	Refs.
b_2	3	Asym. stretch	858.2	Ar	IR	1
			866.7T	N_2	IR	1

Reference

[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. A **101**, 8547 (1997).

$OReO^-$

Threshold for electron detachment from ground-state $OReO^-$ = 20200(800) gas PE[2]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type. meas.	Refs.
	3	Asym. stretch	893.8	Ne	IR	1
			885.5	Ar	IR	1

References

[1] M. Zhou, A. Citra, B. Liang, and L. Andrews, J. Phys. Chem. A **104**, 3457 (2000).
[2] A. Pramann and K. Rademann, Chem. Phys. Lett. **343**, 99 (2001).

$ORuO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	3	Asym. stretch	860.6	Ne	IR	1
			851.8	Ar	IR	1

Reference

[1] M. Zhou, A. Citra, B. Liang, and L. Andrews, J. Phys. Chem. A **104**, 3457 (2000).

$OOsO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	3	Asym. stretch	897.5	Ne	IR	1

Reference

[1] M. Zhou, A. Citra, B. Liang, and L. Andrews, J. Phys. Chem. A **104**, 3457 (2000).

$AgOO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	1030.7	Ne	IR	1

Reference

[1] X. Wang and L. Andrews, J. Phys. Chem. A **105**, 5812 (2001).

$OCeO^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	712.0	Ar	IR	1
b_2	3	Asym. stretch	662.0	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 3171 (1999).

$OPrO^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	665.0	Ar	IR	1
b_2	3	Asym. stretch	667.6	Ne	IR	1
			653.8	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 3171 (1999).

$ONdO^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	660.6	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 3171 (1999).

$OSmO^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	676.4	Ar	IR	1
b_2	3	Asym. stretch	575.5	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 3171 (1999).

$OEuO^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	661.0	Ar	IR	1
b_2	3	Asym. stretch	560.8	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 3171 (1999).

$OGdO^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	685.9	Ar	IR	1
b_2	3	Asym. stretch	589.4	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 3171 (1999).

$OTbO^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	711.2	Ar	IR	1
b_2	3	Asym. stretch	669.0	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 6972 (1999).

$ODyO^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	693.9	Ar	IR	1
b_2	3	Asym. stretch	591.2	Ne	IR	1
			574.6	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 6972 (1999).

$OHoO^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	696.2	Ar	IR	1
b_2	3	Asym. stretch	547.2	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 6972 (1999).

$OErO^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	702.3	Ar	IR	1
b_2	3	Asym. stretch	613.4	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 6972 (1999).

$OYbO^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	701.2	Ar	IR	1
b_2	3	Asym. stretch	604.2	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 6972 (1999).

$OLuO^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	626.9T	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 6972 (1999).

OUO^-

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	857.2	Ne	IR	1

Reference

[1] M. Zhou, L. Andrews, N. Ismail, and C. Marsden, J. Phys. Chem. A **104**, 5495 (2000).

BO_2

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

$T_0 = 24508.0$ gas AB[1] $\tilde{B}-\tilde{X}$ 405–410 nm
24529.5 Ne AB[16]
24481 Ar AB[2] $\tilde{B}-\tilde{X}$ 408–412 nm

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

$B_0 = 0.325$ AB[1]

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

$T_0 = 18291.597$ gas UV[1]LF[3–5,14] $\tilde{A}-\tilde{X}$ 396–700 nm
18162 Ne AB[16]LF[16] $\tilde{A}-\tilde{X}$ 419–1465 nm
17915[b] Ar AB[2] $\tilde{A}-\tilde{X}$ 423–558 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	994	gas	UV	1
			1027	Ne	AB	16
Π_u	2	Bend (ω)	477.29	gas	UV,LF	1,14
		($\kappa^2\Sigma_u^-$)	633.15	gas	UV,LF	1,14
		($^2\Delta_{u,3/2}$)	588.21	gas	UV,LF	1,14
		($^2\Delta_{u,5/2}$)	442.07	gas	UV,LF	1,14
		($\mu^2\Sigma_u^+$)	404.96	gas	UV,LF	1,14
Σ_u^+	3	Asym. stretch	2357H	gas	UV	1
			2361H	Ne	AB	16

$\tau_0 = 91(4)$ ns gas LF[6,9]
A systematic study of the dependence of τ on rotational and vibrational level has been given by Ref. 10.
$A = -101.281$; $\epsilon\omega_2 = -13.896$ gas UV[1]LF[14]
$B_0 = 0.311$ UV[1]LF[13,14]

$\tilde{X}\,^2\Pi_g$ $D_{\infty h}$ Structure: UV[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1056.4	gas	UV,LF	1,3–5
			1058	Ne	LF	16
Π_u	2	Bend (ω)	448.18	gas	UV,LF	1,3–5,14
		($\kappa^2\Sigma_u^-$)	633.80	gas	DL	11
			446.6wm	Ar	IR	15
			398.2m	Ar	IR	15
			493.4	Kr	IR	15
			394.6	Kr	IR	15
Σ_u^+	3	Asym. stretch	1278.26	gas	DL,IR	8,12
			1322H	Ne	LF	16
			1299.3vs	Ar	IR	15
			1282.8s	Ar	IR	15
			1274.6s	Ar	IR	2,15
			1300.7vs	Kr	IR	15
			1285.5s	Kr	IR	15
			1292.2vs	Xe	IR	15
			1279.0	O_2	IR	15

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

[a] Estimated from isotopic shifts.
[b] Independent analysis of the matrix spectrum not given. Each argon-matrix absorption is shifted to lower frequency by approximately 400 cm^{-1} from the corresponding gas-phase R_1 branch band head.

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[1] J. W. C. Johns, Can. J. Phys. **39**, 1738 (1961).
[2] A. Sommer, D. White, M. J. Linevsky, and D. E. Mann, J. Chem. Phys. **38**, 87 (1963).
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$AlNO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO stretch	1380.6	Ar	IR	1

Reference

[1] L. Andrews, M. Zhou, and W. D. Bare, J. Phys. Chem. A **102**, 5019 (1998).

cyc-TlO_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	OO stretch	1082.0	Ar	IR	1–3
			1089	N_2	IR	1
			1081	O_2	IR	1
	2	OTlO s-stretch	295.2s	Ar	IR	1–3
			296	N_2	IR	1
			296	O_2	IR	1

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OTlO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	698.0	Ar	IR	1

Reference

[1] L. Andrews, G. P. Kushto, J. T. Yustein, E. Archibong, R. Sullivan, and J. Leszczynski, J. Phys. Chem. A **101**, 9077 (1997).

CCO^-

Threshold for electron detachment from ground-state CCO^- is 18640(100) gas PE[2,3]

$\tilde{A}\,^2\Sigma^+$ $C_{\infty v}$
$T_0 = 12234$ Ne AB[4] $\tilde{A}-\tilde{X}$ 541–818 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	2082(3)	Ne	AB	4
Π	2	Bend	656(3)	Ne	AB	4
Σ^+	3	CC stretch	1185(3)	Ne	AB	4

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1900T	gas	PE	1,2
			1876.7(1.0)	Ne	IR	4

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$SiCO^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1706.7	Ar	IR	1

Reference

[1] L. Zhang, J. Dong, and M. Zhou, J. Chem. Phys. **113**, 8700 (2000).

$GeCO^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1708.7	Ar	IR	1
			1705.2			
			1701.0			

Reference

[1] L. Zhang, J. Dong, and M. Zhou, J. Chem. Phys. **113**, 8700 (2000).

$SnCO^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1729.1	Ar	IR	1

Reference

[1] L. Zhang, J. Dong, and M. Zhou, J. Chem. Phys. **113**, 8700 (2000).

NCN^-

Threshold for electron detachment from ground-state $NCN^- = 20040(50)$ gas PE[1,2]

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NCO

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

$T_0 = 31768.5$T gas UV[2]LF[18,30,31]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.[27,33]

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

$\tau_0 = 63(3)-152(5)$ ns for various rovibronic bands gas LF[13,30,31]
$A = -76.6$ 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[23,30,31]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

$\tau_0 = 435(10)$ 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, SEP	14,15,17,19, 23,26,29
			1275vw	Ar	IR,LF	3,8
			1269.0	Xe	IR	32
Π	2	Bend (ω)	534.06(3)	gas	UV,LF,SEP	7,15,23,29
		($^2\Sigma^-$)	669.28	gas	UV,LF	7,15,23
			672	Ar	LF	8
		($^2\Delta_{3/2}$)	628.45	gas	UV,LF	7,15,23
			626	Ar	LF	8
		($^2\Delta_{5/2}$)	534.64	gas	UV,LF	7,15,23
			529.5	Ar	LF	8
		($^2\Sigma^+$	488.43	gas	UV,LF	7,15,23
			487	Ar	IR,LF	3,8
Σ^+	3	Asym. stretch	1921.28[c]	gas	LMR,LF,DL, EM,SEP	10,14,15,21, 23,28,25
			1923m	Ar	IR,LF	3,8
			1921.6	Kr	IR	32
			1917.8	Xe	IR	32
			1915.8			
			1935	N_2	IR	3

$A_0 = -95.589(3)$, $\epsilon\omega_2 = -78.37(3)$ 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] For $\tilde{X}\,^2\Pi_{1/2}$, 2017.7(5) gas LF[14,15,23,24]

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NCS

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

$T_0 = 26987.8$ gas EM[1]AB^{2}LF[4,6] $\tilde{B}-\tilde{X}$ 353–485 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	343(10)	gas	AB	2
Σ^+	3	CS stretch	921.5	gas	LF	4

$\tau_{001} = 225(5)$ ns gas LF[4]
$B_0 = 0.197$ AB^2

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

$T_0 = 26054.56(1)$ gas EM[1]AB^{2}LF[4,6] $\tilde{A}-\tilde{X}$ 337–417 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CN stretch	1920.61	gas	AB,LF	2,4
Π	2	Bend ($\kappa\,^2\Sigma^-$)	487.2	gas	LF	4
		($^2\Delta_{3/2}$)	445.3T	gas	LF	4
		($^2\Delta_{5/2}$)	363.7	gas	LF	4
		($\mu\,^2\Sigma^+$)	304.5	gas	LF	4
Σ^+	3	CS stretch	771.12	gas	LF	4

$\tau_0 = 160(5)$ ns gas LF[3,4]EF[5]
$A = -91.58(1)$; $|\epsilon\omega_2| = 103(5)$ gas AB^{2}LF^4
$B_0 = 0.191$ AB^{2}LF[6]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CN stretch	1942.2	gas	LF	4
Π	2	Bend (ω)	376.0(3)	gas	AB,LF,SEP	2,4,6
		($\kappa\,^2\Sigma^-$)	704.84	gas	LF	4,6
		($^2\Delta_{3/2}$)	688.17	gas	LF	4,6
		($^2\Delta_{5/2}$)	375.1	gas	LF	4,6
		($\mu\,^2\Sigma^+$)	364.44	gas	LF	4,6
Σ^+	3	CS stretch	761.9[a]	gas	SEP	6

$A = -327.6(2)$; $\epsilon\omega_2 = -60.06(44)$ gas AB^{2}LF[4,6]SEP[6]
$B_0 = 0.204$ AB^{2}LF[4,6]MW[7]

[a] In Fermi resonance with $2\nu_2$.

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AsCO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1919.3	Ar	IR	1

Reference

[1] L. Zhang, J. Dong, and M. Zhou, Chem. Phys. Lett. **335**, 334 (2001).

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	1284(10)	gas	TPE,PE	21,23,36
Π_u	2	Bend	590(10)	gas	EM,PE,TPE	9,23,36
Σ_u^+	3	Asym. stretch	1891(10)	gas	PE,EM,TPE	17,23,30 36

$\tau_0 = 140(7)$ 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,TPE	2,5,11 23,31,36
Π_u	2	Bend (ω)	461	gas	EM,PE	11,23,31
		($\kappa\,^2\Sigma_u^-$)	568.8	gas	EM,TPE	23,31,36
		($\mu\,^2\Sigma_u^+$)	440.9	gas	EM,TPE	23,31,36
Σ_u^+	3	Asym. stretch	2685.3	gas	LF,EM,TPE	30,36

$\tau_0 = 102(8)$ 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	4,5,8,12
					PE,TPE	22,31,35
Π_u	2	Bend (ω)	511.4(3)	gas	EM,DL	11,22,28,
					PE,TPE	31,35
		($\kappa\,^2\Sigma_u^-$)	719.17	gas	EM,DL,TPE	11,22,35
		($^2\Delta_{3/2}$)	668.04	gas	EM,DL,TPE	11,22,35
		($^2\Delta_{5/2}$)	511.60	gas	EM,DL,TPE	11,22,35
		($\mu\,^2\Sigma_u^+$)	467.26	gas	EM,DL,TPE	11,20,22,35
			462.6	Ne	IR	34
Σ_u^+	3	Asym. stretch	1423.08	gas	DL,PE,TPE	19,31,35
			1421.7	Ne	IR	25,32–34

$A = -161.02(6)$; $\epsilon\omega_2 = -98.8(3)$ gas EM[1,9,11]DL[20,22]TPE[28] (Reanalysis by Ref. 26 gives $A = -161.48(5)$ and $\epsilon\omega_2 = -100.4$.)
$B_0 = 0.380$ EM[1,3,9,11]

[a]Corrected for Fermi resonance.
[b]Measured from lowest rotational level of $\tilde{X}$ state,[29] 34672.33.

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OCS^+

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

$T_0 = 54640(30)$ gas PI^4PE^{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 $PI^4PF^9PE^{10}$

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 $EF^1LF^8PF^{9,11}$ $\tilde{A}-\tilde{X}$ 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

$\tau_0 = 93(9)$ ns[c] gas PEFCO[5]
$\tau_0(\omega = 3/2) = 105(3)$ ns; $\tau_0(\omega = 1/2) = 77(3)$ ns gas HFD[6]EF[7]
$A = -111.8$ gas $EF^1PF^{9,11}$
$B_0 = 0.186$ $LF^8PF^{9,11}$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	2066	gas	EF,PF,TPE	1,11,12
			2071.1	Ne	IR	13
Π	2	Bend	476(16)	gas	PE	10
		($\kappa\,^2\Sigma^-$)	830	gas	TPE	12
		($^2\Delta_{3/2}$)	792	gas	TPE	12
		($\mu\,^2\Sigma^+$)	419	gas	TPE	12
Σ^+	3	CS stretch	697[d]	gas	PF,TPE	9,11,12
			702.5	Ne	IR	13

$A=-367.2$ gas $EF^1PF^9TPE^{12}$
$B_0=0.194$ $LF^8PF^{9,11}$

[a]Ref. 10 gives value of 742(7).
[b]817 for $\omega=1/2$.[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 $CO+S^+(^4S°)$, as was later confirmed.[3] PEFCO studies[5] have yielded the branching ratio for photoexcitation vs. predissociation for the transition origin, permitting an estimate of 550(50) ns for the radiative lifetime.
[d]699.7 for $\omega=1/2$.[9,11]

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CS_2^+

$\tilde{C}\,^2\Sigma_g^+$ $D_{\infty h}$ Structure: MP[15]
$T_0=49064$ gas $PI^5PF^{13}MP^{15}$ $\tilde{C}-\tilde{B}$ 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, PF,MP	5,9,11 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

$\tau_0=11(2)$ 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 35226 Ne LF^7

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

$\tau_0=290(10)$ ns gas $EF^2PIFCO^4PEFCO^8UV^{12}$
There is also a long-lifetime component, with $\pi=1.44(22)$ 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^3LF^{22} $\tilde{A}-\tilde{X}$ 426–512 nm
21010.6 Ne $LF^{6,7,17,24}$ $\tilde{A}-\tilde{X}$ 400–642 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	613(5)[ab]	gas	PE	25
			551[b]	Ne	LF	6,7,18,24
Π_u	2	Bend ($\kappa\,^2\Sigma_u^-$)	510(5)	gas	PE	25
		($^2\Delta_{u,5/2}$)	286(5)	gas	PE	25
			309H	Ne	LF	6,7,18,24
Σ_u^+	3	Asym. stretch	1723(5)[a]	gas	PE	25
			1644H	Ne	LF	7

$\tau=4.09(19)$ μs gas $PIFCO^4ID^{10}UV^{12}$
2.3(1) μs Ne $LF^{6,7}$
$A=-177$ gas $EM^3PE^{14,19,25}LF^{22}$
$B_0=0.101$ 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[b]	gas	EM,TPE	3,16,21
			618[b]	Ne	LF	6,7,17,18
Π_u	2	Bend	332	gas	TPE	16,21
		($^2\Delta_{u,5/2}$)	333.8	gas	TPE	21
		($\mu\,^2\Sigma_u^+$)	328.3	gas	TPE	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 20,23,24
			1200.5	Ar	IR	23

$A=-440.39(3)$ gas $EM^{1,2}TPE^{16,21}$
$B_0=0.109$ EM[1]

[a]Vibrational fundamentals given for $\tilde{A}\,^2\Pi_{3/2}$. For $\tilde{A}\,^2\Pi_{1/2}$, Ref. 25 gives $\nu_1=740(5)$ and $\nu_3=1870(5)$.
[b]Strong Fermi resonance with $2\nu_2$.

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$ClCN^+$

$\tilde{C}\,^2\Sigma^+$ $C_{\infty v}$
$T_0 = 54000(300)$ gas PE[1,2]

$\tilde{B}\,^2\Pi_{3/2}$ $C_{\infty v}$
$T_0 = 22515.54$ gas EF[8]LF[10–12]PE[13] $\tilde{B}-\tilde{X}$ 365–569 nm
22598(5) Ne AB[6] $\tilde{B}-\tilde{X}$ 380–442 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CN stretch	2128.5(7)	gas	LF	10
Π	2	Bend	303.1(7)	gas	LF	10
Σ^+	3	CCl stretch	531.90	gas	LF,PE	10,11,13
			539(4)	Ne	AB	6

$\tau_1 = 205(40)$ ns gas EF[3]
280(56) ns gas PEFCO[5]
170(20) ns gas PIFCO[4,7]
$\tau_2 = 900(100)$ ns gas EF[3]
970(80) ns gas PIFCO[7]
Both lifetimes are dependent on extent of vibrational excitation.[5]
$A = -368(2)$ gas EF[8,9]LF[10]
$B_0 = 0.177$ LF[11]

$\tilde{A}\,^2\Sigma^+$ $C_{\infty v}$
$T_0 = 11690(1)$ gas EF[3,8]PE[13] $\tilde{A}-\tilde{X}$ 843–881 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	CCl stretch	774(2)	gas	EF,PE	8,13

$\tau = 4.4(1.0)$ μs gas EF[3]

$\tilde{X}\,^2\Pi_{1/2}$ $C_{\infty v}$
$T_0 = 276(2)$ gas EF[3,8,9]PE[13] $\tilde{A}-\tilde{X}$ 843–881 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡N stretch	1914(2)	gas	EF,PE	8,13
	3	CCl stretch	827(2)	gas	EF,PE	8,13

$\tilde{X}\,^2\Pi_{3/2}$ $C_{\infty v}$ Structure: UV,PE[3]LF[12]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡N stretch	1915(2)	gas	EF,LF,PE	8–10,13
Π	2	Bend	376T	gas	LF	10
Σ^+	3	CCl stretch	827(2)	gas	EF,LF, PE	8–10,13

$B_0 = 0.205$ LF[11]

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CNN^-

Threshold for electron detachment from ground-state $CNN^- = 14290(80)$ gas PE[1]

Reference

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N_3

$\tilde{B}\,^2\Sigma_u^+$ $D_{\infty h}$ Structure: AB^2
$T_0^a = 36738.750(2)$ gas $AB^{1,2}LF^{3,8}PD^7$ $\tilde{B}-\tilde{X}$ 260–273 nm

All bands above 37000 are diffuse. Fast beam photodissociation studies[7] show that predissociation into $N(^2D)+N_2(X\,^1\Sigma_g^+)$ occurs throughout the 260–273 nm spectral region.

An absorption maximum was observed at 272 nm in mixed argon-nitrogen matrix studies.[6]
$\tau \geqslant 0.37$, $\leqslant 20$ ns gas $LF^{3,8}$
$B_0 = 0.432$ gas AB^2

$\tilde{X}\,^2\Pi_g$ $D_{\infty h}$ Structure: AB^2IR^6

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1320T	gas	LF	3
			1287[b]	N_2[c]	IR	4
Π_u	2	Bend	457T	gas	LF	3
			472.0	N_2	IR	4,9
Σ_u^+	3	Asym. stretch	1644.68	gas	LMR,IR	5,6
			1636.1	Ar	IR	10
			1657.7	N_2	IR	4,9,10

$A_{\text{eff}} = -71.3$; $\epsilon\omega_2 = -94.38$ gas AB^2IR^6
$B_0 = 0.431$ $AB^2LMR^5IR^6$

[a]Revised value resulting from reanalysis by Ref. 6.
[b]$(\nu_1+\nu_3)-\nu_3$.
[c]Mixed with argon.

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As_3

$\tilde{X}\,^2E''$ D_{3h}
Jahn–Teller splitting occurs, with the $^2A_2$ and $^2B_1$ levels separated by ~ 2900 cm^{-1} gas PE^1

Reference

[1] T. P. Lippa, S.-J. Xu, S. A. Lyapustina, J. M. Nilles, and K. H. Bowen, J. Chem. Phys. **109**, 10727 (1998).

N_2O^+

$\tilde{C}\,^2\Sigma^+$ $C_{\infty v}$
$T_0 = 58245(32)$ gas $PE^{1,8}PI^5$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Sym. stretch	1242(24)	gas	PE	1,8,21
Π	2	Bend	508(16)	gas	PE	8
Σ^+	3	Asym. stretch	2283(24)	gas	PE	1,8,21

$\tilde{B}\,^2\Pi$ $C_{\infty v}$
$T_0 = 38440(100)$[a] gas PE^1PF^{17} $\tilde{B}-\tilde{A}$ 538–866 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Sym. stretch	960	gas	PE	1,13
Π	2	Bend	368	gas	PE	13

$\tilde{A}\,^2\Sigma^+$ $C_{\infty v}$ Structure: EM^3PF^{17}
$T_0 = 28162.33$ gas $EM^{3,16}PF^{6,11,12,18,20}$ $\tilde{A}-\tilde{X}$ 317–421 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Sym. stretch	1345.38	gas	EM,PF	3,11,22
Π	2	Bend	614.45	gas	EM	3,16
Σ^+	3	Asym. stretch	2451.7	gas	EM	3

$\tau = 230(10)$ ns gas $EF^{2,10}PIFCO^4PEFCO^7ID^9EM^{14}HFD^{15}$
$B_0 = 0.433$ $EM^{3,16}PF^{11,12}$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Sym. stretch	1126.28	gas	EM	3,22
			1135.5	Ne	IR	19
Π	2	Bend	452.42	gas	EM,PF	3,12,16
Σ^+	3	Asym. stretch	1737.37	gas	EM	3,22
			1741.4wm	Ne	IR	19

[a]Calculated using the first ionization potential of 12.886(2) eV, from Ref. 5.

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$NiCl_2$

In an argon matrix,[11] a relatively weak absorption has its onset near 41500.

UV3

$T_0 = 34652$ Ar AB[5,10,11] 270–289 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	290(15)	Ar	AB	5,10,11

UV2

$T_0 = 30760$ Ar AB[5,10,11] 298–325 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			250T	Ar	AB	5,10,11

UV1

gas AB[1,3]LF[19,21] 353–374 nm

Molecular beam studies of this spectral region with vibrational[19] and rotational[21] resolution reveal an extremely complicated pattern of transitions for which a definitive assignment has not been achieved. It has been suggested that several mutually perturbing electronic states of $NiCl_2$ lie in this spectral region.

$T_0 = 27166$ Ar AB[5,10,11] 327–368 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	260(15)	Ar	AB	5,10,11

$\tau = 0.25(2)$ μs gas LF[19]

$^3\Delta_g$? $D_{\infty h}$ Structure: LF[20]

$T_0 = 21480.64$ gas AB[1,3,6,7]LF[16,17,20,22] ^3A_g–$\tilde{X}$ 439–495 nm
20500(2)[a] gas LF[22] ^3A_g–$\tilde{A}$ 487–539 nm
21590 Ne AB[15] ^3A_g–$\tilde{X}$ 439–486 nm
21465 Ne EM[15]
19405 Ne EM[15] ^3A_g–$\tilde{A}$ 515–591 nm
21300 Ar AB[15] ^3A_g–$\tilde{X}$ 446–491 nm
21257 Ar EM[8,11]
19537 Ar EM[8,11] ^3A_g–$\tilde{A}$ 509–529 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	357.21 (ω)	gas	LF	16,17,20
			355T	Ne	AB	15
			350T	Ar	AB	15
Π_u	2	Bend	60.66 (ω)	gas	LF	17,20
Σ_u^+	3	Asym. stretch	530.95 (ω)	gas	LF	20

$\tau > 1.2$ μs gas LF[16]
$= 3.5(2)$ μs Ne EM[15]
$B_0 = 0.055$ LF[20]

In an argon matrix,[8] weak emission appears between 582 and 583 nm.

In a neon matrix,[15] structured absorption appears between 595 and 648 nm, and, in an argon matrix,[15] between 610 and 632 nm.

In the gas phase,[6,7] an absorption maximum appears near 14510 (689 nm).

In the gas phase,[3,6,7] a relatively weak absorption maximum has been observed near 13000. In a neon matrix,[15] absorption bands are seen at 12783 and 12808 (780–783 nm). In an argon matrix,[15] three bands appear between 12470 and 12635 (791–802 nm).

In the gas phase,[6,7] a relatively sharp absorption maximum has been observed at 11727.

In the gas phase,[3,6,7] an absorption maximum has been observed near 4000. The absorption extends up to at least 8000.

$\tilde{A}\,^3\Pi_g$ $D_{\infty h}$

$T_0 = 1572$[a] gas LF[22] ^3A_g–$\tilde{A}$ 487–539 nm
2060 Ne EM,LF[15] ^3A_g–$\tilde{A}$ 515–591 nm
1720T Ar EM[8,11] ^3A_g–$\tilde{A}$ 509–529 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	366.3(8)	gas	LF	22
			370	Ne	EM,LF	15
			360	Ar	EM	8,11

$\tilde{X}\,^3\Sigma_g^-$ $D_{\infty h}$ Structure: LF[20]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	359.2(3)	gas	LF	14,16,20,22
			357	Ne	Ra	15
			360	Ar	EM,Ra	8,11,15
Π_u	2	Bend	87.28	gas	LF	14,17,20,22
			85	Ar	IR	9
Σ_u^+	3	Asym. stretch	520.4H	gas	IR,LF	2,4,14,20,22
			529.6	Ne	IR	12
			520.9	Ar	IR	5,12,13,18

$B_0 = 0.057$ LF[20]

[a] $0^+ - 0^+$ band separation.

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$CuCl_2$

In the gas phase, an absorption maximum has been observed[3] near 44800.

$2\,^2\Pi_g$ $D_{\infty h}$
$T^a = 19900(1000)$ gas PE[16]

$^2\Sigma_u^+$ $D_{\infty h}$
$T^a = 17800(900)$ gas PE[16]

$^2\Pi_u$ $D_{\infty h}$
$T_0 = 15500T$ gas AB[1,3]LF[7–12,15]PE[16]
15416.0 Ne AB[13]LF[13]
14920.5 Ar AB[4]LF[13]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			240T	Ne	AB	13
			255T	Ar	AB	13

$^2\Delta_{g,3/2}$ $D_{\infty h}$
From maxima in the photoelectron spectrum[16] of $CuCl_2^-$, the origin of this transition is estimated at 8700 cm^{-1}. A revised estimate of 9450 cm^{-1} has also been suggested.[17]
$T_0 = 9567.5$ Ne LF[13]
9427T Ar LF[13]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	364.5	Ne	LF	13
			354.6T	Ar	LF	13
Π_u	2	Bend	80.2	Ne	LF	13

$^2\Delta_{g,5/2}$ $D_{\infty h}$
In the gas phase, absorption[1,3,6] has been reported between 760 and 1454 nm and emission[5,6] between 1150 and 1460 nm, with the origin estimated at $\leqslant$6877. From maxima in the photoelectron spectrum[16] of $CuCl_2^-$, the origin of this transition is estimated at 7100 cm^{-1}. A revised estimate of 7780 cm^{-1} has also been suggested.[17]
$T_0 = 7893.5$ Ne LF[13]
7753.1 Ar LF[13]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	360(15)	gas	AB	3
			360.6(ω)	Ne	LF	13
Π_u	2	Bend	88.76(ω)	Ne	LF	13

$^2\Sigma_g^+$ $D_{\infty h}$
$T_0 = 1910.9$ Ne LF[13]
1616.5 Ar LF[13]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	389.4(ω)	Ne	LF	13
			391.7T (ω)	Ar	LF	13
Π_u	2	Bend	102.6(ω)	Ne	LF	13
			100.3 (ω)	Ar	LF	13

$^2\Pi_{g,1/2}$ $D_{\infty h}$
$T_0 = 474.1$ Ne LF[13]
303.6T Ar LF[13]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	350.1 (ω)	Ne	LF	13
			344.5 (ω)	Ar	LF	13
Π_u	2	Bend	103.6(ω)	Ne	LF	13
			111.1 (ω)	Ar	LF	13

$\tilde{X}\,^2\Pi_{g,3/2}$ $D_{\infty h}$ Structure: LF[8,9,15]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	371.69(ω)	gas	LF	7,9,11,12,14
			370.6 (ω)	Ne	LF	13
			367.3 (ω)	Ar	LF	13
Π_u	2	Bend	95.81 (ω)	gas	LF	10,12,14
			97.0 (ω)	Ne	LF	13
			98.6 (ω)	Ar	LF	13
Σ_u^+	3	Asym. stretch	525.90 (ω)	gas	IR,LF	2,7,9,11,12,14
			522.3 (ω)	Ne	LF	13
			514.4 (ω)	Ar	LF	13

$A = -253.9T$ gas LF[15]
$B_0 = 0.058$ LF[7–9,12,14]

[a] From vertical detachment energies.

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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.
Σ^+	1	B=O stretch	1972.18	gas	DL	3
			1958s	Ar	IR	1
Π	2	Bend	404s	Ar	IR	1
Σ^+	3	BCl stretch	676.04	gas	DL	2
			673wm	Ar	IR	1

$B_0 = 0.174$ MW,DL[2]

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BrBO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	B=O stretch	1937vs	Ar	IR	1
Π	2	Bend	374s	Ar	IR	1
Σ^+	3	BBr stretch	535w	Ar	IR	1

$B_0 = 0.120$ MW[2]

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FBS

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	B=S stretch	1644.38	gas	IR	3
Π	2	Bend	370(50)	gas	MW	1,2

$B_0 = 0.165$ MW[1,2]IR[3]

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ClBS

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BS stretch	1407.56	gas	IR	3–5
Π	2	Bend	300(40)	gas	MW	2
Σ^+	3	BCl stretch	529.90	gas	IR	3–5

$B_0 = 0.093$ MW[1,2]IR[5]

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cyc-GaO_2^-

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			568.5	Ar	IR	1,2

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cyc-InO_2^-

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			462.4	Ar	IR	1,2

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cyc-TlO_2^-

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			473.9	Ar	IR	1

Reference

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NCO^-

Threshold for electron detachment from ground-state $NCO^- = 29120(40)$ gas PE[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	Asym. stretch	2124.31	gas	DL	1
			2124.5T	Xe	IR	3

$B_0 = 0.384$ DL[1]

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$AsCO^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1756.4	Ar	IR	1

Reference

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cyc-CS_2

$^1B_1$ C_{2v}
$T_0 = 27607(5)$ Ar AB[2] $^1B_1 - \tilde{X}$ 334–363 nm

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

$^1B_2$ C_{2v}
$T_0 \leqslant 26586(5)$ Ar AB[2] $^1B_2 - \tilde{X}$ 366–376 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			350T	Ar	AB	2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CS_2 s-stretch	876.5	Ar	IR	1
			881.3	N_2	IR	1
b_2	3	CS_2 a-stretch	517.7	Ar	IR	1
			520.9	N_2	IR	1

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OCTe

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1970.7	Ar	IR	1
			1965.3	CO	IR	1

Reference

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SiS_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	514	CH_4	Ra	2
Σ_u^+	3	Asym. stretch	918.0	Ar	IR	1

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GeO_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	GeO s-stretch	870.1	CH_4	Ra	4
Π_u	2	Bend	195.5	Ar	IR	2
Σ_u^+	3	GeO a-stretch	1052.3	Ar	IR	2,3
			1061.6	N_2	IR	1

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GeS_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	GeS s-stretch	474.7	CH_4	Ra	3
Σ_u^+	3	GeS a-stretch	653.4	Ar	IR	1,2

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N_3^-

Threshold for electron detachment from ground-state N_3^- is 21620(80).[1,5]

$\tilde{X}\,^1\Sigma_g^+$ $D_{\infty h}$ Structure: DL[2,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	1986.47	gas	DL	2,3
			1991.9	Ar	IR	6
			2002.9	N_2	IR	4,6

$B_0 = 0.426$ DL[2,3]

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NO_2^+

$\tilde{D}\,^1B_2$ C_{2v}
$T_0 = 75485$ gas TPE[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1102	gas	TPE	11

$\tilde{e}\,^3B_2$ C_{2v}
$T_0 = 74799$ gas PE[1,2,10]TPE[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1114	gas	PE,TPE	1,2, 10,11

$\tilde{d}\,^3A_1$ C_{2v}
$T_0 = 71622$ gas TPE[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1402	gas	TPE	11
	2	Bend	941	gas	TPE	11
b_2	3	Asym. stretch	2054	gas	TPE	11

$\tilde{C}\,^1B_1$ C_{2v}
$T_0 = 60902$ gas PE[2,10]TPE[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1009	gas	PE,TPE	1,2,10,11

$\tilde{c}\,^3B_1$ C_{2v}
$T_0 = 60354$ gas PE[1,2,10]TPE[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1024	gas	PE,TPE	1,2,10,11

$\tilde{B}\,^1B_2$ C_{2v}
$T_0 = 39166$ gas PE[1,2,10]TPE[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1038	gas	PE,TPE	2,10,11
	2	Bend	576	gas	PE,TPE	1,2,10,11
b_2	3	Asym. stretch	1495	gas	TPE	11

$\tilde{A}\,^1A_2$ C_{2v}
$T_0 = 36150$ gas PE[1,2,10]TPE[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	963	gas	PE,TPE	1,2,10,11
	2	Bend	615	gas	TPE	11

$\tilde{b}\,^3A_2$ C_{2v}
$T_0 = 32318$ gas PE[1,2,10]TPE[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	685	gas	PE,TPE	1,2,10,11

$\tilde{a}\,^3B_2$ C_{2v}
$T_0=26422$ gas PE[1,2,10]TPE[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	639	gas	PE,TPE	1,2,10,11

$A=6.5$ TPE[11]
$\tilde{X}\,^1\Sigma_g^+$ $D_{\infty h}$ Structure: TPE[4,5,7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1401.1	gas	TPE	8,9,11
			1362.4[a]	Ne	IR	6
Π	2	Bend	627.7	gas	TPE	5,7–9,11
Σ_u^+	3	Asym. stretch	2376.5	gas	TPE	5,7,11
			2348.2	Ne	IR	6

$B_0=0.417$ TPE[4,7]

[a] $(\nu_1+\nu_3)-\nu_3$.

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PNO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NO stretch	1756.65	gas	DL	2
			1754.7	Ar	IR	1
	3	PN stretch	865.2	Ar	IR	1

$B_0=0.206$ DL^2MW^3

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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	1277.645	gas	DL	2,3
			1270.4	Ar	IR	1,5

$B_0=0.130$ DL^3MW^4

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XeC_2

Structured absorptions centered at 50500 (198 nm) and 23640 (423 nm) which appear when C_2H_2 isolated in solid xenon is subjected to 193 or 248 nm irradiation[1] are tentatively attributed to XeC_2.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CC stretch	1767.0	Xe	IR	1

Reference

[1] G. Maier and C. Lautz, Eur. J. Org. Chem. **1998**, 769.

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[8,9,11] 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

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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	1,2
	2	Bend	253.7	Ar	IR	2
b_2	3	Asym. stretch	887.5	Ar	IR	1,2

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CO_2^-

Maximum in the photoelectron spectrum of CO_2^- near 11300 (1.4 eV) 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	1253.8w	Ne	IR	6
	2	Bend	714.1w	Ne	IR	6
b_2	3	Asym. stretch	1658.3vs	Ne	IR	2,3,5,6
			1657.0	Ar	IR	4

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FCO

$\tilde{B}$[a]

$T_0 \leqslant 35741$ gas $AB^{2,7,8}$ $\tilde{B}-\tilde{X}$ 220–280 nm
35587 Ar AB^{3} $\tilde{B}-\tilde{X}$ 234–281 nm
35211 CO $AB^{1,3}$ $\tilde{B}-\tilde{X}$ 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.
			651T	gas	AB	2,7,8
			650T	Ar	AB	3
			650T	CO	AB	1,3

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

$T_0 \leqslant 27000$ gas $CL^{5}AB^{7,8}CR^{9}$ $\tilde{A}-\tilde{X}$ 280–455 nm
$T_0 \geqslant 24000$ gas AB^{8}

Bands are somewhat broadened because of predissociation.[9]

$T_0 \leqslant 29586$ Ar AB^{3} $\tilde{A}-\tilde{X}$ 284–338 nm
29516 CO $AB^{1,3}$ $\tilde{A}-\tilde{X}$ 289–339 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	360HT	gas	AB,CR	8,9
			350HT	Ar	AB	3
			350HT	CO	AB	1,3
Σ^+	3	CF stretch	1080T	gas	CR	9
			1050T	Ar	AB	3
			1050T	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

$A_0 = 6.38$; $B_0 = 0.382$; $C_0 = 0.360$ $DL^{4}MW^{10}$

[a]The designation of this state as $\tilde{B}$ is arbitrary. See the discussion in Ref. 9.

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ClCO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CO stretch	1884.59	gas	IR	4
			1876.7vs	Ar	IR	1–3
			1880vs	CO	IR	1
	2	Bend	334.6	Ar	IR	2
	3	CCl stretch	570.1s	Ar	IR	1–3
			570s	CO	IR	1

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ClSiO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SiO stretch	1160.9	Ar	IR	1
	3	SiCl stretch	509.4	Ar	IR	1

Reference

[1] M. Junker and H. Schnöckel, J. Chem. Phys. **110**, 3769 (1999).

OCS^-

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CO stretch	1646.4	Ne	IR	1
	3	CS stretch	718.2	Ne	IR	1

Reference

[1] C. L. Lugez, W. E. Thompson, and M. E. Jacox, J. Chem. Phys. **115**, 166 (2001).

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	1,2
			1160.4	Ar	IR	2

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[2] M. Zhou and L. Andrews, J. Chem. Phys. **112**, 6576 (2000).

CCl_2^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	1213.5	Ne	IR	4
			1195.40	Ar	IR	1–3,5
			1197	Kr	IR	5

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$CClBr^+$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CCl stretch	1120.6	Ar	IR	1–3

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[1] L. Andrews and B. W. Keelan, J. Am. Chem. Soc. **101**, 3500 (1979).
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PO_2

$^2B_1$? C_{2v}

$T_0 = 30393(2)$ gas $AB^1LF^{3,11}$ $^2B_1 - \tilde{X}$ 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,LF	1,11
			942	Ar	AB	6
	2	Bend	389	gas	AB,LF	1,11

$\tau<500$ ns gas LF[3,11]
$\tau_{cont}\cong 4.5\ \mu s$ gas LF[3]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PO s-stretch	1076(12)	gas	MW,LF,LMR	2,3,11
	2	Bend	397(12)	gas	MW,LF,LMR	2,3,11
			386.4	Ar	IR	7
b_2	3	PO a-stretch	1327.53	gas	DL	8,9
			1319.1	Ar	IR	4,5,7,10

$A_0=3.486$; $B_0=0.287$; $C_0=0.264$ MW,LMR[2]

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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
			1527.2	N_2	IR	4
	3	NS stretch	790.2m	Ar	IR	1–3
			792.3	N_2	IR	4

[a]In Fermi resonance with $2\nu_3$.

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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
b_2	3	Asym. stretch	1275.9	Ne	IR	8

Barrier to linearity ~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]

$T_0 = 37216$ gas EM[1]AB[2,3,5,10]LF[20,42,43] $\tilde{A}-\tilde{X}$ 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	1012.1(5)	gas	LF	42,43
	2	Bend	496.7(5)	gas	UV,LF	1–3,5,10,43
			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(5)	gas	LF	42,43

$\tau_0 = 63.5(1.5)$ ns gas LF[20,21,28,30,33,44]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[34,35] $\tilde{a}-\tilde{X}$ 430–800 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1020(30)	gas	PE	45
	2	Bend	517	gas	CL,PE	18,22,24,29,45

$\tau \cong 1$ 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, 36,45
			1221.9	Ne	IR,LF	12,17,40
			1222vs	Ar	IR,LF	6,11,17
	2	Bend	666.25	gas	UV,PE	1,10,34,45
					DL	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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CFCl

$\tilde{A}\,^1A''$ C_s Structure: LF[9,10]

$T_0 = 25284.0$ gas LF[6,7,9–11] $\tilde{A}-\tilde{X}$ 342–466 nm
24983 Ar AB[1]LF[2,3] $\tilde{A}-\tilde{X}$ 340–667 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CF stretch	1229(2) (ω)	gas	LF	11
	2	Bend	391	gas	LF	6,9–11
			392(1)	Ar	LF	3
	3	CCl stretch	713	gas	LF	9–11
			712(2)	Ar	LF	3

$\tau_0 = 620(30)$ ns gas LF[4,5,9,11]EM[8]
330(20) ns Ar LF[3]
$A_{020} = 4.354$; $B_{020} = 0.185$; $C_{020} = 0.177$ LF[9,10]

$\tilde{X}\,^1A'$ C_s Structure: LF[9,10]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CF stretch	1154	gas	LF	6,7,9,10,11
			1146vs	Ar	IR	1
	2	Bend	447	gas	LF	6,7,9,10,11
			442	Ar	LF	2,3
	3	CCl stretch	753	gas	LF	6,7,9,10,11
			742s	Ar	IR	1

$A_0 = 2.349$; $B_0 = 0.214$; $C_0 = 0.196$ LF[9,10]

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CFBr

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

$T_0 = 20906$ gas LF[3–5] $\tilde{A}-\tilde{X}$ 415–580 nm
Ar LF[1] $\tilde{A}-\tilde{X}$ 442–535 nm

The barrier to dissociation is estimated[5] to be 3250(150) above the origin of the $\tilde{A}$ state.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CF stretch	1140	gas	LF	4,5
	2	Bend	340	gas	LF	4,5
			240(40)	Ar	LF	1
	3	CBr stretch	645	gas	LF	4,5

$\tau_{011} = 3100(250)$ ns gas LF[5]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CF stretch	1157vs	Ar	IR	2
	2	Bend	345	gas	LF	3,5
			340(5)	Ar	LF	1
	3	CBr stretch	648	gas	LF	5
			656s	Ar	IR	2

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CCl_2

$\tilde{A}\,^1B_1$ C_{2v} Structure: LF[17]

$T_0 = 17255.67(2)$ gas CL[8]LF[7,9,10,15–18]EM[11] $\tilde{A}-\tilde{X}$ 400–800 nm
17092 Ar AB[1,3]LF[4–6] $\tilde{A}-\tilde{X}$ 440–827 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	634.3	gas	LF	10,15,17
			624	Ar	LF	6
	2	Bend	302.6	gas	LF	9,10,15,17
			304	Ar	AB,LF	1,3,6

$\tau = 3.81(30)$ μs gas LF[7];
$\tau_1 = 1.83(2)$ μs, $\tau_2 = 3.72(6)$ μs gas EM[11,13]
$\tau = 3.6$ μs Ar LF[6]
$A_0 = 3.640$; $B_0 = 0.106$; $C_0 = 0.103$ LF[17]

$\tilde{a}\,^3B_1$ C_{2v}
$T_0=970(800)$ gas PE[20]

$\tilde{X}\,^1A_1$ C_{2v} Structure: MW[14]LF[17]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	730.0	gas	PE,LF	12,17,20
			725.6	Ne	IR	19
			721wm	Ar	IR,LF	1–3,5,6
	2	Bend	335.2	gas	PE,LF	12,17,20
			333	Ar	LF	4–6
b_2	3	Asym. stretch	757.9	Ne	IR	19
			748vs	Ar	IR	1–3,21
			756	Kr	IR	21
			741			

$A_0=1.675$; $B_0=0.123$; $C_0=0.115$ MW[14,22]LF[16,17]

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CClBr

$\tilde{A}$ C_s Structure: LF[5]
$T_0=16190$ gas LF[5,6] $\tilde{A}-\tilde{X}$ 497–600 nm
16044 Ar LF[3,4] $\tilde{A}-\tilde{X}$ 540–776 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CCl stretch	684	Ar	LF	4
	2	Bend	246	gas	LF	5
			246	Ar	LF	4
	3	CBr stretch	532	gas	LF	5
			526	Ar	LF	4

$\tau=5.6(6)$ μs Ar LF[4]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CCl stretch	744	Ar	IR	1,2,7
	2	Bend	262	gas	LF	6
			260	Ar	LF	3,4
	3	CBr stretch	618T	gas	LF	6
			611	Ar	IR	1,2,7

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CBr_2

$\tilde{A}\,^1B_1$ C_{2v} Structure: LF[6]
$T_0=15092.5(1.7)$ gas LF[5,6] $\tilde{A}-\tilde{X}$ 560–663 nm
14962 Ar LF[3,4] $\tilde{A}-\tilde{X}$ 600–857 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	474.8(1.2)	gas	LF	5,6
			468	Ar	LF	4
	2	Bend	185.5(4)	gas	LF	5,6
			186	Ar	LF	4

$\tau=14.5(1.5)$ μs Ar LF[4]

$\tilde{a}\,^3B_1$ C_{2v}
$T_0=810(800)$ gas PE[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	525(20)	gas	PE	7
	2	Bend	200(40)	gas	PE	7

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	598	gas	LF	6
			595w	Ar	IR	1,2
	2	Bend	196	Ar	LF	3,4
b_2	3	Asym. stretch	641s	Ar	IR	1,2

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Cl_2

$\tilde{a}\,^1A_1$ C_{2v}
$T_0 = 480(800)$ gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	500(20)	gas	PE	1
	2	Bend	120(40)	gas	PE	1

Reference

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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[1,2,20]AB[5,9]LF[14,17] $\tilde{A}-\tilde{X}$ 213–276 nm
$\cong 43964$ Ne AB[7] $\tilde{A}-\tilde{X}$ 216–225 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	250.1(3)	gas	AB,LF	5,9,17,18
			253T	Ne	AB	7

$\tau = 11.2(1.5)$ ns gas LF[17]EM[20]
$A_0 = 1.446$; $B_0 = 0.241$; $C_0 = 0.206$ AB[9]

$\tilde{a}\,^3B_1$ C_{2v} Structure: LF[18]
$T_0 = 26319.478(6)$ gas EM[10,20]MPI[16,19]LF[18,21] $\tilde{a}-\tilde{X}$ 364–420 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	278.2	gas	EM,LF,MPI	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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SiFCl

$\tilde{X}$ C_s Structure: MW[1]
$A_0 = 0.793$; $B_0 = 0.151$; $C_0 = 0.127$ MW[1]

Reference

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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]EM[11] $\tilde{A}-\tilde{X}$ 215–265 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

$\tau = 9.3(1)$ ns gas EM[11]

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

$T_0 = 30582.1$ gas $EM^{6,8,9,11}LF^{10}$ $\tilde{a}-\tilde{X}$ 300–380 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

$\tau > 500$ ns gas EM^{11}

$\tilde{X}\,^1A_1$ 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 $AB^2LF^{11}EM^{13}$ $\tilde{A}-\tilde{X}$ 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

$\tau = 89.7(6.8)$ ns gas EM^{10}

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

$T_0 = 22315(2)$ gas $CL^1LF^{11}EM^{13}$ $\tilde{a}-\tilde{X}$ 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

$\tau = 17.4(6)$ μs gas EM^{10}

$\tilde{X}\,^1A_1$ C_{2v} Structure: ED^8MW^{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,Ra	1,2,4
			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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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	1198.6	Ar	IR	1,3

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FPO

$\tilde{X}$ C_s Structure: $MW^{3,5}IR^{5}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	PO stretch	1297.54	gas	IR	4,5
			1292.2	Ar	IR	1
	2	Bend	412T	gas	IR	2,5
			416.0	Ar	IR	1
	3	PF stretch	819.57	gas	IR	2,4,5
			811.4	Ar	IR	1

$A_0=1.397$; $B_0=0.310$; $C_0=0.253$ $MW^{3,5}IR^{4,5}$

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ClPO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	PO stretch	1263.01	gas	IR,DL	5,6,8
			1258vs	Ar	IR	1–4
	2	Bend	308wm	Ar	IR	1
	3	PCl stretch	492T	gas	IR	5
			489vs	Ar	IR	1–3

$A_0=1.115$; $B_0=0.151$; $C_0=0.133$ $DL^{6}MW^{7}$

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BrPO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	PO stretch	1257.84	gas	IR,DL	3,4
			1253.0	Ar	IR	1,2
	2	Bend	253.7	Ar	IR	1
	3	PBr stretch	408	gas	IR	3
			407.1	Ar	IR	1,2

$A_0\cong1.021$; $B_0=0.092$; $C_0=0.084$ DL^{4}

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IPO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	PO stretch	1253	gas	IR	1

Reference

[1] I. Boustani and A. W. Allaf, Vib. Spectrosc. **16**, 157 (1998).

FPS

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	PF stretch	803.25	gas	IR	2,3
			791.4	Ar	IR	1
	2	Bend	313.6	Ar	IR	1
	3	PS stretch	726.27	gas	IR	3
			720.2	Ar	IR	1

$A_0=0.948$; $B_0=0.163$; $C_0=0.139$ $MW^{2,3}$

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PF_2^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	PF stretch	980(30)	gas	PE	1,2
			1012.3	Ne	IR	3
b_2	3	PF stretch	1049.3	Ne	IR	3

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ClON

In an argon matrix, an absorption between 320 and 550 nm, with maximum at 22980 (417 nm) has been assigned[2] to ClON.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO stretch	1842.2vs	Ar	IR	1,2
			1852.1vs	N_2	IR	1,2
	2	Bend	409.4w	Ar	IR	1,2
			405.2w	N_2	IR	1,2
	3	ClO stretch	247T	Ar	IR	2

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[1] A. Hallou, L. Schriver-Mazzuoli, A. Schriver, and P. Chaquin, Chem. Phys. **237**, 251 (1998).
[2] G. Maier, H. P. Reisenauer, and M. De Marco, Chem. Eur. J. **6**, 800 (2000).

BrON

In an argon matrix, an absorption between 330 and 550 nm, with maximum at 22730 (440 nm) has been assigned[1] to BrON.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ON stretch	1820.0vs	Ar	IR	1
			1816.2vs	N_2	IR	1
	2	Bend	350T	Ar	IR	1
			365.4	N_2	IR	1
	3	BrO stretch	190T	N_2	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, and M. De Marco, Chem. Eur. J. **6**, 800 (2000).

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[12,13,16–18] $\tilde{C}-\tilde{X}$ 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	1033.9(6)	gas	AB,LF	11,13,16,18
	2	Bend	253.8(6)	gas	AB,LF	11,13,16,18
	3	SS stretch	410.6	gas	AB,LF	7,11,13,16–18
			415(20)	Xe	AB	4

$\tau = 66(4)$ 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,LF	1,3,14,18
			1156.2	Ar	IR,Ra	8,9
	2	Bend	380	gas	LF	16,18
			382	Ar	IR,Ra	8,9
	3	SS stretch	679.1	gas	IR,LF	1,3,13,18
			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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SeO_2

$^1\tilde{B}_2$ C_{2v} Structure: AB[10]

$T_0 = 31957.4$ gas AB[4,9,10]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

$\tau < 200(100)$ 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	364	gas	AB,IR	9,11,14
			366.0s	Ar	IR	8,13
			365T	Kr,Xe	EM	6
b_2	3	Asym. stretch	968	gas	IR,AB	3,11,14
			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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TeO_2

$^1B_2$? C_{2v}

$T_0 = 25526$ gas LF[4] 345–406 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	679 (ω)	gas	LF	4
	2	Bend	220 (ω)	gas	LF	4

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	823 (ω)	gas	LF	4
			826.4	Ne	IR	1
			822.6	Ar	IR	1
			831.7	N_2	IR	2
	2	Bend	282 (ω)	gas	IR,LF	3,4
			294	N_2	IR	2
b_2	3	Asym. stretch	853	gas	IR	3
			844.8	Ne	IR	1
			839.4	Ar	IR	1
			848.3	N_2	IR	2

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$OClO^+$

$\tilde{D}\,^1A_2$ C_{2v}

$T_0 = 62200(80)$ gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			485(40)	gas	PE	3

$\tilde{d}\,^3A_2$ C_{2v}

$T_0 = 59460(80)$ gas PE[1–3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ClO s-stretch	605(40)	gas	PE	3

$\tilde{C}\,^1B_2$ C_{2v}
$T_0 = 39530(80)$ gas PE[1–3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ClO s-stretch	765(40)	gas	PE	3

$\tilde{B}\,^1B_1$[a] C_{2v}
$T_0 = 25410(80)$ gas PE[3]

Vib. sym.	No.	Approximate typeofmode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ClO s-stretch	725(40)	gas	PE	3

$\tilde{A}\,^1A_2$[a] C_{2v}
$T_0 = 24040(80)$ gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ClO s-stretch	810(40)	gas	PE	3

$\tilde{c}\,^3B_1$[a] C_{2v}
$T_0 = 19690(80)$ gas PE[1–3]

$\tilde{b}\,^3A_2$[a] C_{2v}
T[b] $= 20330(80)$ gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	485(40)	gas	PE	3

$\tilde{a}\,^3B_2$[a] C_{2v}
$T_0 = 16540(80)$ gas PE[1–3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ClO s-stretch	765(40)	gas	PE	3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ClO s-stretch	1015(40)	gas	PE	2,3
	2	Bend	520(40)	gas	PE	2,3

[a]Assignments from Ref. 4.

[b]From vertical ionization potential.

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CF_2^-

Threshold for electron detachment from ground-state CF_2^- = 1450(160) gas PE[1–3]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF stretch	860(30)	gas	PE	1

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[1] K. K. Murray, D. G. Leopold, T. M. Miller, and W. C. Lineberger, J. Chem. Phys. **89**, 5442 (1988).
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CCl_2^-

Threshold for electron detachment from ground-state CCl_2^- = 12830(560) gas PE[1–3]

References

[1] K. K. Murray, D. G. Leopold, T. M. Miller, and W. C. Lineberger, J. Chem. Phys. **89**, 5442 (1988).
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CBr_2^-

Threshold for electron detachment from ground-state CBr_2^- = 15170(560) gas PE[1]

Reference

[1] R. L. Schwartz, G. E. Davico, T. M. Ramond, and W. C. Lineberger, J. Phys. Chem. A **103**, 8213 (1999).

CI_2^-

Threshold for electron detachment from ground-state CI_2^- = 16860(560) gas PE[1]

Reference

[1] R. L. Schwartz, G. E. Davico, T. M. Ramond, and W. C. Lineberger, J. Phys. Chem. A **103**, 8213 (1999).

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]
The $\tilde{E}$–$\tilde{A}$ emission of gas-phase PF_2 is observed[5] near 30800 (325 nm) when PF_3 is excited by 14.4 eV radiation.

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

$\tau = 7.9$ ns gas EM[5]

$\tilde{C}\,^2A_1$ C_{2v}
$T_0 = 45000T$ gas EM[5]
$\tau = 14.7$ ns gas EM[5]

$\tilde{B}\,^2B_2$ C_{2v}
$T_0 = 23998(6)$ gas EM[3,5] $\tilde{B}$–$\tilde{X}$ 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	219T	gas	EM	3

$\tau \geqslant 1.9$ ms gas EM[3]

$\tilde{A}\,^2A_1$ C_{2v}
gas EM[5] $\tilde{A}$–$\tilde{X}$ 320–550 nm

$\tilde{X}\,^2B_1$ 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

$\tilde{E}$ (**4*p***) 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

$\tilde{D}\,^2A_1$(**4*s***) 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

$\tilde{B}\,^2B_2$ C_{2v}
In the gas phase, unstructured emission at wavelengths longer than 320 nm, with a maximum at approximately 460 nm, has been attributed[2,4] to PCl_2.
$\tau = 29(6)$ 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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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
			1442.5	Ne	IR	8,9
			1439.6			
			1442.5vs[b]	Ar	IR	2,7,9
			1416.7			
			1440.7[b]	Kr	IR	9
			1412.1			
			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 1417, 435, and 227 cm^{-1} in argon-matrix experiments and at 1412 in krypton-matrix experiments are contributed by ClOO trapped in a metastable site in the rare-gas lattice.[7–9]

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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.
	1	OO stretch	1487.0	Ne	IR	5
			1485.1	Ar	IR	1–4

References

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SO_2^-

Threshold for electron detachment from ground-state $SO_2^- = 8930(65)$ gas PE[2,3]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	944(48)	gas	PE	3
			990.8	Ne	IR	5
			985m Cs	Ar	IR,Ra	1,4
			990 Na	Ar	IR	1,4
	2	Bend	435(100)	gas	PE	3
			495wm Cs	Ar	IR	1,4
			495 Na	Ar	IR	1,4
b_2	3	Asym. stretch	1086.2	Ne	IR	5
			1089.7	Ar	IR	4
			1081.8			
			1042s Cs	Ar	IR	1,4
			1041 Na	Ar	IR	1,4

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S_3^-

Threshold for electron detachment from ground-state $S_3^- = 17000(110)$ gas PE[1,3]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	594.2T	Ar	IR	2

References

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OF_2^+

$\tilde{E}$ C_{2v}
$T^a = 51560(400)$ gas PE[1,2]

$\tilde{D}$ C_{2v}
$T_0 \cong 38650$ gas PE[1,2]

$\tilde{C}\,^2A_2$ C_{2v}
$T_0 = 26880(120)$ gas PE[1–3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	OF_2 s-stretch	900(50)	gas	PE	3
	2	Bend	480(50)	gas	PE	3

$\tilde{A}\,^2B_2$ C_{2v}
$T_0 = 21950(120)$ gas PE[1–3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	440(30)	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	OF s-stretch	1000(20)	gas	PE	1–3

[a] From vertical ionization potential.

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[1] A. B. Cornford, D. C. Frost, F. G. Herring, and C. A. McDowell, J. Chem. Phys. **55**, 2820 (1971).
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Cl_2O^+

$\tilde{F}\,^2B_1$ C_{2v}
$T^a = 54380(320)$ gas PE[1]

$\tilde{E}\,^2A_1$ C_{2v}
$T^a = 46070(320)$ gas PE[1]

$\tilde{D}\,^2B_2$ C_{2v}
$T^a = 40020(320)$ gas PE[1]

$\tilde{C}\,^2A_2$ [b] C_{2v}
$T_0 = 14970(70)$ gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	613(40)	gas	PE	2
	2	Bend	306T	gas	PE	2

$\tilde{B}\,^2A_1$ [b] C_{2v}
$T_0 \geqslant 12630(70)$ gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	282(40)	gas	PE	2

$\tilde{A}\,^2B_2$ [b] C_{2v}
$T_0 = 9110(70)$ gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	290(40)	gas	PE	2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	ClO s-stretch	678(40)	gas	PE	1,2
	2	Bend	274(40)	gas	PE	1,2

[a]From vertical ionization potential.
[b]For assignment, see Ref. 3.

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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.[21,24,29,35,40,46–48]

$\tilde{A}\,^2A_2$ C_{2v}[a] Structure: AB[25]
$T_0 = 21017.2$ gas AB[1,2,5,14,25,31,32,34,35,45]LF[15,16,50]MPI[33,36]PF[41,43,47] $\tilde{A}-\tilde{X}$ 260–780 nm
20991.3 Ne AB[48]LF[48] $\tilde{A}-\tilde{X}$ 415–755 nm
20827.8 Ar AB[48]LF[48] $\tilde{A}-\tilde{X}$ 417–765 nm
20684.8 Kr AB[48]LF[48] $\tilde{A}-\tilde{X}$ 425–748 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	708.0	gas	AB,LF	5,14,34,50
			707.9	Ne	AB	48
			716.0	Ar	AB	48
			712.5	Kr	AB	48
	2	Bend	289.7	gas	AB,LF	5,14,34,50
			292.5	Ne	AB	48
			302.3	Ar	AB	48
			303.0	Kr	AB	48
b_2	3	Asym. stretch	441.2	gas	AB	25,34
			443.8H	Ne	AB	48
			448.6H	Kr	AB	48

$\tau_1^b = 56(20)$ ps gas AB[21,24]LF[29]
$\tau_2^c = 336(27)$ 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,Ra	20,23,26,
					LMR	49
					DL,LS	28,37,39
			944.8m	Ne	IR	44,48
			947.6m	Ar	IR,Ra	13,17,18
						44,48
			944.1	Kr	Ra,IR	18,48
			940(2)	Xe	Ra	18
			950(2)	N_2	Ra	18
	2	Bend	447.70s	gas	IR,AB	4,5,14–16,
					LF,Ra	22,25,38,39,49
			448.7m	Ne	IR	44
			451s	Ar	IR,LF	13,17,18,44
			447s			
			447	Kr	LF	18
b_2	3	Asym. stretch	1110.11vs	gas	IR,Ra	3,14,26
						38,39,49
			1107.6vs	Ne	IR	44,48
			1106.5vs	Ar	IR	13,17,44,
			1100.8vs			48
			1102.2	Kr	IR	48

$A_0 = 1.737$; $B_0 = 0.332$; $C_0 = 0.278$ 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 $F_1(J = N + 1/2)$ spin states.
[c]For $F_2(J = N - 1/2)$ spin states.

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OBrO

$\tilde{C}\,^2A_2$ C_{2v}

$T_0 = 15863$ gas AB[2,6,10] $\tilde{C}-\tilde{X}$ 388–645 nm
15818.4(2) Ne AB[8] $\tilde{C}-\tilde{X}$ 482–632 nm
16785(20) Ar AB[3,5] $\tilde{C}-\tilde{X}$ 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	641.5[a]	gas	AB	2,6
			642.77(13)[a]	Ne	AB	8
			631T	Ar	AB	5
	2	Bend	210.7[a]	gas	AB	2,6
			223.2(4)[a]	Ne	AB	8
			221T	Ar	AB	5
b_2	3	Asym. stretch	463H	Ne	AB	8

$\tilde{X}\,^2B_1$ C_{2v} Structure: MW[4,7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	799.4	gas	AB,IR	6,9
			797.6	Ne	IR	8
			795.7	Ar	IR	3,5
	2	Bend	317.5	gas	AB	6
			317.0	Ar	IR	5
b_2	3	Asym. stretch	848.6	gas	IR	4,9
			848.4	Ne	IR	8
			845.2	Ar	IR	1,3,5

$A_0 = 0.935$; $B_0 = 0.275$; $C_0 = 0.212$ MW[4,7]

[a] ω.

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BrOCl

Gas-phase absorption maxima of BrOCl have been observed[2] at 36760 (272 nm) and 31250 (320 nm).

$\tilde{X}$ 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

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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. A more recent gas-phase study[6] supports the assignment of the absorption maximum near 31800 (314 nm) to BrOBr and proposes the assignment of absorption maxima at 28570 (350 nm), 19230 (520 nm), and 15150 (660 nm) to that species, as well.

In an argon matrix, very slow photoisomerization of BrOBr to BrBrO is observed[8] on exposure of the sample to radiation between 16700 (600 nm) and 25000 (400 nm). Rapid photoisomerization occurs between 25000 and 28600 (350 nm).

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[5,7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	533	gas	IR	10
			526.1s	Ar	IR	1,2,8
			528	N_2	IR	3
b_2	3	Asym. stretch	629	gas	IR	10
			621.4	Ne	IR	9
			623.4w	Ar	IR	2,8
			626	N_2	IR	3

$A_0 = 1.108$; $B_0 = 0.046$; $C_0 = 0.044$ MW[5,7]

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SF_2

$\tilde{J}\,{}^1B_1(5s)$ C_{2v}
$T_0 = 68951$ gas MPI[14]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	942(3)	gas	MPI	14

$\tilde{I}(3d)$ C_{2v}
$T_0 = 68847$ gas MPI[14]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	933(4)	gas	MPI	14

$\tilde{H}(3d)$ C_{2v}
$T_0 = 68571$ gas MPI[14]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	936(4)	gas	MPI	14

$\tilde{G}(3d)$ C_{2v}
$T_0 = 68378$ gas MPI[14]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	939(12)	gas	MPI	14

$\tilde{F}(4p)$ C_{2v}
$T_0 = 63812$ gas MPI[14]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	966(6)	gas	MPI	14
	2	Bend	417(23)	gas	MPI	14

$\tilde{E}(4p)$ C_{2v}
$T_0 = 62025(30)$ gas MPI[10,14]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	941(27)	gas	MPI	10,14
	2	Bend	413(12)	gas	MPI	10,14

$\tilde{C}$
gas MPI[10,14] $\tilde{C}-\tilde{X}$ 165–175 nm

$\tilde{B}\,{}^1B_1(4s)$ C_{2v}
$T_0 = 54433(30)$ gas MPI[10,14]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	991(12)	gas	MPI	10,14
	2	Bend	361(24)	gas	MPI	10,14

$\tilde{B}'\ ^1A_1$ C_{2v}

$T_0 = 38623$ gas MPI[14,15] $\tilde{B}'-\tilde{X}$ 235–260 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	926(4)	gas	MPI	15

$\tilde{A}$

$T_0 = 18100(1000)$ 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]

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ClSBr

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SCl stretch	515.6	Ar	IR	1
			517.8	Kr	IR	1
			519.2	N_2	IR	1
	3	SBr stretch	416.0	Ar	IR	1
			413.0	Kr	IR	1
			416.0	N_2	IR	1

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$OClO^-$

Threshold for electron detachment from ground-state $OClO^- = 17310(20)$ gas PE[2,3]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	774(25)	gas	PE	2
			790 Cs	Ar	IR	1
	2	Bend	418 Cs	Ar	IR	1
b_2	3	Asym. stretch	823 Cs	Ar	IR	1

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FClO

$\tilde{X}$ C_s Structure: IR^2MW^3

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ClO stretch	1037.69	gas	IR	2
			1038s	Ar	IR	1
	2	Bend	310H	gas	IR	2
			315.2m	Ar	IR	1
	3	FCl stretch	596.9	gas	IR	2
			593.5vs	Ar	IR	1

$A_0 = 1.223$; $B_0 = 0.278$; $C_0 = 0.226$ IR^2MW^3

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BrBrO

In an argon matrix, irradiation at 870 nm results in photoisomerization to BrOBr.[3] Rapid photoisomerization also ensues on irradiation beyond 29400 (340 nm).[4]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	BrO stretch	804.8	Ne	IR	5
			805.4	Ar	IR	1–4
	3	BrBr stretch	236	Ar	IR	1

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I_3

$\tilde{C}$

A band in the photoelectron spectrum of I_3^- 5700 (0.707 eV) above the band for I_3 ($\tilde{X}$) has been assigned[2] to I_3 ($\tilde{C}$).

$\tilde{B}$

A band in the photoelectron spectrum of I_3^- 5190 (0.643 eV) above the band for I_3 ($\tilde{X}$) has been assigned[2] to I_3 ($\tilde{B}$).

$\tilde{A}$

A band in the photoelectron spectrum of I_3^- 2480 (0.307 eV) above the band for I_3 ($\tilde{X}$) has been assigned[1,2] to I_3 ($\tilde{A}$).

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	115(5)	gas	PE	1

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Cl_3^-

In the gas phase, a photodetachment peak at 47360 (211 nm) has been assigned[6] to the formation of Cl_3 ($1\,^2\Pi_g$)$+e$. The doublet structure of this peak is attributed to spin-orbit interaction. This state of Cl_3 is expected to be bound.

In the gas phase, a broad photodetachment peak with maximum at 41700 (240 nm) has been assigned[6] to the formation of Cl_3 ($\tilde{X}\,^2\Pi_u$,$1\,^2\Sigma_g^+$)$+e$, where both states of Cl_3 are dissociative. An absorption maximum which appears at 39840 (251 nm) when CsCl is codeposited with Cl_2 in an argon matrix[3] and at 39530 (253 nm) when an Ar:Cl_2 sample is subjected to electron bombardment during deposition[5] has also been assigned to Cl_3^-.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	225T Cs	Ar	Ra	2
			253 Rb	Ar	Ra	2
			258 K	Ar	Ra	2
			276 Na	Ar	Ra	2
Σ_u^+	3	Asym. stretch	327 Cs	Ar	IR,Ra	2
			340 Rb	Ar	IR,Ra	2
			345 K	Ar	IR,Ra	2
			375 Na	Ar	IR,Ra	2
			374[a]	Kr	IR	1

[a] Attributed in Ref. 1 to the uncharged species. Reassigned by Ref. 4 to the anion.

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I_3^-

Threshold for electron detachment from ground-state $I_3^- = 34100(100)$ gas PE[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	112(1)	gas	Ra[a]	3
			113 Cs	Ar	Ra[a]	1

[a] Resonance Raman.

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8.4. Four-Atomic Trihydrides

$HPd(H_2)$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	PdH stretch	1900.8	Ar	IR	1

$DPd(D_2)$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	PdD stretch	1366.4	Ar	IR	1

Reference

[1] L. Andrews, X. Wang, M. E. Alikhani, and L. Manceron, J. Phys. Chem. A **105**, 3052 (2001).

PtH_3

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	PtH s-stretch	2064.7	Ar	IR	1
a''	5	PtH a-stretch	1802.4	Ne	IR	1
			1784.3	Ar	IR	1

PtD_3

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a''	5	PtD a-stretch	1293.8	Ar	IR	1

Reference

[1] L. Andrews, X. Wang, and L. Manceron, J. Chem. Phys. **114**, 1559 (2001).

$HAu(H_2)$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		2170.1	Ne	IR	1
			2167.9			
			2173.6	Ar	IR	1
			2170.6			

$DAu(D_2)$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		1559.0	Ne	IR	1
			1559.3	Ar	IR	1
			1556.5	D_2	IR	1
b_2			939.6	D_2	IR	1
			434.8	D_2	IR	1

Reference

[1] X. Wang and L. Andrews, J. Am. Chem. Soc. **123**, 12899 (2001).

CeH_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	CeH_3 stretch	1283.1	Ar	IR	1

CeD_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	CeD_3 stretch	918.0	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **104**, 1640 (2000).

NdH_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	NdH_3 stretch	1150.0	Ar	IR	1

NdD_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	NdD_3 stretch	824.6	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **104**, 1640 (2000).

SmH_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	SmH_3 stretch	1203.5	Ar	IR	1

SmD_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	SmD_3 stretch	857.0	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **104**, 1640 (2000).

GdH_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	GdH_3 stretch	1323.6	Ar	IR	1

GdD_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	GdD_3 stretch	947.5	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **104**, 1640 (2000).

TbH_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	TbH_3 stretch	1375.5	Ar	IR	1

TbD_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	TbD_3 stretch	985.2	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **104**, 1640 (2000).

LuH_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	LuH_3 stretch	1386.4	Ar	IR	1

LuD_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	LuD_3 stretch	993.9	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **104**, 1640 (2000).

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	1,2
	4	Deformation	758.7s	Ar	IR	1,2

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

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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	1359(7)	gas	PE,PD	1,2,6
e'	3	CH stretch	3108.38	gas	LD	3–5
	4	Deformation	1370(7)	gas	PD	6

$B_0 = 9.362$ 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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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^2IR[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,Ra	13,16,23,26,32
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,CC	11,25,27
					CR,IR	30,34–36
			3162wm	Ne	IR	4
			3150	Ar	IR	6
			3171.4	H_2	IR	29,33
			3170.6			
	4	Deformation	1396w	Ne	IR	4
			1398[c]	Ar	IR	8
			1402.7	H_2	IR	29,33
			1401.6			

$B_0 = 9.578$ AB^2DL[9]LD[34]IR[36]; $C_0 = 4.743$ DL[9]LD[34]

CD_3

df $^2E'$[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]$R(0_0)$ transition.
[d]Approximate value; perturbed by Fermi resonance.

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SiH_3

$\tilde{M}\,^2A_2''(6p)$ D_{3h}
$T_0 = 60341$ gas MPI[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	800(30)	gas	MPI	7

$\tilde{L}(5d)$ D_{3h}
$T_0 = 59615(30)$[c] gas MPI[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	839(26)	gas	MPI	8

$\tilde{J}'(4d)$ D_{3h}
$T_0 = 57726(30)$ gas MPI[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	835(26)	gas	MPI	8

$\tilde{J}\,^2A_2''(5p)$ D_{3h}
$T_0 = 56929$ gas MPI[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	821(4)	gas	MPI	7

$\tilde{I}'(4d)$ D_{3h}
$T_0 = 56253(30)$ gas MPI[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	814(25)	gas	MPI	8

$\tilde{D}\,^2A_1'(3d)$ D_{3h}
$T_0 = 49787(30)$ gas MPI[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	810(31)	gas	MPI	8

$\tilde{E}\,^2A_2''(4p)$ D_{3h}
$T_0 = 48438$ gas MPI[5,7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	796(7)	gas	MPI	5,7
e'	4	Deformation	870(5)H	gas	MPI	7

$\tilde{A}\,^2A_1$ C_{3v}
gas AB[9,12] $\tilde{A}$–$\tilde{X}$ 205–256 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
			733.6	Ar	IR	13
			732.4	Kr	IR	11
			730.0			
e	3	SiH_3 stretch	2185.2	gas	DL	10
	4	Deformation	929T	Kr	IR	11

Barrier to inversion = 1935 gas PE[4]MPI[7]
$B_0 = 4.763$ DL[3]

SiD_3

$\tilde{P}\,^2A_2''(7p)$ D_{3h}
$T_0 = 62002$ gas MPI[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	615(3)	gas	MPI	7

$\tilde{N}\,^2E'(5f)$ D_{3h}
$T_0 = 61005$ gas MPI[7,8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	619(7)	gas	MPI	7

$\tilde{M}\,^2A_2''(6p)$ D_{3h}
$T_0 = 60267$ gas MPI[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	615(4)	gas	MPI	7

$\tilde{K}\,^2E'(4f)$ D_{3h}
$T_0 = 58417$ gas MPI[7,8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	602(10)	gas	MPI	8

$\tilde{J}'(4d)$ D_{3h}

$T_0 = 57840(30)$[c] gas MPI[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	603(20)	gas	MPI	8

$\tilde{J}\,^2A_2''(5p)$ D_{3h}

$T_0 = 56874$ gas MPI[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	608(3)	gas	MPI	7

$\tilde{I}'(4d)$ D_{3h}

$T_0 = 56205(30)$ gas MPI[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	600(17)	gas	MPI	8

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

$T_0 \cong 50000$ gas MPI[7,8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	602(5)	gas	MPI	7

$\tilde{D}\,^2A_1''(3d)$ D_{3h}

$T_0 = 49685(30)$[c] gas MPI[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	600(28)	gas	MPI	8

$\tilde{E}\,^2A_2''(4p)$ D_{3h}

$T_0 = 48391$ gas MPI[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	SiD_3 stretch	1576(3)	gas	MPI	7
a_2''	2	OPLA	589(3)	gas	MPI	7
e'	4	Deformation	635(6)H	gas	MPI	7

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Umbrella	545[a]	gas	MPI	7
			542[b]	gas	MPI	7
			545.5	Ar	IR	13
			548.9	Kr	IR	11
			547.2			
			545.8	D_2	IR	13

Barrier to inversion = 1925 gas MPI[7]

[a] $1^- - 0^+$ transition.
[b] $1^+ - 0^-$ transition.
[c] Extrapolated value.

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NH_3^+

$\tilde{A}\,^2E$ D_{3h}

$T_0 = 36470(100)$ gas PE[3,4,12]

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	3,7,11,12
			916.8	Ne	IR	13
e'	3	NH stretch	3388.65	gas	LD	6
			3404.6	Ne	IR	13
	4	Bend	1507.1	gas	PE,TPE	8–11
			1516.8	Ne	IR	13

$B_0 = 10.644$; $C_0 = 5.247$ 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	684(4)	gas	PE	2,11
			683.3	Ne	IR	13
e'	3	ND stretch	2551.8	Ne	IR	13
	4	Bend	1138(56)	gas	PE	10
			1114.6	Ne	IR	13

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H_3O^+

$\tilde{X}$ C_{3v} Structure: CC[4]MW[19]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	OH stretch	3491.17[a]	gas	LD	18
			3389.66[b]	gas	LD	18
	2	Umbrella	954.40[a]	gas	DL	2,3,5,7
			525.82[b]	gas	DL	5–7
e	3	OH stretch	3535.56[c,d]	gas	CC	1,4,10,15
			3518.95[c,e]	gas	CC	1,4,10,14,15
	4	Deformation	1625.95[d]	gas	DL	11
			1638.53[e]	gas	DL	11

$B(0^+)=11.254$; $C(0^+)=6.129$; $B(0^-)=11.054$; $C(0^-)=6.211$
IR,MW[9,12,15]CC[16]LD[16,18]

D_3O^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Umbrella	645.13[a]	gas	DL	8
			438.39[b]	gas	DL	8
e	3	OD stretch	2629.65[d]	gas	LD	13
			2624.24[e]	gas	LD	13

$B(0^+)=5.675$; $C(0^+)=3.15(5)$; $B(0^-)=5.644$; $C(0^-)=3.16(5)$
DL[8]LD[13]MW[19]

[a] $1^- - 0^+$ transition.
[b] $1^+ - 0^-$ transition. For H_3O^+, $0^- - 0^+ = 55.35\ cm^{-1}$,[6,12] and for D_3O^+, $15.36\ cm^{-1}$.[8,17,19]
[c] $\nu - C'\zeta + 7/4\,\eta_K$.
[d] $1^+ - 0^+$ transition.
[e] $1^- - 0^-$ transition.

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H_3S^+

$\tilde{X}$ C_{3v} Structure: MW[6,7]

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]

D_3S^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SD stretch	1827.22	gas	DL	5
e	3	SD stretch	1838.62	gas	DL	5

$B_0=2.542$; $C_0=2:12(3)$ DL[5]MW[6]

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8.5. Four-Atomic Dihydrides

cyc-Pd_2H_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}		PdH stretch	1345.8	Ne	IR	1
			1347.7	Ar	IR	1

cyc-Pd_2D_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}		PdD stretch	953.9	Ne	IR	1
			950.2	Ar	IR	1

Reference

[1] L. Andrews, X. Wang, M. E. Alikhani, and L. Manceron, J. Phys. Chem. A **105**, 3052 (2001).

cyc-$(CeH)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Asym. stretch	1128.0	Ar	IR	1

cyc-$(CeD)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Asym. stretch	808.3	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **104**, 1640 (2000).

cyc-$(PrH)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Asym. stretch	1135.6	Ar	IR	1

cyc-$(PrD)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Asym. stretch	813.4	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **104**, 1640 (2000).

cyc-$(GdH)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Asym. stretch	1201.9	Ar	IR	1

cyc-$(GdD)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Asym. stretch	860.9	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **104**, 1640 (2000).

cyc-$(TbH)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Asym. stretch	1212.1	Ar	IR	1

cyc-$(TbD)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Asym. stretch	868.8	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **104**, 1640 (2000).

cyc-$(LuH)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Asym. stretch	1273.2	Ar	IR	1

cyc-$(LuD)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Asym. stretch	912.1	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **104**, 1640 (2000).

$LiNH_2$

$\tilde{X}$ C_{2v} Structure: MW[1]
$A_0 = 13.161(2)$; $B_0 = 1.011$; $C_0 = 0.933$ MW[1]

$LiND_2$

$\tilde{X}$ C_{2v}
$A_0 = 6.584$; $B_0 = 0.894$; $C_0 = 0.781$ MW[1]

Reference

[1] D. B. Grotjahn, P. M. Sheridan, I. A. Jihad, and L. M. Ziurys, J. Am. Chem. Soc. **123**, 5489 (2001).

$NaNH_2$

$\tilde{X}$ C_{2v} Structure: MW[2]
$A_0 = 12.933(3)$; $B_0 = 0.375$; $C_0 = 0.364$ MW[1]

$NaND_2$

$\tilde{X}$ C_{2v}
$A_0 = 6.506$; $B_0 = 0.330$; $C_0 = 0.313$ MW[2]

References

[1] J. Xin, M. A. Brewster, and L. M. Ziurys, Astrophys. J. **530**, 323 (2000).
[2] D. B. Grotjahn, P. M. Sheridan, I. Al Jihad, and L. M. Ziurys, J. Am. Chem. Soc. **123**, 5489 (2001).

HCBeH

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	BeH stretch	2087.3	Ar	IR	1
	3	CBe stretch	983.7	Ar	IR	1
Π	4	Deformation	534.2	Ar	IR	1

DCBeD

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	BeD stretch	1593.5	Ar	IR	1
	3	CBe stretch	935.2	Ar	IR	1
Π	4	Deformation	430.2	Ar	IR	1
			427.8			

Reference

[1] T. M. Greene, D. V. Lanzisera, L. Andrews, and A. J. Downs, J. Am. Chem. Soc. **120**, 6097 (1998).

$MgCH_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s-stretch	2786.8	Ar	IR	1
	3	MgC stretch	502.2	Ar	IR	1

$MgCD_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_2 s-stretch	2040.3	Ar	IR	1
	3	MgC stretch	472.1	Ar	IR	1

Reference

[1] W. D. Bare, A. Citra, C. Trindle, and L. Andrews, Inorg. Chem. **39**, 1204 (2000).

$MgNH_2$

$\tilde{X}\,^2A_1$ C_{2v} Structure: MW[2]
$A_0 = 12.626$; $B_0 = 0.444$; $C_0 = 0.428$ MW[1,2]

$MgND_2$

$\tilde{X}\,^2A_1$ C_{2v}
$A_0=6.334$; $B_0=0.388$; $C_0=0.365$ MW[2]

References

[1] P. M. Sheridan and L. M. Ziurys, Astrophys. J. **540**, L61 (2000).
[2] P. M. Sheridan and L. M. Ziurys, Can. J. Phys. **79**, 409 (2001).

$CaNH_2$

$\tilde{C}\,^2A_1$ C_{2v} Structure: LF[2,7]
$T_0=17375.167$ gas CL[1]LF[2,7] $\tilde{C}-\tilde{X}$ 575 nm
$A=12.95$; $1/2(B+C)=0.302$; $1/4(B-C)=0.0018$ LF[2,7]

$\tilde{B}\,^2B_1$ C_{2v} Structure: LF[7]
$T_0=15885.28$ gas CL[1]LF[3–5,7,8] $\tilde{B}-\tilde{X}$ 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

$A_0=14.365$; $1/2(B_0+C_0)=0.302$; $1/4(B_0-C_0)=0.004$ LF[5,7,8]

$\tilde{A}\,^2B_2$ C_{2v} Structure: LF[7]
$T_0=15464.367$ gas CL[1]LF[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]MW[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CaN stretch	524(10)	gas	LF	3

$A=13.080(3)$; $B_0=0.300$; $C_0=0.293$ LF[2,5,6]MW[9]

$CaND_2$

$\tilde{X}\,^2A_1$ C_{2v}
$A_0=6.527$; $B_0=0.260$; $C_0=0.250$ MW[9]

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$SrNH_2$

$\tilde{C}\,^2A_1$ C_{2v}
$T_0=15862(10)$ gas CL[1]LF[2] $\tilde{C}-\tilde{X}$ 632 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	SrN stretch	458(5)	gas	LF	2,3
b_1	4	OPLA	290(30)	gas	LF	3
b_2	6	Deformation	290(30)	gas	LF	3

$\tilde{B}\,^2B_1$ C_{2v} Structure: LF[3]
$T_0=14689.32$ gas CL[1]LF[2,3] $\tilde{B}-\tilde{X}$ 670–725 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	SrN stretch	444(5)	gas	LF	2,3

$A_0=14.714$; $(B_0+C_0)=0.455$; $(B_0-C_0)=0.004$ LF[3]

$\tilde{A}\,^2B_2$ C_{2v} Structure: LF[3]
$T_0=14230.62$ gas CL[1]LF[2,3] $\tilde{A}-\tilde{X}$ 670–725 nm
$A_0=12.103$; $(B_0+C_0)=0.457$; $(B_0-C_0)=0.005$ LF[3]

$\tilde{X}\,^2A_1$ C_{2v} Structure: LF[3]MW[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NH_2 s-stretch	3293(10)	gas	LF	3
	2	NH_2 scissors	1678(10)	gas	LF	3
	3	SrN stretch	459(5)	gas	LF	2,3
b_1	4	OPLA	320(30)	gas	LF	3
b_2	6	Deformation	320(30)	gas	LF	3

$A_0=13.154(5)$; $B_0=0.226$; $C_0=0.222$ LF[3]MW[4]

$SrND_2$

$\tilde{X}\,^2A_1$ C_{2v}
$A_0=6.557$; $B_0=0.194$; $C_0=0.188$ MW[4]

References

[1] R. F. Wormsbecher, M. Trkula, C. Martner, R. E. Penn, and D. O. Harris, J. Mol. Spectrosc. **97**, 29 (1983).
[2] A. M. R. P. Bopegedera, C. R. Brazier, and P. F. Bernath, J. Phys. Chem. **91**, 2779 (1987).
[3] C. R. Brazier and P. F. Bernath, J. Mol. Spectrosc. **201**, 116 (2000).
[4] J. M. Thompsen, P. M. Sheridan, and L. M. Ziurys, Chem. Phys. Lett. **330**, 373 (2000).

$HYOH^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		YH stretch	1534.2	Ar	IR	1
		YO stretch	695.1	Ar	IR	1

$DYOD^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		YD stretch	1099.6	Ar	IR	1
		YO stretch	681.6	Ar	IR	1

Reference

[1] L. Zhang, L. Shao, and M. Zhou, Chem. Phys. **272**, 27 (2001).

$HCCH^+$

$\tilde{C}\,^2\Sigma^+$ $D_{\infty h}$
$T_0 = 92460(80)$ 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

$\tau < 14$ 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

$\tau_0 = 150$ 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	Nc	IR	8,12
			3105.5	Ar	IR	4,8,12
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	8,12
			2311.5	Ar	IR	4,8,12
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. $\epsilon_4 = 0.30$.[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 $DCCD^+$.

References

[1] C. Baker and D. W. Turner, Proc. R. Soc. London, Ser. A **308**, 19 (1968).
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[4] M. E. Jacox and W. B. Olson, J. Chem. Phys. **86**, 3134 (1987).
[5] M. W. Crofton, M.-F. Jagod, B. D. Rehfuss, and T. Oka, J. Chem. Phys. **86**, 3755 (1987).
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HScOH

In an argon matrix,[1] photolyzes with 300–400 nm radiation, producing H_2 + ScO.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ScH stretch	1482.6	Ar	IR	1,2
		ScO stretch	713.0	Ar	IR	1,2

DScOD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ScD stretch	1068.5	Ar	IR	1,2
		ScO stretch	693.6	Ar	IR	1,2

References

[1] J. W. Kauffman, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **89**, 3547 (1985).
[2] L. Zhang, J. Dong, and M. Zhou, J. Phys. Chem. A **104**, 8882 (2000).

HYOH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		YH stretch	1399.1	Ar	IR	1
		YO stretch	641.5	Ar	IR	1

DYOD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		YD stretch	1002.9	Ar	IR	1
		YO stretch	623.1	Ar	IR	1

Reference

[1] L. Zhang, L. Shao, and M. Zhou, Chem. Phys. **272**, 27 (2001).

HLaOH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		LaH stretch	1263.7	Ar	IR	1
		LaO stretch	576.4	Ar	IR	1

DLaOD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		LaD stretch	905.8	Ar	IR	1
		LaO stretch	559.7	Ar	IR	1

Reference

[1] L. Zhang, L. Shao, and M. Zhou, Chem. Phys. **272**, 27 (2001).

HTiOH

In an argon matrix,[1] photolyzes with 400–500 nm radiation, producing H_2 + TiO.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		TiH stretch	1538.9	Ar	IR	1,2
		TiO stretch	699.7	Ar	IR	1

DTiOD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		TiD stretch	1107.7	Ar	IR	1
		TiO stretch	697.3	Ar	IR	1

References

[1] J. W. Kauffman, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **89**, 3547 (1985).
[2] M. Zhou, L. Zhang, J. Dong, and Q. Qin, J. Am. Chem. Soc. **122**, 10680 (2000).

H_2TiO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		TiH_2 s-stretch	1646.8	Ar	IR	1
		TiH_2 a-stretch	1611.9	Ar	IR	1
		TiO stretch	1010.5	Ar	IR	1

D_2TiO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		TiD_2 a-stretch	1168.2	Ar	IR	1
		TiO stretch	1009.6	Ar	IR	1

Reference

[1] M. Zhou, L. Zhang, J. Dong, and Q. Qin, J. Am. Chem. Soc. **122**, 10680 (2000).

HZrOH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ZrH stretch	1530.9	Ar	IR	1

DZrOD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ZrD stretch	1098.2	Ar	IR	1

Reference

[1] M. Zhou, L. Zhang, J. Dong, and Q. Qin, J. Am. Chem. Soc. **122**, 10680 (2000).

H_2ZrO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ZrH_2 s-stretch	1577.6	Ar	IR	1
		ZrH_2 a-stretch	1539.4	Ar	IR	1
		ZrO stretch	924.7	Ar	IR	1

D_2ZrO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ZrD_2 s-stretch	1130.3	Ar	IR	1
		ZrD_2 a-stretch	1107.8	Ar	IR	1
		ZrO stretch	922.4	Ar	IR	1

Reference

[1] M. Zhou, L. Zhang, J. Dong, and Q. Qin, J. Am. Chem. Soc. **122**, 10680 (2000).

H_2HfO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		HfH_2 s-stretch	1646.4	Ar	IR	1
		HfH_2 a-stretch	1615.6	Ar	IR	1
		HfO stretch	921.0	Ar	IR	1

D_2HfO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		HfD_2 a-stretch	1158.1	Ar	IR	1
		HfO stretch	918.7	Ar	IR	1

Reference

[1] M. Zhou, L. Zhang, J. Dong, and Q. Qin, J. Am. Chem. Soc. **122**, 10680 (2000).

HVOH

In an argon matrix,[1] photolyzes with radiation having a short wavelength cutoff of 400 nm.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		VH stretch	1567.0	Ar	IR	1,2
		VO stretch	703.3T	Ar	IR	1
		Bend	414.5T	Ar	IR	1

DVOD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		VD stretch	1128.4	Ar	IR	1,2
		VO stretch	696.6T	Ar	IR	1

References

[1] J. W. Kauffman, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **89**, 3547 (1985).
[2] M. Zhou, J. Dong, L. Zhang, and Q. Zin, J. Am. Chem. Soc. **123**, 135 (2001).

H_2VO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	VH s-stretch	1710.6	Ar	IR	1
	2	VO stretch	1029.4	Ar	IR	1
		VH a-stretch	1680.4	Ar	IR	1

D_2VO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	VD s-stretch	1235.1	Ar	IR	1
	2	VO stretch	1029.1	Ar	IR	1
		VD a-stretch	1215.3	Ar	IR	1

Reference

[1] M. Zhou, J. Dong, L. Zhang, and Q. Qin, J. Am. Chem. Soc. **123**, 135 (2001).

HNbOH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	NbH stretch	1587.5	Ar	IR	1

DNbOD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	NbD stretch	1141.2	Ar	IR	1

Reference

[1] M. Zhou, J. Dong, L. Zhang, and Q. Qin, J. Am. Chem. Soc. **123**, 135 (2001).

H_2ONb

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		H_2O bend	1569.1	Ar	IR	1

D_2ONb

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		D_2O bend	1153.2	Ar	IR	1

Reference

[1] M. Zhou, J. Dong, L. Zhang, and Q. Qin, J. Am. Chem. Soc. **123**, 135 (2001).

H_2NbO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NbH s-stretch	1704.5	Ar	IR	1
	2	NbO stretch	976.9	Ar	IR	1
		NbH a-stretch	1665.2	Ar	IR	1

D_2NbO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NbD s-stretch	1224.0	Ar	IR	1
	2	NbO stretch	976.9	Ar	IR	1
		NbD a-stretch	1197.7	Ar	IR	1

Reference

[1] M. Zhou, J. Dong, L. Zhang, and Q. Qin, J. Am. Chem. Soc. **123**, 135 (2001).

H_2TaO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	TaH s-stretch	1780.4	Ar	IR	1
	2	TaO stretch	986.9	Ar	IR	1
		TaH a-stretch	1762.3	Ar	IR	1

D_2TaO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	TaO stretch	984.9	Ar	IR	1
		TaD a-stretch	1264.7	Ar	IR	1

Reference

[1] M. Zhou, J. Dong, L. Zhang, and Q. Qin, J. Am. Chem. Soc. **123**, 135 (2001).

HMnOH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	MnH stretch	1663.4	Ar	IR	1,2
		MnO stretch	648.1	Ar	IR	1,2

DMnOD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	MnD stretch	1197.1	Ar	IR	1,2
		MnO stretch	628.5	Ar	IR	1,2

References

[1] J. W. Kauffman, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **89**, 3541 (1985).
[2] M. Zhou, L. Zhang, L. Shao, W. Wang, K. Fan, and Q. Qin, J. Phys. Chem. A **105**, 5801 (2001).

HFeOH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	FeH stretch	1731.9	Ar	IR	1,2
		FeO stretch	682.4	Ar	IR	1,2
		Bend	457.6	Ar	IR	1

DFeOD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	FeD stretch	1245.3	Ar	IR	1,2
		FeO stretch	660.5	Ar	IR	1,2

References

[1] J. W. Kauffman, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **89**, 3541 (1985).
[2] L. Zhang, M. Zhou, L. Shao, W. Wang, K. Fan, and Q. Qin, J. Phys. Chem. A **105**, 6998 (2001).

$AlNH_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	NH_2 scissors	1520.3	Ar	IR	1,2
	3	AlN stretch	726.3	Ar	IR	1,2
b_1	4	OPLA	406.7	Ar	IR	1,2
b_2	5	NH_2 a-stretch	3495.1	Ar	IR	1,2

$AlND_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	ND_2 scissors	1137.7	Ar	IR	1,2
	3	AlN stretch	694.8	Ar	IR	1,2
b_1	4	OPLA	314.6	Ar	IR	2

References

[1] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **101**, 5082 (1997).
[2] H.-J. Himmel, A. J. Downs, and T. M. Greene, J. Am. Chem. Soc. **122**, 9793 (2000).

$GaNH_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	NH_2 scissors	1505.9	Ar	IR	1,2
	3	GaN stretch	589.3	Ar	IR	1,2
b_1	4	OPLA	303.3	Ar	IR	2
b_2	5	NH_2 a-stretch	3471.6	Ar	IR	1,2

$GaND_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	ND_2 scissors	1132.6	Ar	IR	2
	3	GaN stretch	557.9	Ar	IR	2

References

[1] H.-J. Himmel, A. J. Downs, and T. M. Greene, Chem. Commun. 871 (2000).
[2] H.-J. Himmel, A. J. Downs, and T. M. Greene, J. Am. Chem. Soc. **122**, 9793 (2000).

$InNH_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	NH_2 scissors	1498.1	Ar	IR	1
	3	InN stretch	498.7	Ar	IR	1
b_1	4	OPLA	237.0	Ar	IR	1
b_2	5	NH_2 a-stretch	3481.7	Ar	IR	1
	6	NH_2 rock	469.6	Ar	IR	1

$InND_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	ND_2 scissors	1116.3	Ar	IR	1
	3	InN stretch	480.6	Ar	IR	1

Reference

[1] H.-J. Himmel, A. J. Downs, and T. M. Greene, J. Am. Chem. Soc. **122**, 9793 (2000).

H_2CSi

$\tilde{B}\,^1B_2$ C_{2v} Structure: LF^4
$T_0 = 29312.88$ gas AB^1LF^{3-5} $\tilde{B}-\tilde{X}$ 300–342 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 stretch	2997	gas	LF	4,5
	2	CH_2 scissors	1101.96	gas	AB,LF	1,4,5
	3	CSi stretch	702.00	gas	AB,LF	1,3–5
b_1	4	OPLA	697	gas	LF	5
b_2	6	CH_2 rock	731	gas	LF	4,5

$A_0 = 8.533$; $B_0 = 0.510$; $C_0 = 0.479$ AB^1LF^4

$\tilde{X}\,^1A_1$ C_{2v} Structure: MW^2LF^4

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s-stretch	2947(5)	gas	LF	6
	2	CH_2 scissors	1273(3)	gas	SEP	6
	3	CSi stretch	933(3)	gas	SEP	6
b_1	4	OPLA	687(5)H	gas	SEP	6
b_2	6	CH_2 rock	263(5)	gas	LF	6

$A_0 = 10.186$; $B_0 = 0.552$; $C_0 = 0.521$ $AB^1MW^2LF^4$

D_2CSi

$\tilde{B}\,^1B_2$ C_{2v}
$T_0 = 29237.35$ gas $AB^1LF^{4,5}$ $\tilde{B}-\tilde{X}$ 308–342 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_2 stretch	2180	gas	LF	4,5
	2	CD_2 scissors	831	gas	AB,LF	1,4,5
	3	CSi stretch	681	gas	AB,LF	1,4,5
	4	OPLA	547	gas	LF	5
b_2	6	CD_2 rock	549	gas	LF	4,5

$A_0 = 4.286$; $B_0 = 0.443$; $C_0 = 0.400$ LF^4

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_2 s-stretch	2185(3)	gas	SEP	6
	2	CD_2 scissors	1054(3)	gas	SEP	6
	3	CSi stretch	808(3)	gas	SEP	6
b_1	4	OPLA	539(3)H	gas	SEP	6
b_2	6	CD_2 rock	216(5)	gas	LF	6

$A_0 = 5.084$; $B_0 = 0.468$; $C_0 = 0.425$ LF^4

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H_2CGe

$\tilde{B}\,^1B_2$ C_{2v} Structure: LF[2]
$T_0 = 27330.42$ gas LF[1,2] $\tilde{B}-\tilde{X}$ 354–367 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_2 scissors	1024	gas	LF	2
	3	CGe stretch	548	gas	LF	1,2
b_1	4	OPLA	613	gas	LF	2
b_2	6	CH_2 rock	692	gas	LF	2

$\tau = 2\ \mu s$ gas LF[2]
$A_0 = 8.318$; $B_0 = 0.368$; $C_0 = 0.351$ LF[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_2 scissors	1238	gas	LF	3
	3	GeC stretch	782	gas	LF	3
b_1	4	OPLA	673	gas	LF	3
b_2	6	CH_2 rock	351	gas	LF	3

$A_0 = 10.055$; $B_0 = 0.401$; $C_0 = 0.385$ LF[2]

D_2CGe

$\tilde{B}\,^1B_2$ C_{2v}
$T_0 = 27278.45$ gas LF[2] $\tilde{B}-\tilde{X}$ 354–367 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_2 scissors	782	gas	LF	2
	3	CGe stretch	528	gas	LF	2
b_1	4	OPLA	465	gas	LF	2
b_2	6	CD_2 rock	513	gas	LF	2

$A_0 = 4.179$; $B_0 = 0.315$; $C_0 = 0.293$ LF[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_2 s-stretch	2089	gas	LF	3
	2	CD_2 scissors	1000	gas	LF	3
	3	GeC stretch	694	gas	LF	3
b_1	4	OPLA	520	gas	LF	3
b_2	6	CD_2 rock	282	gas	LF	3

$A_0 = 5.025$; $B_0 = 0.334$; $C_0 = 0.312$ LF[2]

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br-Si_2H_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		890.3w	Ar	IR	3
b_1	5		1475.6vw	Ar	IR	3
b_2	6		1092.8vs	Ar	IR	3

$A_0 = 5.244$; $B_0 = 0.243$; $C_0 = 0.240$ MW[1,2]

br-Si_2D_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	6		818	Ar	IR	3

$A_0 = 2.688$; $B_0 = 0.240$; $C_0 = 0.234$ MW[2]

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$HCNH^+$

$\tilde{X}$ $C_{\infty v}$ Structure: LD[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NH stretch	3482.84	gas	LD	1,2
	2	CH stretch	3187.86	gas	LD	1,2
	3	CN stretch	2155.70	gas	DL	7,8
Π	4	HCN bend	801.59	gas	DL	5
	5	HNC bend	645.92	gas	DL	6

$B_0 = 1.236$ LD[1,2]MW[3,9]

$DCND^+$

$\tilde{X}$ $C_{\infty v}$
$B_0 = 0.892$ MW[9]

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H_2CN

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

$T_0 = 35620$ gas AB[2,3,5] $\tilde{C}-\tilde{X}$ 280–285 nm
35436(25) Ar AB[6] $\tilde{C}-\tilde{X}$ 270–285 nm

Gas-phase absorption is diffuse.[5] Photolysis is observed in an argon matrix.[6]

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

$T_0 = 35075$[a] gas AB[2,3,5] $\tilde{B}-\tilde{X}$ 280–285 nm
34990(25) Ar AB[6] $\tilde{B}-\tilde{X}$ 270–285 nm

All gas-phase bands are diffuse.[5] Photolysis is observed in an argon matrix.[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s-stretch	2774(50)T	Ar	AB	6
	2	CN stretch	1883(50)	Ar	AB	6
	3	CH_2 scissors	1413(50)	Ar	AB	6

$\tilde{X}\,^2B_2$ C_{2v} Structure: ESR[1,4] MW[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s-stretch	2820T	gas	PE	7
	2	CN stretch	1725.4vw	Ar	IR	6
	3	CH_2 scissors	1337T	gas	PE	7
			1336.6m	Ar	IR	6
			1332.7	Kr	IR	9
			1328.7	Xe	IR	9
b_1	4	OPLA	954.1wm	Ar	IR	6
			950.3	Kr	IR	9
b_2	5	CH_2 a-stretch	3103.2m	Ar	IR	6
	6	CH_2 rock	912.8w	Ar	IR	6
			909.0	Kr	IR	9

$A_0 = 9.484$; $B_0 = 1.306$; $C_0 = 1.142$ MW[8]

D_2CN

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

$T_0 = 35481$[a] gas AB[2,5] $\tilde{C}-\tilde{X}$ 271–285 nm

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

$T_0 = 35036$[a] gas AB[2,5] $\tilde{B}-\tilde{X}$ 271–285 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CN stretch	1894T	gas	AB	2,5
	3	CD_2 scissors	1079T	gas	AB	2,5

$\tilde{X}\,^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_2 s-stretch	2080T	gas	PE	7
	3	CD_2 scissors	990T	gas	PE	7
			1073.4	Ar	IR	6
b_1	4	OPLA	776	Ar	IR	6
b_2	5	CD_2 a-stretch	2427.5T	Ar	IR	6

[a] Tentative assignment.

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HCNH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1217.9T	Kr	IR	2
		CNH deform.	886.3T	Ar	IR	1
			882.8T	Kr	IR	2

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H_2CP

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

$A_0 = 9.879$; $B_0 = 0.566$; $C_0 = 0.534$ MW[1]

D_2CP

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

$A_0 = 4.951$; $B_0 = 0.477$; $C_0 = 0.434$ MW[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_2 s-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	1,4,5,7
b_1	4	OPLA	919(24)	gas	PE	7
b_2	5	CH_2 a-stretch	2718(24)	gas	PE	7
	6	CH_2 deform.	777(4)	gas	PE	4,5,7

$A_0 = 8.875(3)$; $B_0 = 1.31(1)$; $C_0 = 1.14(1)$ 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
			648(4)	gas	PE	4,5

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InH_2Cl

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	InH_2 s-stretch	1804.0	Ar	IR	1
	2	InH_2 scissors	575.8	Ar	IR	1
	3	InCl stretch	343.4	Ar	IR	1
b_1	4	OPLA	541.4	Ar	IR	1
b_2	5	InH_2 a-stretch	1820.3	Ar	IR	1
	6	HInCl deform.	415.7	Ar	IR	1

InD_2Cl

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	InD_2 s-stretch	1291.9	Ar	IR	1
	2	InD_2 scissors	415.3	Ar	IR	1
	3	InCl stretch	339.3	Ar	IR	1
b_1	4	OPLA	389.1	Ar	IR	1
b_2	5	InD_2 a-stretch	1310.9	Ar	IR	1
	6	DInCl deform.	298.2	Ar	IR	1

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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]DR[34] $\tilde{A}-\tilde{X}$ 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]DR[34] $\tilde{a}-\tilde{X}$ 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]

$\tilde{X}\ ^1A_1$ 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

$\tau_0 = 182\ \mu s$ 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

$A_0=4.883$; $B_0=0.497$; $C_0=0.450$ $MW^2AB^{10}LF^{27}$

[a]Barrier to inversion≅50.[18]
[b]From fit to combination bands.

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H_2CSe

$\tilde{A}\,^1A_2$ C_{2v} Structure: LF^7
$T_0\cong13555$ 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 $AB^1CL^{3,8}LF^{5,6,9}$ $\tilde{a}-\tilde{X}$ 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 $LF^{6,9,10}$ $\tilde{a}-\tilde{X}$ 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

$A_0=4.865$; $B_0=0.344$; $C_0=0.321$ $MW^4LF^{7,9}$

[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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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[2,6,13]

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	10,11,13
			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	10,11,13
			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}
$T_0\cong58086$[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	12,13
			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	12,13
			972	N_2	IR	7

$A_0=6.025$; $B_0=1.089$; $C_0=0.920$ IR[6,12]

[a]$4p\pi$ Rydberg transition.
[b]$3p\pi$ Rydberg transition.
[c]5_0^1 vibronic band origin.[8]
[d]1–0 subband origin.

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H_2CF

5*p* Rydberg state C_{2v}
$T_0 = 67265(10)$ gas MPI[8]

4*p* Rydberg state C_{2v}
$T_0 = 63275(10)$ gas MPI[8] $4p-\tilde{X}$ 147–158 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF stretch	1580(20)	gas	MPI	8
	3	CH_2 scissors	1443(20)	gas	MPI	8
b_1	4	OPLA	1259(20)	gas	MPI	8

3*p* Rydberg state C_{2v}
$T_0 = 52863(10)$ gas MPI[8] $3p-\tilde{X}$ 167–193 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF stretch	1575(20)	gas	MPI	8
	3	CH_2 scissors	1420(20)	gas	MPI	8
b_1	4	OPLA	1223(20)	gas	MPI	8

Threshold for photodecomposition, producing CF, observed[5] near 280 nm in an argon matrix.

$\tilde{X}\,^2B_1$ C_{2v} Structure: ESR[1]MW[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CF stretch	1170.42	gas	DL	7
			1163m	Ar	IR	2,3,5
b_1	4	OPLA	300(30)	gas	MW	6
			260(30)	gas	MPI	8

$A_0 = 8.846$; $B_0 = 1.032$; $C_0 = 0.925$ LMR[4,9]MW[6]

D_2CF

5*p* Rydberg state C_{2v}
$T_0 = 67186(10)$ gas MPI[8]

4*p* Rydberg state C_{2v}
$T_0 = 63195(10)$ gas MPI[8] $4p-\tilde{X}$ 154–159 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_2 s-stretch	2190(20)	gas	MPI	8
	2	CF stretch	1513(20)	gas	MPI	8
	3	CD_2 scissors	1076(20)	gas	MPI	8
b_1	4	OPLA	1004(20)	gas	MPI	8

3*p* Rydberg state C_{2v}
$T_0 = 52786(10)$ gas MPI[8] $3p-\tilde{X}$ 167–193 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_2 s-stretch	2176(20)	gas	MPI	8
	2	CF stretch	1504(20)	gas	MPI	8
	3	CD_2 scissors	1080(20)	gas	MPI	8
b_1	4	OPLA	976(10)	gas	MPI	8

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF stretch	1191m	Ar	IR	2,3,5
	3	CD_2 scissors	1013w	Ar	IR	5
b_1	4	OPLA	170(30)	gas	MPI	8

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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	2,6
	3	CCl stretch	827s	Ar	IR	1,2,6
			827	Kr	IR	6
			829	Xe	IR	6
b_1	4	OPLA	402s	Ar	IR	1,2,6
			395	Kr	IR	6
			389	Xe	IR	6

$A_0 = 9.152(3)$; $B_0 = 0.532$; $C_0 = 0.502$ 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	1,2,6
			791	Kr	IR	6
			793	Xe	IR	6
b_1	4	OPLA	291m	Ar	IR	1,2

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H_2NS

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_1	4	OPLA	325T	gas	MW	1

$A_0 = 11.123(5)$; $B_0 = 0.538$; $C_0 = 0.513$ MW[1]

D_2NS

$\tilde{X}\,^2B_1$ C_{2v}
$A_0 = 5.605$; $B_0 = 0.466$; $C_0 = 0.430$ MW[1]

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$HOOH^+$

$\tilde{C}$ C_2
$T_0 = 49000(500)$ gas PE[1–3]

$\tilde{B}\,^2A$ C_2
$T_0 = 32430(220)$ gas PE[1–3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	2	OO stretch	1100(50)	gas	PE	3

$\tilde{A}\,^2A$ C_2
$T^a = 16070(500)$ gas PE[1–3]

$\tilde{X}\,^2B$ C_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a		Deformation	1080(50)	gas	PE,PI	2–4

[a] From vertical ionization potential. The first ionization potential of HOOH is taken to equal 10.63 eV, from the photoionization study of Ref. 4.

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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	3,16,24
			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.

References

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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
			2553.8	Ar	IR	18
	2	Deformation	883	gas	IR	3
			880.3	Ar	IR	18
	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
			2556.6	Ar	IR	18
	6	Deformation	882.0	gas	IR	1,3

$A_0 = 4.899$; $B_0 = 0.233$; $C_0 = 0.232$ MW[4,8,9,12,17]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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$HFFH^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_u	5	HF a-stretch	3064.7	Ne	IR	1

$DFFD^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_u	5	DF a-stretch	2287.6	Ne	IR	1

Reference

[1] C. L. Lugez, M. E. Jacox, and R. D. Johnson III, J. Chem. Phys. **110**, 5037 (1999).

$HClClH^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_u	5	HCl a-stretch	2704.1	Ne	IR	1

$DClClD^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_u	5	DCl a-stretch	1962.2	Ne	IR	1

Reference

[1] D. Forney, M. E. Jacox, and W. E. Thompson, J. Chem. Phys. **103**, 1755 (1995).

$HBrBrH^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_u	5	HBr a-stretch	2440.3	Ne	IR	1

$DBrBrD^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_u	5	DBr a-stretch	1756.4	Ne	IR	1

Reference

[1] C. L. Lugez, M. E. Jacox, and W. E. Thompson, J. Chem. Phys. **105**, 3901 (1996).

$HIIH^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_u	5	HI a-stretch	2143.0	Ne	IR	1

$DIID^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_u	5	DI a-stretch	1537.0	Ne	IR	1

Reference

[1] C. L. Lugez, M. E. Jacox, and W. E. Thompson, J. Chem. Phys. **105**, 3901 (1996).

HXeOH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	XeH stretch	1577.6	Xe	IR	1

DXeOD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	XeD stretch	1141.2	Xe	IR	1

Reference

[1] M. Pettersson, L. Khriachtchev, J. Lundell, and M. Räsänen, J. Am. Chem. Soc. **121**, 11904 (1999).

HXeSH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		XeH stretch	1118.6	Xe	IR	1,2

DXeSD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		XeD stretch	832.8	Xe	IR	2

References

[1] L. Khriachtchev, M. Pettersson, E. Isoniemi, and M. Räsänen, J. Chem. Phys. **108**, 5747 (1998).
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8.6. Four-Atomic Monohydrides

LiCCH

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	5	Deformation	136T	gas	MW	2

$B_0 = 0.352$ MW[1,2]

LiCCD

$\tilde{X}$ $C_{\infty v}$
$B_0 = 0.321$ MW[1,2]

References

[1] D. B. Grotjahn, A. J. Apponi, M. A. Brewster, J. Xin, and L. M. Ziurys, Angew. Chem. **110**, 2824 (1998); Angew. Chem. Int. Ed. Engl. **37**, 2678 (1998).
[2] A. J. Apponi, M. A. Brewster, and L. M. Ziurys, Chem. Phys. Lett. **298**, 161 (1998).

NaCCH

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	5	Deformation	102T	gas	MW	1

$B_0 = 0.150$ MW[1]

NaCCD

$\tilde{X}\,^1\Sigma$ $C_{\infty v}$
$B_0 = 0.139$ MW[1]

Reference

[1] M. A. Brewster, A. J. Apponi, J. Xin, and L. M. Ziurys, Chem. Phys. Lett. **310**, 411 (1999).

KCCH

$\tilde{X}$ $C_{\infty v}$ Structure: MW[1,2]
$B_0 = 0.099$ MW[1,2]

KCCD

$\tilde{X}$ $C_{\infty v}$
$B_0 = 0.092$ MW[1,2]

References

[1] J. Xin and L. M. Ziurys, Astrophys. J. **501**, L151 (1998).
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$YbCCH^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	5	YbCC bend	97(5)	gas	MPI	1

Reference

[1] H.-P. Loock, A. Bérces, B. Simard, and C. Linton, J. Chem. Phys. **107**, 2720 (1997).

MgCCH

$\tilde{A}\,^2\Pi$ $C_{\infty v}$
$T_0 = 22807$ gas LF[1,3] $\tilde{A}-\tilde{X}$ 415–440 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		MgC stretch	552	gas	LF	1

$A = 36.4$ gas LF[1]
$B_0 = 0.175$ gas LF[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	CC stretch	1984.2	Ar	IR	2
	3	MgC stretch	496(2)	gas	LF	3
			491.8	Ar	IR	2
Π	4	HCC bend	660.8	Ar	IR	2
	5	MgCC bend	143(2)	gas	LF	3

$B_0 = 0.166$ MW[4]

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	2
	3	MgC stretch	485.1	Ar	IR	2

References

[1] G. K. Corlett, A. M. Little, and A. M. Ellis, Chem. Phys. Lett. **249**, 53 (1996).
[2] C. A. Thompson and L. Andrews, J. Am. Chem. Soc. **118**, 10242 (1996).
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CaCCH

$\tilde{C}\,^2\Delta$ $C_{\infty v}$
$T_0 = 21900$T gas LF[9] $\tilde{C}-\tilde{X}$ 440–452 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		HCC deform.	573(5)	gas	LF	9
		CaC stretch	394(5)	gas	LF	9
		CaCC deform.	99(5)	gas	LF	9

$\tilde{B}\,^2\Sigma^+$ $C_{\infty v}$
$T_0 = 16600$T gas LF[5]

$\tilde{A}\,^2\Pi$ $C_{\infty v}$
$T_0 = 15525.393$ gas LF[1–3,5–8,10] $\tilde{A}-\tilde{X}$ 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]
$\epsilon_4\omega_4 = 1.85(4)$ gas LF[10]
$\epsilon_5\omega_5 = 3.528(14)$ 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	397.40	gas	LF	1,8
Π	5	CaCC bend	102.94	gas	LF	6

$B_0 = 0.113$ LF[2,3,5] MW^4

References

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[10] M. Li and J. A. Coxon, J. Mol. Spectrosc. **196**, 14 (1999).

SrCCH

$\tilde{B}'\,^2\Delta$ $C_{\infty v}$
$T_0 \leqslant 21129.6$ gas LF[3] $\tilde{B}'-\tilde{X}$ 457–475 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	SrC stretch	339	gas	LF	3

$A = 106$ gas LF[3]

$\tilde{A}\,^2\Pi$ $C_{\infty v}$
$T_0 = 14176(10)$ 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

SrCCD

$\tilde{B}'\,^2\Delta$ $C_{\infty v}$
$T_0 \leqslant 21103.6$ gas LF[3] $\tilde{B}'-\tilde{X}$ 457–474 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	SrC stretch	334	gas	LF	3

$A = 104$ gas LF[3]

References

[1] A. M. R. P. Bopegedera, C. R. Brazier, and P. F. Bernath, Chem. Phys. Lett. **136**, 97 (1987).
[2] B. P. Nuccio, A. J. Apponi, and L. M. Ziurys, Chem. Phys. Lett. **247**, 283 (1995).
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PdCCH

$\tilde{A}$
$T_0 = 2820(1210)$ gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	CC stretch	1720(170)	gas	PE	1

Reference

[1] V. D. Moravec and C. C. Jarrold, J. Chem. Phys. **112**, 792 (2000).

YbCCH

$\tilde{A}\,^2\Pi_{3/2}$ $C_{\infty v}$
$T_0 = 18250(5)$ gas LF,MPI[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	5	YbCC bend	99(5)	gas	MPI	1

$\tilde{A}\,^2\Pi_{1/2}$ $C_{\infty v}$
$T_0 = 16850(5)$ gas LF,MPI[1] $\tilde{A}-\tilde{X}$ 587–594 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	5	YbCC bend	103(5)	gas	MPI	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	YbC stretch	328(20)	gas	LF	1
Π	5	YbCC bend	96(10)	gas	MPI	1

YbCCD

$\tilde{A}\,^2\Pi_{3/2}$ $C_{\infty v}$
$T_0 = 18250(5)$ gas LF,MPI[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	5	YbCC bend	93(5)	gas	MPI	1

$\tilde{A}\,^2\Pi_{1/2}$ $C_{\infty v}$
$T_0 = 16850(5)$ gas LF,MPI[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	5	YbCC bend	99(5)	gas	MPI	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	5	YbCC bend	94(5)	gas	LF,MPI	1

Reference

[1] H.-P. Loock, A. Bérces, B. Simard, and C. Linton, J. Chem. Phys. **107**, 2720 (1997).

$PdCCH^-$

Threshold for electron detachment from ground-state $PdCCH^-$ = 15980(240) gas PE[1]

Reference

[1] V. D. Moravec and C. C. Jarrold, J. Chem. Phys. **112**, 792 (2000).

HBeCN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CN stretch	2202.8	Ar	IR	1
	2	BeH stretch	2128.6	Ar	IR	1
	3	BeC stretch	800.1	Ar	IR	1
	4	H deformation	530.1	Ar	IR	1

DBeCN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CN stretch	2194.2	Ar	IR	1
	2	BeD stretch	1642.1	Ar	IR	1
	3	BeC stretch	750.9	Ar	IR	1
	4	H deformation	436.1 431.5	Ar	IR	1

Reference

[1] D. V. Lanzisera and L. Andrews, J. Am. Chem. Soc. **119**, 6392 (1997).

HBeNC

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	BeH stretch	2153.2	Ar	IR	1
	2	NC stretch	2085.7	Ar	IR	1
	3	BeN stretch	912.4	Ar	IR	1
	4	H deformation	525.4 521.7	Ar	IR	1

DBeNC

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NC stretch	2098.6	Ar	IR	1
	2	BeD stretch	1631.3	Ar	IR	1
	3	BeN stretch	895.6	Ar	IR	1
	4	D deformation	422.1 418.0	Ar	IR	1

Reference

[1] D. V. Lanzisera and L. Andrews, J. Am. Chem. Soc. **119**, 6392 (1997).

HBCC

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BH stretch	2763.2	Ar	IR	2
	2	C≡C stretch	1995.3	Ar	IR	1,2

DBCC

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BD stretch	2173.3	Ar	IR	1
	2	C≡C stretch	1907.7	Ar	IR	1,2

References

[1] L. Andrews, P. Hassanzadeh, J. M. L. Martin, and P. R. Taylor, J. Phys. Chem. **97**, 5839 (1993).
[2] L. Andrews, D. V. Lanzisera, P. Hassanzadeh, and Y. Hannachi, J. Phys. Chem. A **102**, 3259 (1998).

HBCN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	BH stretch	2664.8	Ar	IR	1
	2	CN stretch	2108.0	Ar	IR	1
	3	BC stretch	938.4	Ar	IR	1

DBCN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CN stretch	1971.2	Ar	IR	1
	3	BC stretch	908.6	Ar	IR	1

Reference

[1] D. V. Lanzisera, L. Andrews, and P. R. Taylor, J. Phys. Chem. A **101**, 7134 (1997).

HBNC

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	NC stretch	1952.2	Ar	IR	1
	3	BN stretch	1046.4	Ar	IR	1

DBNC

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	3	BN stretch	1024.7	Ar	IR	1

Reference

[1] D. V. Lanzisera, L. Andrews, and P. R. Taylor, J. Phys. Chem. A **101**, 7134 (1997).

cyc-HB(CN)

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	BH stretch	2708.6	Ar	IR	1
			1081.0	Ar	IR	1
			736.8	Ar	IR	1

cyc-DB(CN)

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	BD stretch	2037.9	Ar	IR	1
			1042.7	Ar	IR	1
			737.4T	Ar	IR	1

Reference

[1] D. V. Lanzisera, L. Andrews, and P. R. Taylor, J. Phys. Chem. A **101**, 7134 (1997).

HC_3

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

$T_0 = 23171$ gas MPI[8] $\tilde{C}-\tilde{X}$ 424–432 nm

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

$T_0 = 20538$ gas MPI[8] $\tilde{B}-\tilde{X}$ 454–487 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	4	CCH bend	783.5	gas	MPI	8
	5	C_3 bend	493	gas	MPI	8

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

$T_0 = 19187$ gas MPI[8] $\tilde{A}-\tilde{X}$ 445–521 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	2800	gas	MPI	8
	2		1836	gas	MPI	8
	3		1091	gas	MPI	8
	4	CCH bend	881.3	gas	MPI	8
	5	C_3 bend	460	gas	MPI	8

$A \cong 19.2$ MPI[8]

$\tilde{X}\,^2\Pi_{1/2}$ $C_{\infty v}$ 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	CH 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.

References

[1] M. E. Jacox and D. E. Milligan, Chem. Phys. **4**, 45 (1974).
[2] C. A. Gottlieb, J. M. Vrtilek, E. W. Gottlieb, P. Thaddeus, and A. Hjalmarson, Astrophys. J. **294**, L55 (1985).
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[8] H. Ding, T. Pino, F. Güthe, and J. P. Maier, J. Chem. Phys. **115**, 6913 (2001).

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

$A_{eff} = 72.4$ MW[3]
$B_0 = 0.181$ MW[2,3]

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

References

[1] D. Han, C. M. L. Rittby, and W. R. M. Graham, J. Chem. Phys. **106**, 6222 (1997).
[2] A. J. Apponi, M. C. McCarthy, C. A. Gottlieb, and P. Thaddeus, Astrophys. J. **536**, L55 (2000).
[3] M. C. McCarthy, A. J. Apponi, C. A. Gottlieb, and P. Thaddeus, J. Chem. Phys. **115**, 870 (2001).

cyc-HSi_3

$\tilde{X}\,^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3		398(20)	gas	PE	1

Reference

[1] C. Xu, T. R. Taylor, G. R. Burton, and D. M. Neumark, J. Chem. Phys. **108**, 7645 (1998).

cyc-HSi_3^-

Threshold for electron detachment from ground-state *cyc*-HSi_3^- = 20410(80) gas PE[1]

Reference

[1] C. Xu, T. R. Taylor, G. R. Burton, and D. M. Neumark, J. Chem. Phys. **108**, 7645 (1998).

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.[4,11] 254-nm irradiation of HCCN isolated in an argon matrix results in photoisomerization to HCNC.[11]

$\tilde{X}\,^3\Sigma^-$ $C_{\infty v}$[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
			3229.4s	Ar	IR	4,11
			3213.3	N_2	IR	11
	2	CCN a-stretch	1734.9s	Ar	IR	4,11
			1750.3	N_2	IR	11
	3	CCN s-stretch	1178.6wm	Ar	IR	4,11
			1189.2	N_2	IR	11
Π	4	CCN deform.	383(20)	gas	CC,MW	8,9
	5	H deform.	128.91	gas	MW,CC,LMR	9,12,14

$B_0 = 0.366$ MW[5,7,9]LMR[14]

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	2436.37	gas	LD	10
			2424.0ms	Ar	IR	4,11
			2432.3	N_2	IR	11
	2	CCN a-stretch	1729.0s	Ar	IR	4,11
			1739.5	N_2	IR	11
	3	CCN s-stretch	1149.2wm	Ar	IR	11
			1148.5	N_2	IR	11
Π	4	CCN deform.	367(15)	gas	MW	9
	5	D deform.	74.84	gas	MW,LD,LMR	9,10,13

$B_0 = 0.330$ MW[6,9]LMR[13]

[a]Quasi-linear,[6,7] with barrier to linearity of 256 for HCCN[9,12,15] and of 229 for DCCN.[10,15]

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[12] J.-X. Han, P. Y. Hung, J. DeSain, W. E. Jones, and R. F. Curl, J. Mol. Spectrosc. **198**, 421 (1999).
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[15] P. Y. Hung, F. Sun, N. T. Hunt, L. A. Burns, and R. F. Curl, J. Chem. Phys. **115**, 9331 (2001).

HCNC

In an argon matrix, absorption occurs between 200 and 240 nm, with maximum near 45900 (218 nm).[1]

$T_0 = 32150$ Ar AB[1] 270–311 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		NC stretch	1950T	Ar	AB	1
			400T	Ar	AB	1

In an argon matrix, weak absorption is observed between 600 and 1100 nm, with maximum near 11700 (855 nm) and a band spacing of approximately 520. Irradiation at wavelengths longer than 700 nm leads to isomerization to *cyc*-HC=NC:.[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	2834.5wm	Ar	IR	1
			2852.8	N_2	IR	1
	2	N=C stretch	1859.5vs	Ar	IR	1
			1874.2	N_2	IR	1
	3	C–N stretch	1173.5m	Ar	IR	1
			1182.9	N_2	IR	1
	4	HCN bend	1080.5w	Ar	IR	1
			1090.9	N_2	IR	1

DCNC

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CD stretch	2110.9wm	Ar	IR	1
			2124.8	N_2	IR	1
	2	N=C stretch	1856.4vs	Ar	IR	1
			1871.2	N_2	IR	1
	3	C–N stretch	1082.9w	Ar	IR	1
			1091.6	N_2	IR	1
	4	DCN bend	904.5wm	Ar	IR	1
			911.2	N_2	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, and K. Rademacher, Chem. Eur. J. **4**, 1957 (1998).

cyc-HC=NC:

In an argon matrix, unstructured absorption occurs between 240 and 300 nm, with a maximum near 37900 (264 nm).[1]

In an argon matrix, irradiation at wavelengths between ~350 and 450 nm leads to isomerization to HCCN.[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	3140.2wm	Ar	IR	1
			3154.4	N_2	IR	1
	2	C=N stretch	1571.0wm	Ar	IR	1
			1573.3	N_2	IR	1
	3		1290.5s	Ar	IR	1
			1289.6	N_2	IR	1
	4		1009.2m	Ar	IR	1
			1018.2	N_2	IR	1
	5		828.6vs	Ar	IR	1
			843.1	N_2	IR	1
a''	6	H–CC OPLA	895.7w	Ar	IR	1
			903.2	N_2	IR	1

cyc-DC=NC:

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CD stretch	2365.8wm	Ar	IR	1
			2376.3	N_2	IR	1
	2	C=N stretch	1532.1wm	Ar	IR	1
			1533.3	N_2	IR	1
	3		1268.5vs	Ar	IR	1
			1268.9	N_2	IR	1
	4		957.9s	Ar	IR	1
			964.5	N_2	IR	1
	5	DCN deform.	668.2s	Ar	IR	1
			677.5	N_2	IR	1
a''	6	D–CC OPLA	829.3wmT	Ar	IR	1
			843.1T	N_2	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, and K. Rademacher, Chem. Eur. J. **4**, 1957 (1998).

HCNSi

In an argon matrix,[1] irradiation at wavelengths longer than 700 nm results in photoisomerization to *cyc*-(HCSiN).

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	2753.5wm	Ar	IR	1
	2	CN stretch	1538.1wm	Ar	IR	1
	3	CH deform.	977.0vs	Ar	IR	1
	4	SiN stretch	734.8w	Ar	IR	1

DCNSi

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CD stretch	2059.0w	Ar	IR	1
	2	CN stretch	1485.9s	Ar	IR	1
	3	CD deform.	854.7vs	Ar	IR	1
	4	SiN stretch	665.3wm	Ar	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, H. Egenolf, and J. Glatthaar, Eur. J. Org. Chem. **1998**, 1307.

cyc-(HCSiN)

In an argon matrix,[1] irradiation at wavelengths longer than 395 nm or with a 366 nm laser leads to photoisomerization to HSiNC.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	2974.2m	Ar	IR	1
	2	CN stretch	1466.2wm	Ar	IR	1
	3	CH deform.	1124.7vs	Ar	IR	1
	4	SiC stretch	769.8vs	Ar	IR	1
	5	Ring deform.	635.5vs	Ar	IR	1
a''	6	CH deform.	820.6vs	Ar	IR	1

cyc-(DCSiN)

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CN stretch	1452.2wm	Ar	IR	1
	3	CD deform.	944.0wm	Ar	IR	1
	4	SiC stretch	718.3m	Ar	IR	1
	5	Ring deform.	591.6vs	Ar	IR	1
a''	6	CD deform.	634.1w	Ar	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, H. Egenolf, and J. Glatthaar, Eur. J. Org. Chem. **1998**, 1307.

HSiNC

In an argon matrix,[1] irradiation at 254 nm leads to photoisomerization to HSiCN.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NC stretch	2039.5s	Ar	IR	1
	2	SiH stretch	2017.8vs	Ar	IR	1
	3	SiH deform.	867.9m	Ar	IR	1
	4	SiN stretch	622.0m	Ar	IR	1

DSiNC

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NC stretch	2035.9vs	Ar	IR	1
	2	SiD stretch	1470.1m	Ar	IR	1
	3	SiD deform.	662.6m	Ar	IR	1
	4	SiN stretch	607.4wm	Ar	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, H. Egenolf, and J. Glatthaar, Eur. J. Org. Chem. **1998**, 1307.

HSiCN

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CN stretch	2142.7s	Ar	IR	1
	2	SiH stretch	2026.7vs	Ar	IR	1
	3	SiH deform.	826.4vs	Ar	IR	1
	4	SiC stretch	563.5wm	Ar	IR	1

DSiCN

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CN stretch	2143.2m	Ar	IR	1
	2	SiD stretch	1470.0vs	Ar	IR	1
	3	SiD deform.	642.1m	Ar	IR	1
	4	SiC stretch	547.3wm	Ar	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, H. Egenolf, and J. Glatthaar, Eur. J. Org. Chem. **1998**, 1307.

HCCP

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

$B_0 = 0.188$ MW[1]

DCCP

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

$B_0 = 0.171$ MW[1]

Reference

[1] I. K. Ahmad, H. Ozeki, and S. Saito, J. Chem. Phys. **107**, 1301 (1997).

HCBF

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3261.7	Ar	IR	1
	2	B=C stretch	1822.3	Ar	IR	1

DCBF

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2468.5	Ar	IR	1
	2	B=C stretch	1786.8	Ar	IR	1

Reference

[1] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **104**, 9295 (2000).

HCBCl

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3251.2	Ar	IR	1
	2	B=C stretch	1691.1	Ar	IR	1

DCBCl

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2464.1	Ar	IR	1
	2	B=C stretch	1644.3	Ar	IR	1

Reference

[1] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **104**, 9295 (2000).

HCBBr

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3248.2	Ar	IR	1
	2	B=C stretch	1665.1	Ar	IR	1

DCBBr

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2461.9	Ar	IR	1
	2	B=C stretch	1616.3	Ar	IR	1

Reference

[1] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **104**, 9295 (2000).

HCCO

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

$T_0 = 33464.75(5)$ gas PF[6,7]LF[8,9] $\tilde{B}-\tilde{X}$ 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	7–9
Π	4	HCC deform. ($^2\Sigma$)	750.7	gas	LF	9
		($^2\Sigma$)	564.3	gas	LF	9
	5	CCO deform. ($^2\Sigma$)	382.0	gas	LF	9
		($^2\Sigma$)	346.6	gas	LF	9

$A_{eff} = -46.74(3)$ LF[9]
$B_0 = 0.324$ PF[7]LF[8,9]

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]
Barrier to linearity between 700 and 900 PE[10]

DCCO

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

$T_0 = 33448.99(5)$ gas LF[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	4	DCC deform. ($^2\Sigma$)	652.5	gas	LF	9
		($^2\Sigma$)	465.6	gas	LF	9
	5	CCO deform. ($^2\Sigma$)	380.0	gas	LF	9

$A_{eff} = -37.10(4)$ LF[9]
$B_0 = 0.294$ LF[9]

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

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[1] Y. Endo and E. Hirota, J. Chem. Phys. **86**, 4319 (1987).
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[10] B. Schäfer-Bung, B. Engels, T. R. Taylor, D. M. Neumark, P. Botschwina, and M. Perić, J. Chem. Phys. **115**, 1777 (2001).

HNCN

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

$T_0 = 31521$ gas AB[2,3]PF[8] $\tilde{C}-\tilde{X}$ 289–317 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		NCN s-stretch	1024	gas	AB,PF	2,3,8

$\tilde{B}\,^2A'$ C_s Structure: AB[1]

$T_0 = 28994.1$ gas AB[1]LF[4]PF[8] $\tilde{B}-\tilde{X}$ 344–364 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a''	6	NCN deform.	560(10)	gas	PF	8

$\tau_0 = 20(5)$ ns gas LF[4]
$A_0 = 22.30$; $B_0 = 0.376$; $C_0 = 0.369$ AB[1]LF[4]

$\tilde{X}\,^2A''$ 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	6
	2	NCN a-stretch	1879(106)	gas	PE	7
			1843s	Ar	IR	6
	3	NCN s-stretch	1049(162)	gas	PE	7
			1146vs	Ar	IR	6
a''	6	NCN deform.	440T	gas	LF	4

$A_0=21.18(11)$; $B_0=0.370$; $C_0=0.363$ AB[1]LF[4]MW[5]

DNCN

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

$T_0=31506$ gas AB[2]PF[8] $\tilde{C}-\tilde{X}$ 307–317 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		NCN s-stretch	1036	gas	PF	8

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	NCN a-stretch	1879(106)	gas	PE	7
	3	NCN s-stretch	1049(162)	gas	PE	7

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HCNN

$\tilde{B}$

$T_0=30500$ 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

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

$T_0=4830(720)$ gas PE[7]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	3233.7wm	Ar	IR	3,6
			3229m	N_2	IR	3
	2	CNN a-stretch	1780(77)	gas	PE	7
			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			
	5	CNN deform.	485(70)	gas	PE	7

DCNN

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

$T_0=4840(720)$ gas PE[7]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CNN a-stretch	1790(74)	gas	PE	7
			1771vs	Ar	IR	3
		D deform.	725vs	Ar	IR	3
	5	CNN deform.	460(70)	gas	PE	7

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$HCCO^-$

Threshold for electron detachment from ground-state $HCCO^-=18860(65)$ gas PE[1,2]

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$HNCN^-$

Threshold for electron detachment from ground-state $HNCN^- = 7330(20)$ gas PE[1]

$DNCN^-$

Threshold for electron detachment from ground-state $DNCN^- = 7330(20)$ gas PE[1]

Reference

[1] E. P. Clifford, P. G. Wenthold, W. C. Lineberger, G. A. Petersson, and G. B. Ellison, J. Phys. Chem. A **101**, 4338 (1997).

$HCNN^-$

Threshold for electron detachment from ground-state $HCNN^- = 13600(50)$ gas PE[1]

$DCNN^-$

Threshold for electron detachment from ground-state $DCNN^- = 13540(50)$ gas PE[1]

Reference

[1] E. P. Clifford, P. G. Wenthold, W. C. Lineberger, G. A. Petersson, K. M. Broadus, S. R. Kass, S. Kato, C. H. DePuy, V. M. Bierbaum, and G. B. Ellison, J. Phys. Chem. A **102**, 7100 (1998).

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

$T_0 = 32449(20)$ gas AB^4PF^{18} $\tilde{A}-\tilde{X}$ 228–282 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	HNC bend	1192(10)	gas	PF	18
	4	NC stretch	1034(20)	gas	PF	18
	5	NCO bend	599(7)	gas	PF	18

$A \cong 4.37$; $B \cong 0.388$; $C \cong 0.357$ 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			
			3514.7	Kr	IR	17
			3500.6			
			3485.2	Xe	IR	17
			3483.0			
			3479.9			
	2	NCO a-stretch	2268.89vs	gas	IR,Ra	1,2,9,10,16
			2259.0vs	Ar	IR	12,13
			2261.6	Kr	IR	17
			2254.4	Xe	IR	17
	3	NCO s-stretch	1327vw	gas	IR,Ra	1,2,16
	4	HNC, NCO bend	776.62wm	gas	IR	6
			769.8wm	Ar	IR	12,13
			763.6	Kr	IR	17
			765.1	Xe	IR	17
			760.3			
	5	HNC, NCO bend	577.35w	gas	IR	1,2,6
			573.7wm	Ar	IR	12,13
			572.9	Kr	IR	17
			571.3			
			574.2	Xe	IR	17
			570.3			
a''	6	Torsion	656.29	gas	IR	6,11
			695.6 (1-0)	Kr	IR	17
			694.7 (1-0)	Xe	IR	17

$A_0 = 30.638$; $B_0 = 0.369$; $C_0 = 0.364$ MW^7IR^{14}

DNCO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ND stretch	2637.20	gas	IR	8
			2606.9m	Ar	IR	12
	2	NCO a-stretch	2235vs	gas	IR	3
			2231.0vs	Ar	IR	12
	3	NCO s-stretch	1310	gas	IR	3
	4	DNC, NCO bend	578.6w	Ar	IR	12
	5	DNC, NCO bend	475.4w	Ar	IR	12
a''	6	Torsion	602.9	gas	IR	3

$A_0 = 17.09$; $B_0 = 0.344$; $C_0 = 0.336$ MW^7

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HOCN

$\tilde{X}$ C_s Structure: MO[2–4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3610	Ne	IR	5
			3569.6s	Ar	IR	1,6
			3536	Kr	IR	8
			3506s	N_2	IR	1
	2	C≡N stretch	2302	gas	IR	9
			2294	Ne	IR	5
			2286.3vs	Ar	IR	1,6,7
			2291.1	Kr	IR	8
			2294s	N_2	IR	1
	3	OH deform.	1227	Ne	IR	5
			1227.9s	Ar	IR	1,6,7
			1220.6	Kr	IR	8
			1241m	N_2	IR	1
	4	C–O stretch	1082	Ne	IR	5
			1081.3m	Ar	IR	1,6,7
			1088.6	Kr	IR	8
			1098s	N_2	IR	1
	5	OCN deform.	460wm	N_2	IR	1

DOCN

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2635.0vs	Ar	IR	1,6
			2590sh	N_2	IR	1
	2	C≡N stretch	2284.6vs	Ar	IR	1,6
			2292s	N_2	IR	1
	3	OD deform.	1077.8ms	Ar	IR	1,6
			1093m	N_2	IR	1
	4	C–O stretch	949.4m	Ar	IR	1,6
			957m	N_2	IR	1
	5	OCN deform.	437wm	N_2	IR	1

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HCNO

$\tilde{A}$ C_s

$T_0 \leqslant 35053$ gas AB[8] $\tilde{A}-\tilde{X}$ 244–285 nm Underlying absorption continuum, with increasing intensity at shorter wavelengths.[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Bend	345(5)	gas	AB	8

$\tilde{X}$ $C^a_{\infty v}$ Structure: MW,IR[13]MO[15]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3336.12	gas	IR	1,10,18
			3338	Ne	IR	14
			3317.2s	Ar	IR	17
			3311	N_2	IR	17
	2	CNO a-stretch	2195.76	gas	IR	1,2,10,18
			2200	Ne	IR	14
			2192.7vs	Ar	IR	17
			2200	N_2	IR	17
	3	CNO s-stretch	1254.23	gas	IR	1,2,10,18
			1250	Ne	IR	14
			1244.1m	Ar	IR	17
			1232	N_2	IR	17
Π	4	CNO bend	537.18	gas	IR	1,2,9,16 18,19
			539	Ne	IR	14
			538.2w 536.9w	Ar	IR	17
			528	N_2	IR	17
	5	HCN bend	224.10	gas	IR	9,11,18, 19
			560	Ne	IR	17
			566.6m	Ar	IR	17
			582	N_2	IR	17

$B_0 = 0.383$ MW[3,4]

DCNO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2620.73	gas	IR	7
			2612.7vs	Ar	IR	17
	2	CNO a-stretch	2070.92	gas	IR	12
			2063.2s	Ar	IR	17
	3	CNO s-stretch	1254	gas	IR	2,6
			1218.5m	Ar	IR	17
Π	5	DCN bend	162.64	gas	IR	9,19
			418.5wm	Ar	IR	17

$B_0 = 0.343$ $MW^{3,5}IR^{7}$

[a]Quasilinear. See discussion in Refs. 13, 15, and 17.

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HSCN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	SH stretch	2581.0	Ar	IR	1
			2580.2	N_2	IR	1
	2	CN stretch	2182.3	Ar	IR	1
			2182.3	N_2	IR	1
		HSC bend	959.7	Ar	IR	1
			960.9	N_2	IR	1

DSCN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CN stretch	2183.0	Ar	IR	1
			2183.8	N_2	IR	1
	2	SD stretch	1874.0	Ar	IR	1
			1873.6	N_2	IR	1
		DSC bend	692.8	Ar	IR	1
			688.5	N_2	IR	1

Reference

[1] M. Wierzejewska and Z. Mielke, Chem. Phys. Lett. **349**, 227 (2001).

HSNC

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	NC stretch	2064.2T	Ar	IR	1
			2065.9T	N_2	IR	1

DSNC

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	NC stretch	2063.5T	Ar	IR	1
			2065.4T	N_2	IR	1

Reference

[1] M. Wierzejewska and Z. Mielke, Chem. Phys. Lett. **349**, 227 (2001).

t-HNNO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH stretch	3254.0wm	Xe	IR	1
	2	NN stretch	1628.9vs	Xe	IR	1
			1627.1			
	3	NO stretch	1296.2m	Xe	IR	1
			1294.5			
	4	HNN bend	1214.7m	Xe	IR	1
			1213.4			
a''	6	Torsion	746.5wm	Xe	IR	1

Reference

[1] S. L. Laursen, A. E. Delia, and K. Mitchell, J. Phys. Chem. A **104**, 3681 (2000).

c-HNNO

In a xenon matrix,[1] irradiation at 700 nm (14290) results in photoisomerization to *t*-HNNO.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	NH stretch	3158vw	Xe	IR	1
	2	NN stretch	1623.7s 1622.3	Xe	IR	1
	3	NO stretch	1273.4wm	Xe	IR	1
	4	HNN bend	1166.9wm	Xe	IR	1
a″	6	Torsion	712.1	Xe	IR	1

Reference

[1] S. L. Laursen, A. E. Delia, and K. Mitchell, J. Phys. Chem. A **104**, 3681 (2000).

HFCN

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	CH stretch	3016w	Ar	IR	1,2
	2	C=N stretch	1672s	Ar	IR	1,2
	3	HCF deform.	1233w	Ar	IR	2
	4	CF stretch	1057vs	Ar	IR	1,2
	5	FCN bend	536m	Ar	IR	1,2
a″	6	OPLA	894w	Ar	IR	2

DFCN

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	CD stretch	2252w	Ar	IR	1,2
	2	C=N stretch	1651m	Ar	IR	1,2
	3	CF stretch	1047vs	Ar	IR	1,2
	4	DCF deform.	922w	Ar	IR	2
	5	FCN bend	530wm	Ar	IR	1,2
a″	6	OPLA	735vw	Ar	IR	2

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[2] E. Ya. Misochko, I. U. Goldschleger, A. V. Akimov, and C. A. Wight, J. Am. Chem. Soc. **123**, 5156 (2001).

FCNH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	NH stretch	3405wm	Ar	IR	1
	2	CN stretch	1700s	Ar	IR	1
	3	CF stretch	1172wm	Ar	IR	1
	4	Deformation	905vs	Ar	IR	1
	5	Deformation	595w	Ar	IR	1
a″	6	Torsion	734wm	Ar	IR	1

FCND

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	ND stretch	2532wm	Ar	IR	1
	2	CN stretch	1701vs	Ar	IR	1
	3	CF stretch	1142vs	Ar	IR	1
	4	Deformation	759s	Ar	IR	1
a″	6	Torsion	575wm	Ar	IR	1

Reference

[1] E. Ya. Misochko, I. U. Goldschleger, A. V. Akimov, and C. A. Wight, J. Am. Chem. Soc. **123**, 5156 (2001).

$HAlCl_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	AlH stretch	1968s	Ar	IR	1,2
	2	AlCl s-stretch	481s	Ar	IR	1,2
b_1	4	OPLA	472s	Ar	IR	1,2
b_2	5	AlCl a-stretch	579m	Ar	IR	1,2
	6	H deformation	654vs	Ar	IR	1,2

$DAlCl_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	AlD stretch	1430	Ar	IR	1
	2	AlCl s-stretch	478	Ar	IR	1
b_1	4	OPLA	355	Ar	IR	1
b_2	6	AlCl a-stretch	598	Ar	IR	1

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[2] J. Müller and B. Wittig, Eur. J. Inorg. Chem. **1998**, 1807.

$HAlBr_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	AlH stretch	1952.5	Ar	IR	1
	2	AlBr s-stretch	366.0	Ar	IR	1
b_1	4	OPLA	453.5	Ar	IR	1
b_2	5	HAlBr deform.	634.5	Ar	IR	1
	6	AlBr a-stretch	476.0	Ar	IR	1

Reference

[1] J. Müller and B. Wittig, Eur. J. Inorg. Chem. **1998**, 1807.

$HGaCl_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	GaH stretch	2015.3s	Ar	IR	1,2
	2	$GaCl_2$ s-stretch	414.3wm	Ar	IR	1,2
b_1	4	OPLA	464.3ms	Ar	IR	1,2
b_2	5	H deform.	607.5vs	Ar	IR	1,2
	6	$GaCl_2$ a-stretch	437.3s	Ar	IR	1,2

$DGaCl_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	GaD stretch	1450.2	Ar	IR	1
	2	$GaCl_2$ s-stretch	414.5	Ar	IR	1
b_2	5	Mixed	469.6	Ar	IR	1
	6	Mixed	420.4	Ar	IR	1

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$HGaBr_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	GaH stretch	1991.5s	Ar	IR	1
	2	$GaBr_2$ s-stretch	287.5w	Ar	IR	1
b_1	4	OPLA	445.5wm	Ar	IR	1
b_2	5	HGaBr deform.	597.0vs	Ar	IR	1
	6	$GaBr_2$ a-stretch	333.0m	Ar	IR	1

Reference

[1] J. Müller and H. Sternkicker, J. Chem. Soc., Dalton Trans., 4149 (1999).

$HInCl_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	InH stretch	1846.9	Ar	IR	1
	2	$InCl_2$ s-stretch	369.1	Ar	IR	1
b_1	4	OPLA	402.6	Ar	IR	1
b_2	5	HInCl deform.	469.7	Ar	IR	1
	6	$InCl_2$ a-stretch	358.5	Ar	IR	1

$DInCl_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	InD stretch	1325.6	Ar	IR	1
	2	$InCl_2$ s-stretch	368.8	Ar	IR	1
b_1	4	OPLA	304.8	Ar	IR	1
b_2	5	DInCl deform.	311.2	Ar	IR	1
	6	$InCl_2$ a-stretch	385.1	Ar	IR	1

Reference

[1] H.-J. Himmel, A. J. Downs, and T. M. Greene, J. Am. Chem. Soc. **122**, 922 (2000).

HCOCl

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

$T_0 = 32760$ gas $AB^{5,6}CR^{12}$ $\tilde{A}-\tilde{X}$ 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 = 1642 gas AB^5CR^{12}

$\tilde{X}\,^1A'$ 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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$HCCl_2^+$

A broad, unstructured absorption observed near 250 nm in argon-matrix experiments[2] in which infrared absorptions of $HCCl_2^+$ are prominent has been attributed to an excited state of $HCCl_2^+$ which can undergo proton transfer to the matrix.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	3032.8w	Ar	IR	3,6
	2	CCl stretch	860(30)	gas	PE	4,5
			845w	Ar	IR	3
b_2	5	H deformation	1291m	Ar	IR	1–3,6
	6	CCl stretch	1044s	Ar	IR	1–3,6
			1038	Kr	IR	6

$DCCl_2^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCl stretch	790(30)	gas	PE	4,5
b_2	5	CCl stretch	1122s	Ar	IR	1,2,6
	6	D deformation	864wm	Ar	IR	1,2,6

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$HCClBr^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CCl stretch	994m	Ar	IR	1,2

$DCClBr^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1077s	Ar	IR	1

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HKrCN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	KrH stretch	1497.4	Kr	IR	1

DKrCN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	KrD stretch	1109.0	Kr	IR	1

Reference

[1] M. Pettersson, J. Lundell, L. Khriachtchev, and M. Räsänen, J. Chem. Phys. **109**, 618 (1998).

HXeCN

In a xenon matrix, an unstructured absorption maximum at 42740 (234 nm) has been assigned[3] to HXeCN.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	XeH stretch	1650	Kr	IR	1
			1623.8	Xe	IR	1–3

DXeCN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	XeD stretch	1178.0	Xe	IR	1

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HXeNC

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NC stretch	2048.5	Kr	IR	1
			2043.8	Xe	IR	1
	2	XeH stretch	1878	Kr	IR	1
			1851.0	Xe	IR	1–3

DXeNC

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	XeD stretch	1338.8	Xe	IR	1

References

[1] M. Pettersson, J. Lundell, L. Khriachtchev, and M. Räsänen, J. Chem. Phys. **109**, 618 (1998).
[2] M. Pettersson, L. Khriachtchev, S. Jolkkonen, and M. Räsänen, J. Phys. Chem. A **103**, 9154 (1999).
[3] J. Ahokas, K. Vaskonen, J. Eloranta, and H. Kunttu, J. Phys. Chem. A **104**, 9506 (2000).

t-HONO

$\tilde{B}$

An intense, unstructured absorption between 200 and 275 nm, with a maximum near 46500 (215 nm), has been attributed[13] to HONO.

$\tilde{A}\,^1A''$ C_s
$T_0 = 26034$ gas AB[1–3,6,25] $\tilde{A}-\tilde{X}$ 315–385 nm
Diffuse bands; predissociated into OH+NO.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		NO stretch	1117	gas	AB	6

$\tilde{X}\,^1A'$ C_s Structure: MW[9,11,12]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3590.71m	gas	IR	4,5,8,16,17,21
			3572.6	Ar	IR	24
			3568.5			
			3551.8	Kr	IR	27
			3558	N_2	IR	7
	2	N=O stretch	1699.76s	gas	IR,LS	4,5,8,14
					DL	16–18,23
			1689.1	Ar	IR	10,20,24
			1688.0			
			1684.0	Kr	IR	27
			1684	N_2	IR	7
	3	HON bend	1263.21s	gas	IR,DL	4,5,8,16,17, 19,23,26
			1265.8	Ar	IR	24
			1263.9			
			1265.3	Kr	IR	27
			1298	N_2	IR	7
	4	O–N stretch	790.12s	gas	IR	4,5,8,16
						17,22,26
			800.4	Ar	IR	10,20,24
			796.6			
			794.5	Kr	IR	27
			815	N_2	IR	7
	5	ONO bend	595.6s	gas	IR	4,5,8,17
			608.7	Ar	IR	24
			606.7	Kr	IR	27
			625	N_2	IR	7
a''	6	Torsion	543.0m	gas	IR	4,5,8,17
			549.4	Ar	IR	10,24
			549.1	Kr	IR	27
			583	N_2	IR	7

$A_0 = 3.099$; $B_0 = 0.418$; $C_0 = 0.367$ MW[9,11,15]IR[21]

t-DONO

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

$T_0 = 26050(10)$ gas AB[2,3,6] $\tilde{A}-\tilde{X}$ 315–385 nm

Diffuse bands; predissociated into OD+NO.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		NO stretch	1147(20)	gas	AB	6

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2651.13	gas	IR	4,5,8,17
			2620	N_2	IR	7
	2	N=O stretch	1693.98	gas	IR	4,5,8,17
			1682	N_2	IR	7
	3	DON bend	1012.68	gas	IR	4,5,8,17
			1030	N_2	IR	7
	4	O–N stretch	736.27	gas	IR	4,5,8,17
			769	N_2	IR	7
	5	ONO bend	590.4	gas	IR	4,5,8,17
			618	N_2	IR	7
a''	6	Torsion	416.1	gas	IR	4,8,17
			444	N_2	IR	7

$A_0 = 2.981$; $B_0 = 0.389$; $C_0 = 0.344$ MW[9,11]

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c-HONO

$\tilde{B}$

An intense, unstructured absorption between 200 and 275 nm, with a maximum near 46500 (215 nm), has been attributed[13] to HONO.

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

$T_0 = 26320$ gas AB[1–3,6] $\tilde{A}-\tilde{X}$ 315–385 nm

Diffuse bands; predissociated into OH+NO.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		NO stretch	1107	gas	AB	6

$\tilde{X}\,^1A'$ C_s Structure: MW[10,11]

141(35) higher in energy than *t*-HONO ($\tilde{X}$). MW[12]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3426.20w	gas	IR	4,5,8,16, 17,21
			3412.4	Ar	IR	9,22
			3410.7			
			3399.7	Kr	IR	24
			3410	N_2	IR	7
	2	N=O stretch	1640.52m	gas	IR,LS	4,5,8,14 16,21
			1634.0	Ar	IR	9,19,22
			1632.8			
			1629.0	Kr	IR	24
			1633	N_2	IR	7
	3	HON bend	1315.2	Kr	IR	24
	4	O–N stretch	851.94s	gas	IR,DL	4,5,8, 16–18,20, 23
			853.1	Ar	IR	9,19,22
			850.2			
			851.9	Kr	IR	24
			865	N_2	IR	7
	5	ONO bend	609.0w	gas	IR	8,17
			608	Ar	IR	9,19
			616.6	Kr	IR	24
a''	6	Torsion	638.5m	gas	IR	4,5,8,17
			638.4	Ar	IR	9,19,22
			635.0	Kr	IR	24
			658	N_2	IR	7

$A_0 = 2.805$; $B_0 = 0.439$; $C_0 = 0.379$ MW[10,15]DL[18]IR[21]

c-DONO

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

gas AB[2,3] $\tilde{A}-\tilde{X}$ 315–385 nm

Diffuse bands; predissociated into OD+NO.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	4	O–N stretch	660T	gas	AB	6

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2525	gas	IR	4,5,8
			2518	N_2	IR	7
	2	N=O stretch	1625	gas	IR	5,8
			1612	N_2	IR	7
	3	DON bend	1008	gas	IR	8
	4	O–N stretch	813.50	gas	IR	4,5,8,17
			828	N_2	IR	7
	5	ONO bend	601	gas	IR	8
a''	6	Torsion	508.2	gas	IR	4,8,17
			522	N_2	IR	7

$A_0=2.362$; $B_0=0.430$; $C_0=0.363$ MW[10]

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HNOO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH stretch	3165.5w	Xe	IR	1
	2	HNO bend	1489.8	Ar	IR	1
			1485.5wm	Xe	IR	1
	3	NO stretch	1097.7	Ar	IR	1
			1096.6			
			1092.3vs	Xe	IR	1
	4	OO stretch	1058.0	Ar	IR	1
			1054.5m	Xe	IR	1
a''	6	Torsion	776.3	Ar	IR	1
			764.0ms	Xe	IR	1

Reference

[1] S. L. Laursen, J. E. Grace, Jr., R. L. DeKock, and S. A. Spronk, J. Am. Chem. Soc. **120**, 12583 (1998).

c-HOPO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3550.7	Ar	IR	1
	2	P=O stretch	1252.6	Ar	IR	1
	4	P–O stretch	851.07	gas	DL	2
			841.5	Ar	IR	1
a''	6	Torsion	523.9	Ar	IR	1

$A_0=1.239(3)$; $B_0=0.318$; $C_0=0.254$ DL[2]

c-DOPO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2620.4	Ar	IR	1
	2	P=O stretch	1253.0	Ar	IR	1

References

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HCF_2

$\tilde{F}$ 3*p* Rydberg state C_{2v}
$T_0 = 49312(10)$ gas MPI[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF stretch	1365(8)	gas	MPI	4
	3	CF_2 scissors	660(20)	gas	MPI	4
b_1	4	OPLA	1022(1)	gas	MPI	4

$\tilde{X}$ C_s Structure: ESR[1]MPI[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CF s-stretch	1164s	Ar	IR	2,3
	3	Umbrella	949(10)	gas	MPI	4
a''	5	HCF deform.	1317m	Ar	IR	2,3
	6	CF a-stretch	1173vs	Ar	IR	2,3

Barrier to inversion = 2800(500) gas MPI[4]
$A_0 = 2.242$; $B_0 = 0.368$; $C_0 = 0.320$ MW[5]

DCF_2

$\tilde{F}$ 3*p* Rydberg state C_{2v}
$T_0 = 49323(10)$ gas MPI[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF stretch	1300(21)	gas	MPI	4
	3	CF_2 scissors	650(15)	gas	MPI	4
b_1	4	OPLA	864(2)	gas	MPI	4

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CF s-stretch	1143m	Ar	IR	2,3
	3	Umbrella	794(4)	gas	MPI	4
a''	5	CF a-stretch	1214s	Ar	IR	2,3
	6	DCF deform.	933wm	Ar	IR	2,3

References

[1] R. W. Fessenden and R. H. Schuler, J. Chem. Phys. **43**, 2704 (1965).
[2] T. G. Carver and L. Andrews, J. Chem. Phys. **50**, 5100 (1969).
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$HCCl_2$

3*d* Rydberg state C_{2v}
$T_0 = 54024(10)$ gas MPI[3] $3d-\tilde{X}$ 179–185 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCl_2 s-stretch	845(10)	gas	MPI	3

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a''	5	HCCl deform.	1226m	Ar	IR	1,4
			1222	Kr	IR	4
	6	CCl_2 a-stretch	902vs	Ar	IR	1,4
			896	Kr	IR	4

$DCCl_2$

3*d* Rydberg state C_{2v}
$T_0 = 53980(10)$ gas MPI[3] $3d-\tilde{X}$ 180–185 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCl_2 s-stretch	814(10)	gas	MPI	3

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a''	5	DCCl deform.	974vs	Ar	IR	1,2
	6	CCl_2 a-stretch	814s	Ar	IR	1,2

References

[1] T. G. Carver and L. Andrews, J. Chem. Phys. **50**, 4235 (1969).
[2] E. E. Rogers, S. Abramowitz, M. E. Jacox, and D. E. Milligan, J. Chem. Phys. **52**, 2198 (1970).
[3] G. R. Long and J. W. Hudgens, J. Phys. Chem. **91**, 5870 (1987).
[4] T. D. Fridgen, X. K. Zhang, J. M. Parnis, and R. E. March, J. Phys. Chem. A **104**, 3487 (2000).

HCClBr

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	H deformation	1196m	Ar	IR	1,2
	3	CCl stretch	866s	Ar	IR	1,2

References

[1] T. G. Carver and L. Andrews, J. Chem. Phys. **50**, 4235 (1969).
[2] T. D. Fridgen, X. K. Zhang, J. M. Parnis, and R. E. March, J. Phys. Chem. A **104**, 3487 (2000).

HO_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OH stretch	3361	Ar	IR	1
		OH deform.	1223	Ar	IR	1
		O_3 deform.	566	Ar	IR	1

DO_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OD stretch	2486	Ar	IR	1
		OD deform.	940	Ar	IR	1
		O_3 deform.	552	Ar	IR	1

Reference

[1] B. Nelander, A. Engdahl, and T. Svensson, Chem. Phys. Lett. **332**, 403 (2000); Chem. Phys. Lett. **339**, 295 (2001).

8.7. Four-Atomic Nonhydrides

K_4

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g		Sym. stretch	93.0	Kr	Ra	1
		Deformation	30.0	Kr	Ra	1
b_{3g}		Deformation	61.5	Kr	Ra	1

Reference

[1] A. Kornath, R. Ludwig, and A. Zoermer, Angew. Chem. **110**, 1620 (1998); Angew. Chem. Int. Ed. **37**, 1575 (1998).

Ag_4

Mass-selected Ag_4 trapped in an argon matrix has a prominent fluorescence band at 21830 (458 nm) which is strongest on excitation of the molecule at 24690 (405 nm), 33440 (299 nm), and 36630 (273 nm).

Reference

[1] C. Félix, C. Sieber, W. Harbich, J. Buttet, I. Rabin, W. Schulze, and G. Ertl, Chem. Phys. Lett. **313**, 105 (1999).

Nb_3O^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	Nb_3 deformation	312	gas	TPE	1

Reference

[1] D.-S. Yang, M. Z. Zgierski, D. M. Rayner, P. A. Hackett, A. Martinez, D. R. Salahub, P.-N. Roy, and T. Carrington, Jr., J. Chem. Phys. **103**, 5335 (1995).

V_3O

$\tilde{A}$

$T_0 = 3350(30)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	3		310(15)	gas	PE	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	VO stretch	750(20)	gas	PE	1
	2		415(15)	gas	PE	1
	3		340(15)	gas	PE	1

Reference

[1] S. M. E. Green, S. Alex, N. L. Fleischer, E. L. Millam, T. P. Marcy, and D. G. Leopold, J. Chem. Phys. **114**, 2653 (2001).

Nb_3O

$\tilde{B}$

$T_0 = 6190(120)$ gas PE[2]

$\tilde{A}$

$T_0 = 4300(100)$ gas PE[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NbO stretch	710(15)	gas	PE	2
	3	Nb_3 deformation	320	gas	TPE,PE	1,2

References

[1] D.-S. Yang, M. Z. Zgierski, D. M. Rayner, P. A. Hackett, A. Martinez, D. R. Salahub, P.-N. Roy, and T. Carrington, Jr., J. Chem. Phys. **103**, 5335 (1995).
[2] S. M. E. Green, S. Alex, N. L. Fleischer, E. L. Millam, T. P. Marcy, and D. G. Leopold, J. Chem. Phys. **114**, 2653 (2001).

Ta_3O

$\tilde{B}$

$T_0 = 3870(50)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			250(15)	gas	PE	1

$\tilde{A}$
$T_0 = 3180(40)$ gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	TaO stretch	710(15)	gas	PE	1
	3		225(15)	gas	PE	1

Reference

[1] S. M. E. Green, S. Alex, N. L. Fleischer, E. L. Millam, T. P. Marcy, and D. G. Leopold, J. Chem. Phys. **114**, 2653 (2001).

V_3O^-

Threshold for electron detachment from ground-state $V_3O^- = 9830(65)$ gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	VO stretch	770(20)	gas	PE	1
	3		355(20)	gas	PE	1

Reference

[1] S. M. E. Green, S. Alex, N. L. Fleischer, E. L. Millam, T. P. Marcy, and D. G. Leopold, J. Chem. Phys. **114**, 2653 (2001).

Nb_3O^-

Threshold for electron detachment from ground-state $Nb_3O^- = 11240(50)$ gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3		300(20)	gas	PE	1

Reference

[1] S. M. E. Green, S. Alex, N. L. Fleischer, E. L. Millam, T. P. Marcy, and D. G. Leopold, J. Chem. Phys. **114**, 2653 (2001).

Ta_3O^-

Threshold for electron detachment from ground-state $Ta_3O^- = 12770(80)$ gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3		215(20)	gas	PE	1

Reference

[1] S. M. E. Green, S. Alex, N. L. Fleischer, E. L. Millam, T. P. Marcy, and D. G. Leopold, J. Chem. Phys. **114**, 2653 (2001).

cyc-$(ScN)_2^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}			807.3	Ar	IR	1

Reference

[1] G. V. Chertihin, L. Andrews, and C. W. Bauschlicher, Jr., J. Am. Chem. Soc. **120**, 3205 (1998).

cyc-$(YN)_2^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}			731.5	Ar	IR	1

Reference

[1] G. V. Chertihin, W. D. Bare, and L. Andrews, J. Phys. Chem. A **102**, 3697 (1998).

CAl_3

$\tilde{C}$ D_{3h}
$T_0 = 12260(290)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			440(50)	gas	PE	1

$\tilde{B}$ D_{3h}
$T_0 = 5410(510)$ gas PE[1]

$\tilde{A}$ C_{2v}
$T_0 = 1050(360)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			610(60)	gas	PE	1

$\tilde{X}\,^2B_2$ C_{2v}

Reference

[1] A. I. Boldyrev, J. Simons, X. Li, W. Chen, and L.-S. Wang, J. Chem. Phys. **110**, 8980 (1999).

cyc-$SiAl_3$

$\tilde{C}$ C_{2v}
$T^a = 6540(1030)$ gas PE[1]

$\tilde{B}$ C_{2v}
$T^a = 1210(760)$ gas PE[1]

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

[a]From vertical electron detachment energies.

Reference

[1] X. Li, H.-F. Zhang, L.-S. Wang, A. E. Kuznetsov, N. A. Cannon, and A. I. Boldyrev, Angew. Chem. Int. Ed. **40**, 1867 (2001).

cyc-$GeAl_3$

$\tilde{C}$ C_{2v}
$T^a = 7660(1620)$ gas PE[1]

$\tilde{B}$ C_{2v}
$T^a = 1050(970)$ gas PE[1]

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

[a]From vertical electron detachment energies.

Reference

[1] X. Li, H.-F. Zhang, L.-S. Wang, A. E. Kuznetsov, N. A. Cannon, and A. I. Boldyrev, Angew. Chem. Int. Ed. **40**, 1867 (2001).

cyc-$SnAl_3$

$\tilde{C}$ C_{2v}
$T^a = 8550(580)$ gas PE[1]

$\tilde{B}$ C_{2v}
$T^a = 1780(360)$ gas PE[1]

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

[a]From vertical electron detachment energies.

Reference

[1] X. Li, H.-F. Zhang, L.-S. Wang, A. E. Kuznetsov, N. A. Cannon, and A. I. Boldyrev, Angew. Chem. Int. Ed. **40**, 1867 (2001).

cyc-$PbAl_3$

$\tilde{C}$ C_{2v}
$T^a = 10300(510)$ gas PE[1]

$\tilde{B}$ C_{2v}
$T^a = 4600(180)$ gas PE[1]

$\tilde{A}$ C_{2v}
$T^a = 440(230)$ gas PE[1]

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

[a]From vertical electron detachment energies.

Reference

[1] X. Li, H.-F. Zhang, L.-S. Wang, A. E. Kuznetsov, N. A. Cannon, and A. I. Boldyrev, Angew. Chem. Int. Ed. **40**, 1867 (2001).

cyc-ScC_3

$\tilde{A}$ C_{2v}
$T_0 = 3390(160)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CScC s-stretch	600(50)	gas	PE	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CScC s-stretch	560(30)	gas	PE	1

Reference

[1] L.-S. Wang and X. Li, J. Chem. Phys. **112**, 3602 (2000).

cyc-TiC_3

$\tilde{C}$
$T_0 = 8660(190)$ gas PE[1]

$\tilde{B}$
$T_0 = 6730(190)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			500(60)	gas	PE	1

$\tilde{A}$
$T_0 = 5120(190)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			500(60)	gas	PE	1

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			650(30)	gas	PE	1

Reference

[1] X.-B. Wang, C.-F. Ding, and L.-S. Wang, J. Phys. Chem. A **101**, 7699 (1997).

cyc-VC_3

$\tilde{B}$ C_{2v}
$T_0 = 12180(240)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CVC s-stretch	600(50)	gas	PE	1

$\tilde{A}$ C_{2v}
$T_0 = 2580(160)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CVC s-stretch	450(50)	gas	PE	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CVC s-stretch	600(30)	gas	PE	1

Reference

[1] L.-S. Wang and X. Li, J. Chem. Phys. **112**, 3602 (2000).

cyc-NbC_3

$\tilde{C}$ C_{2v}
$T^a = 12620(230)$ gas PE[1]

$\tilde{B}$ C_{2v}
$T^a = 9710(260)$ gas PE[1]

$\tilde{A}$ C_{2v}
$T^a = 6850(230)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			840(50)	gas	PE	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			610(30)	gas	PE	1

[a]From vertical electron detachment energy.

Reference

[1] H.-J. Zhai, S.-R. Liu, X. Li, and L.-S. Wang, J. Chem. Phys. **115**, 5170 (2001).

cyc-CrC_3

$\tilde{G}$ C_{2v}
$T_0 = 14040(240)$ gas PE[1]

$\tilde{E}$ C_{2v}
$T_0 = 10650(240)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CCrC s-stretch	500(50)	gas	PE	1

$\tilde{D}$ C_{2v}
$T_0 = 7750(160)$ gas PE[1]

$\tilde{C}$ C_{2v}
$T_0 = 3630(160)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CCrC s-stretch	540(30)	gas	PE	1

$\tilde{B}$ C_{2v}
$T_0 = 2500(160)$ gas PE[1]

$\tilde{A}$ C_{2v}
$T_0 = 1210(160)$ gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CCrC s-stretch	560(60)	gas	PE	1

Reference

[1] L.-S. Wang and X. Li, J. Chem. Phys. **112**, 3602 (2000).

cyc-MnC_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CMnC s-stretch	490(20)	gas	PE	1

Reference

[1] L.-S. Wang and X. Li, J. Chem. Phys. **112**, 3602 (2000).

cyc-FeC_3

$\tilde{B}$ C_{2v}
$T_0 = 5490(160)$ gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CFeC s-stretch	500(30)	gas	PE	2

$\tilde{A}$ C_{2v}
$T_0 = 4760(160)$ gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CFeC s-stretch	350(50)T	gas	PE	2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CFeC s-stretch	480(40)	gas	PE	2

References

[1] J. Fan, L. Lou, and L.-S. Wang, J. Chem. Phys. **102**, 2701 (1995).
[2] L.-S. Wang and X. Li, J. Chem. Phys. **112**, 3602 (2000).

cyc-CoC_3

$\tilde{C}$ C_{2v}
$T_0 = 8310T$ gas PE[1]

$\tilde{B}$ C_{2v}
$T_0 = 2420T$ gas PE[1]

$\tilde{A}$ C_{2v}
$T_0 = 1210T$ gas PE[1]

Reference

[1] L.-S. Wang and X. Li, J. Chem. Phys. **112**, 3602 (2000).

cyc-NiC_3

$\tilde{A}$ C_{2v}
$T_0 = 3230T$ gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CNiC s-stretch	480(60)	gas	PE	1

Reference

[1] L.-S. Wang and X. Li, J. Chem. Phys. **112**, 3602 (2000).

Fe_2CO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1897.7	Ar	IR	1,2
			1884	Kr	IR	1

References

[1] C. H. F. Peden, S. F. Parker, P. H. Barrett, and R. G. Pearson, J. Phys. Chem. **87**, 2329 (1983).
[2] M. Zhou, G. V. Chertihin, and L. Andrews, J. Chem. Phys. **109**, 10893 (1998).

cyc-$(ScN)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}			772.2	Ar	IR	1
b_{3u}			672.9	Ar	IR	1

Reference

[1] G. V. Chertihin, L. Andrews, and C. W. Bauschlicher, Jr., J. Am. Chem. Soc. **120**, 3205 (1998).

cyc-$(YN)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}			710.4	Ar	IR	1
b_{3u}			586.9	Ar	IR	1

Reference

[1] G. V. Chertihin, W. D. Bare, and L. Andrews, J. Phys. Chem. A **102**, 3697 (1998).

cyc-$(LaN)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}			652.3	Ar	IR	1
b_{3u}			529.9	Ar	IR	1

Reference

[1] G. V. Chertihin, W. D. Bare, and L. Andrews, J. Phys. Chem. A **102**, 3697 (1998).

cyc-$(TiN)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{1u}			766.3	Ar	IR	1
b_{2u}			680.2	Ar	IR	1

Reference

[1] G. P. Kushto, P. F. Souter, G. V. Chertihin, and L. Andrews, J. Chem. Phys. **110**, 9020 (1999).

cyc-$(ZrN)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{1u}			771.2	Ar	IR	1
			757.2			
b_{2u}			675.2	Ar	IR	1

Reference

[1] G. P. Kushto, P. F. Souter, G. V. Chertihin, and L. Andrews, J. Chem. Phys. **110**, 9020 (1999).

cyc-$(HfN)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{1u}			775.7	Ar	IR	1
b_{2u}			682.7	Ar	IR	1

Reference

[1] G. P. Kushto, P. F. Souter, G. V. Chertihin, and L. Andrews, J. Chem. Phys. **110**, 9020 (1999).

cyc-$(CoN)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}	5		711.1	N_2	IR	1
b_{3u}	6		537.3	N_2	IR	1

Reference

[1] L. Andrews, A. Citra, G. V. Chertihin, W. D. Bare, and M. Neurock, J. Phys. Chem. A **102**, 2561 (1998).

cyc-$(RhN)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			748.1	Ar	IR	1
			756.7	N_2	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **103**, 3410 (1999).

cyc-$(NiN)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}			710.1	Ar	IR	1
			723.3	N_2	IR	1

Reference

[1] L. Andrews, A. Citra, G. V. Chertihin, W. D. Bare, and M. Neurock, J. Phys. Chem. A **102**, 2561 (1998).

Pt_2NN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2132.3	Ar	IR	1
			491.9	Ar	IR	1

Reference

[1] A. Citra, X. Wang, W. D. Bare, and L. Andrews, J. Phys. Chem. A **105**, 7799 (2001).

PtNNPt

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			716.8	Ne	IR	1
			672.1T	Ar	IR	1
			713.8	N_2	IR	1

Reference

[1] A. Citra, X. Wang, W. D. Bare, and L. Andrews, J. Phys. Chem. A **105**, 7799 (2001).

cyc-$(CeN)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}	5		542.8	Ar	IR	1
			526.2	N_2	IR	1
b_{3u}	6		667.6	Ar	IR	1
			639.6	N_2	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **102**, 10238 (1998).

cyc-$(PrN)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}	5		544.9	Ar	IR	1
			531.1	N_2	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **102**, 10238 (1998).

cyc-$(NdN)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}	5		546.7	Ar	IR	1
			530.3	N_2	IR	1
b_{3u}	6		679.2	Ar	IR	1
			657.6	N_2	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **102**, 10238 (1998).

cyc-$(SmN)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}	5		553.9	Ar	IR	1
			533.9	N_2	IR	1
			526.7			
b_{3u}	6		686.7	Ar	IR	1
			666.5	N_2	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **102**, 10238 (1998).

cyc-$(GdN)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}	5		563.5	Ar	IR	1
			545.6	N_2	IR	1
			538.5			
b_{3u}	6		690.2	Ar	IR	1
			688.3			
			686.8			
			668.5	N_2	IR	1
			663.8			

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **102**, 10238 (1998).

cyc-$(TbN)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}	5		569.3	Ar	IR	1
			567.8			
			550.9	N_2	IR	1
b_{3u}	6		698.8	Ar	IR	1
			669.4	N_2	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 1311 (1999).

cyc-$(DyN)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{3u}	6		701.9	Ar	IR	1
			678.2	N_2	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 1311 (1999).

cyc-$(HoN)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}	5		551.9	N_2	IR	1
b_{3u}	6		701	Ar	IR	1
			678.6	N_2	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 1311 (1999).

cyc-$(ErN)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{3u}	6		678.3	N_2	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 1311 (1999).

cyc-$(TmN)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}	5		566.5	N_2	IR	1
			563.4			
b_{3u}	6		684.2	N_2	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 1311 (1999).

cyc-$(LuN)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}	5		589.9	Ar	IR	1
			587.7			
			569.6	N_2	IR	1
b_{3u}	6		703.9	Ar	IR	1
			701.0			
			675.2	N_2	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 1311 (1999).

cyc-$(ThN)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}	5		719.0	Ar	IR	1
b_{3u}	6		605.6	Ar	IR	1

Reference

[1] G. P. Kushto, P. F. Souter, and L. Andrews, J. Chem. Phys. **108**, 7121 (1998).

BNBB

$^5\Sigma^-$ $C_{\infty v}$

$T_0 = 7790(160)$ gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+			1879(60)	gas	PE	1,2
			1403(60)	gas	PE	2

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

$T_0 = 6660(110)$ gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+			1863(60)	gas	PE	1,2
			758(60)	gas	PE	1,2

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

References

[1] K. R. Asmis, T. R. Taylor, and D. M. Neumark, Eur. Phys. J. D **9**, 257 (1999).
[2] K. R. Asmis, T. R. Taylor, and D. M. Neumark, J. Chem. Phys. **111**, 10491 (1999).

BCCB

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	BC a-stretch	955.0	Ar	IR	1

Reference

[1] J. D. Presilla-Márquez, P. G. Carrick, and C. W. Larson, J. Chem. Phys. **110**, 5702 (1999).

AlCCAl

$\tilde{C}$

$T^a = 15490(830)$ gas PE[2]

$\tilde{B}$

$T^a = 12420(630)$ gas PE[2]

$\tilde{A}$

$T^a = 10730(470)$ gas PE[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	AlC a-stretch	605.1	Ar	IR	1

[a] From vertical electron detachment energies.

References

[1] G. V. Chertihin, L. Andrews, and P. R. Taylor, J. Am. Chem. Soc. **116**, 3513 (1994).
[2] N. A. Cannon, A. I. Boldyrev, X. Li, and L.-S. Wang, J. Chem. Phys. **113**, 2671 (2000).

CAl_3^-

Threshold for electron detachment from ground-state CAl_3^- = 20650(160) gas PE[1]

Reference

[1] A. I. Boldyrev, J. Simons, X. Li, W. Chen, and L.-S. Wang, J. Chem. Phys. **110**, 8980 (1999).

cyc-$SiAl_3^-$

Vertical electron detachment energy from ground-state $SiAl_3^-$ = 22030(640) gas PE[1]

Reference

[1] X. Li, H.-F. Zhang, L.-S. Wang, A. E. Kuznetsov, N. A. Cannon, and A. I. Boldyrev, Angew. Chem. Int. Ed. **40**, 1867 (2001).

cyc-$GeAl_3^-$

Vertical electron detachment energy from ground-state $GeAl_3^-$ = 21780(730) gas PE[1]

Reference

[1] X. Li, H.-F. Zhang, L.-S. Wang, A. E. Kuznetsov, N. A. Cannon, and A. I. Boldyrev, Angew. Chem. Int. Ed. **40**, 1867 (2001).

cyc-$SnAl_3^-$

Vertical electron detachment energy from ground-state $SnAl_3^-$ = 21460(320) gas PE[1]

Reference

[1] X. Li, H.-F. Zhang, L.-S. Wang, A. E. Kuznetsov, N. A. Cannon, and A. I. Boldyrev, Angew. Chem. Int. Ed. **40**, 1867 (2001).

cyc-$PbAl_3^-$

Vertical electron detachment energy from ground-state $PbAl_3^-$ = 20040(160) gas PE[1]

Reference

[1] X. Li, H.-F. Zhang, L.-S. Wang, A. E. Kuznetsov, N. A. Cannon, and A. I. Boldyrev, Angew. Chem. Int. Ed. **40**, 1867 (2001).

NAl_3

$\tilde{a}$ C_{2v}
T^a = 14680(690) gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	3	NAl_3 a-stretch	773.1	Ar	IR	2
			777.9	N_2	IR	2
			770.3			

[a]From vertical electron detachment energy.

References

[1] S. K. Nayak, B. K. Rao, P. Jena, X. Li, and L.-S. Wang, Chem. Phys. Lett. **301**, 379 (1999).
[2] L. Andrews, M. Zhou, G. V. Chertihin, W. D. Bare, and Y. Hannachi, J. Phys. Chem. A **104**, 1656 (2000).

NGa_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	3	NGa_3 a-stretch	666.2	N_2	IR	1
			656.0			

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 1648 (2000).

NIn_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	3	NIn_3 a-stretch	604.7	N_2	IR	1
			596.3			

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 1648 (2000).

NTl_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	3	NTl_3 a-stretch	551.9	N_2	IR	1
			544.2			

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 1648 (2000).

cyc-ScC_3^-

Threshold for electron detachment from ground-state *cyc*-ScC_3^- = 13230(160) gas PE[1]

Reference

[1] L.-S. Wang and X. Li, J. Chem. Phys. **112**, 3602 (2000).

cyc-TiC_3^-

Threshold for electron detachment from ground-state *cyc*-TiC_3^- = 12590(120) gas PE[1]

Reference

[1] X.-B. Wang, C.-F. Ding, and L.-S. Wang, J. Phys. Chem. A **101**, 7699 (1997).

cyc-VC_3^-

Threshold for electron detachment from ground-state *cyc*-VC_3^- = 11860(160) gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CVC s-stretch	420(50)	gas	PE	1

Reference

[1] L.-S. Wang and X. Li, J. Chem. Phys. **112**, 3602 (2000).

cyc-NbC_3^-

Threshold for electron detachment from ground-state *cyc*-NbC_3^- = 13600(160) gas PE[1]

Reference

[1] H.-J. Zhai, S.-R. Liu, X. Li, and L.-S. Wang, J. Chem. Phys. **115**, 5170 (2001).

cyc-CrC_3^-

Threshold for electron detachment from ground-state *cyc*-CrC_3^- = 12100(160) gas PE[1]

Reference

[1] L.-S. Wang and X. Li, J. Chem. Phys. **112**, 3602 (2000).

cyc-MnC_3^-

Threshold for electron detachment from ground-state *cyc*-MnC_3^- = 15090(160) gas PE[1]

Reference

[1] L.-S. Wang and X. Li, J. Chem. Phys. **112**, 3602 (2000).

cyc-FeC_3^-

Threshold for electron detachment from ground-state *cyc*-FeC_3^- = 13550(160) gas PE[1,2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CFeC s-stretch	330(40)	gas	PE	2

References

[1] J. Fan, L. Lou, and L.-S. Wang, J. Chem. Phys. **102**, 2701 (1995).
[2] L.-S. Wang and X. Li, J. Chem. Phys. **112**, 3602 (2000).

cyc-CoC_3^-

Threshold for electron detachment from ground-state *cyc*-CoC_3^- = 12510(480) gas PE[1]

Reference

[1] L.-S. Wang and X. Li, J. Chem. Phys. **112**, 3602 (2000).

cyc-NiC_3^-

Threshold for electron detachment from ground-state *cyc*-NiC_3^- = 11210(400) gas PE[1]

Reference

[1] L.-S. Wang and X. Li, J. Chem. Phys. **112**, 3602 (2000).

$BNBB^-$

Threshold for electron detachment from ground-state $BNBB^-$ = 16930(280) gas PE[1]

$^2\Pi$ $C_{\infty v}$
T_0 = 1220(80) gas PE[1]

$\tilde{X}\,{}^4\Sigma^-$ $C_{\infty v}$

Reference

[1] K. R. Asmis, T. R. Taylor, and D. M. Neumark, J. Chem. Phys. **111**, 10491 (1999).

Al_3N^-

Threshold for electron detachment from ground-state Al_3N^- = 7750(650) gas PE[1]

Reference

[1] S. K. Nayak, B. K. Rao, P. Jena, X. Li, and L.-S. Wang, Chem. Phys. Lett. **301**, 379 (1999).

BCCC

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C_3 stretch	2002.1T	Ar	IR	1
	2	BC stretch	1512.5	Ar	IR	1

Reference

[1] J. D. Presilla-Márquez, P. G. Carrick, and C. W. Larson, J. Chem. Phys. **110**, 5702 (1999).

$CAlSi_2$

$\tilde{B}$
$T^a = 8550(870)$ gas PE[1]
$\tilde{A}$
$T^a = 4030(460)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			400(60)T	gas	PE	1

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

[a]From vertical electron detachment energies.

Reference

[1] A. I. Boldyrev, X. Li, and L.-S. Wang, J. Phys. Chem. A **104**, 5358 (2000).

$AlCCAl^-$

Threshold for electron detachment from ground-state quasilinear $AlCCAl^-$ = 5160(400) gas PE[1]

Reference

[1] N. A. Cannon, A. I. Boldyrev, X. Li, and L.-S. Wang, J. Chem. Phys. **113**, 2671 (2000).

cyc-$Al_2C_2^-$

Vertical detachment energy from ground-state *cyc*-$Al_2C_2^-$ to form quasilinear $AlCCAl^-$ = 12750(400) gas PE[1]

Reference

[1] N. A. Cannon, A. I. Boldyrev, X. Li, and L.-S. Wang, J. Chem. Phys. **113**, 2671 (2000).

Al_3O

$\tilde{C}\,^2A_1$ C_{2v}
$T_0 = 20250(800)$ gas PE[1]

$\tilde{B}\,^2B_2$ C_{2v}
$T_0 = 15400(800)$ gas PE[1]MO[2]

$\tilde{A}\,^2A_1$ C_{2v}
$T_0 = 11130(700)$ gas PE[1]MO[2]

$\tilde{X}\,^2B_2$ C_{2v}

References

[1] H. Wu, X. Li, X.-B. Wang, C.-F. Ding, and L.-S. Wang, J. Chem. Phys. **109**, 449 (1998).
[2] T. K. Ghanty and E. R. Davidson, J. Phys. Chem. A **103**, 2867 (1999).

ScOScO

$\tilde{X}$

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

Reference

[1] G. V. Chertihin, L. Andrews, M. Rosi, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **101**, 9085 (1997).

cyc-$(ScO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			699.1	Ar	IR	1
			688.1	N_2	IR	1
			647.8	Ar	IR	1
			635.5	N_2	IR	1

Reference

[1] G. V. Chertihin, L. Andrews, M. Rosi, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **101**, 9085 (1997).

VOVO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		−OVO a-stretch	1042.4	Ar	IR	1

Reference

[1] G. V. Chertihin, W. D. Bare, and L. Andrews, J. Phys. Chem. A **101**, 5090 (1997).

cyc-$(VO)_2$

$\tilde{X}$

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

Reference

[1] G. V. Chertihin, W. D. Bare, and L. Andrews, J. Phys. Chem. A **101**, 5090 (1997).

NbONbO

$\tilde{X}$

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

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 8251 (1998).

cyc-$(TaO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		TaO stretch	689.1	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 8251 (1998).

CrOCrO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			996.6	Ne	IR	2
			984.3	Ar	IR	1

References

[1] G. V. Chertihin, W. D. Bare, and L. Andrews, J. Chem. Phys. **107**, 2798 (1997).
[2] M. Zhou and L. Andrews, J. Chem. Phys. **111**, 4230 (1999).

cyc-$(MnO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			601.0	Ar	IR	1
			603.2	N_2	IR	1
			506.8	Ar	IR	1

Reference

[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. A **101**, 8547 (1997).

MnOMnO

$\tilde{X}$

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

Reference

[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. A **101**, 8547 (1997).

cyc-$(FeO)_2$

$\tilde{A}$

$T_0 = 3550(400)$ gas PE[6]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}			670(70)	gas	PE	6
			660.6	Ar	IR	3,4,7
			657.3	N_2	IR	5
b_{3u}			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).
[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).
[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).
[7] G. V. Chertihin, A. Citra, L. Andrews, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **101**, 8793 (1997).

cyc-$(CoO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}			685.2	Ar	IR	1
			706.0	N_2	IR	1
b_{3u}			469.6	Ar	IR	1
			494.6	N_2	IR	1

Reference

[1] G. V. Chertihin, A. Citra, L. Andrews, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **101**, 8793 (1997).

CoOCoO

$\tilde{X}$

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

Reference

[1] G. V. Chertihin, A. Citra, L. Andrews, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **101**, 8793 (1997).

cyc-$(RhO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			562.4T	Ar	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **103**, 4845 (1999).

cyc-$(PtO)_2$

$\tilde{X}$

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

Reference

[1] W. D. Bare, A. Citra, G. V. Chertihin, and L. Andrews, J. Phys. Chem. A **103**, 5456 (1999).

cyc-$(CeO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CeO stretch	575.0	Ar	IR	1
		CeO stretch	483.6	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 3171 (1999).

cyc-$(PrO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		PrO stretch	713	Ne	IR	1
			699.2	Ar	IR	1
		PrO stretch	605.8	Ar	IR	1
			593.7			

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 3171 (1999).

cyc-$(NdO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NdO stretch	600.0	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 3171 (1999).

cyc-$(SmO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SmO stretch	564.4	Ar	IR	1
		SmO stretch	422.6	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 3171 (1999).

cyc-$(EuO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{2u}			530.5	Ar	IR	1
b_{3u}			444.6	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 3171 (1999).

cyc-$(TbO)_2$

$\tilde{X}$

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

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 6972 (1999).

cyc-$(DyO)_2$

$\tilde{X}$

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

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 6972 (1999).

cyc-$(TmO)_2$

$\tilde{X}$

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

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 6972 (1999).

cyc-$(YbO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			590.9T	Ar	IR	1
			540.1T	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 6972 (1999).

cyc-$(LuO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			569.6T	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 6972 (1999).

cis-$CAlSi_2^-$

Vertical electron detachment energy from ground-state *cis*-$CAlSi_2^-$ = 20490(320) gas PE[1]

Reference

[1] A. I. Boldyrev, X. Li, and L.-S. Wang, J. Phys. Chem. A **104**, 5358 (2000).

Al_2N_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		AlN stretch	651.4	Ar	IR	1
			648.2	N_2	IR	1

Reference

[1] L. Andrews, M. Zhou, G. V. Chertihin, W. D. Bare, and Y. Hannachi, J. Phys. Chem. A **104**, 1656 (2000).

Al_2P_2

$\tilde{b}$ C_{2v}
T^a = 10250(830) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PP s-stretch	420(15)	gas	PE	1

$\tilde{a}\,^3A_2$ C_{2v}
$T^a = 4680(830)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	AIP s-stretch	320(12)	gas	PE	1

$\tilde{X}\,^1A_g$ D_{2h}

[a]From vertical ionization potential.

Reference

[1]H. Gómez, T. R. Taylor, and D. M. Neumark, J. Phys. Chem. A **105**, 6886 (2001).

Al_3O^-

Threshold for electron detachment from ground-state $Al_3O^- = 12670(480)$ gas PE[1]MO[2]

References

[1]H. Wu, X. Li, X.-B. Wang, C.-F. Ding, and L.-S. Wang, J. Chem. Phys. **109**, 449 (1998).
[2]T. K. Ghanty and E. R. Davidson, J. Phys. Chem. A **103**, 2867 (1999).

C_4

$^3\Sigma_u^-$ $D_{\infty h}$
$T_0 = 26384.9(2)$ gas CR[15] $^3\Sigma_u^- - \tilde{X}$ 334–379 nm
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	1821	gas	CR	15
			1822(20)	Ne	AB	11
			869	gas	CR	15
	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

$B_0 = 0.157$ CR[15]

$^1\Pi_g$ $D_{\infty h}$
$T_0 = 11380$ gas PE[14]

$^1\Pi_u$ $D_{\infty h}$
$T_0 = 9360(160)$T gas PE[14]

$^3\Pi_u$ $D_{\infty h}$
$T_0 = 7500(160)$ gas PE[14]

$^3\Pi_g$ $D_{\infty h}$
$T_0 = 6620(160)$ gas PE[14]

$^1\Sigma_g^+$ $D_{\infty h}$
$T_0 = 4030(160)$T gas PE[14]

$^1\Delta_g$ $D_{\infty h}$
$T_0 = 2680(120)$ gas PE[6,14]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	2032(50)	gas	PE	14
Π_g	4	Bend	331(50)	gas	PE	14

$\tilde{X}\,^3\Sigma_g^-$ $D_{\infty h}^a$ 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	2057(50)	gas	PE	6,14
Σ_u^+	3	Asym. stretch	1548.61	gas	DL	3
			1547.0	Ne	IR	8,10,13
			1543.4	Ar	IR	1
			1539.5	Kr	IR	12
Π_g	4	Bend	323(50)	gas	PE,DL	6,9,14
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).
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[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).
[7]N. Moazzen-Ahmadi, J. J. Thong, and A. R. W. McKellar, J. Chem. Phys. **100**, 4033 (1994).
[8]A. M. Smith, J. Agreiter, M. Härtle, C. Engel, and V. E. Bondybey, Chem. Phys. **189**, 315 (1994).
[9]N. Moazzen-Ahmadi and J. J. Thong, Chem. Phys. Lett. **233**, 471 (1995).
[10]D. Forney, M. E. Jacox, and W. E. Thompson, J. Mol. Spectrosc. **170**, 178 (1995).
[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).
[13]S. Tam, M. Macler, and M. E. Fajardo, J. Chem. Phys. **106**, 8955 (1997).
[14]C. Xu, G. R. Burton, T. R. Taylor, and D. M. Neumark, J. Chem. Phys. **107**, 3428 (1997).
[15]H. Linnartz, O. Vaizert, T. Motylewski, and J. P. Maier, J. Chem. Phys. **112**, 9777 (2000).

SiC_3

$\tilde{a}$ $C_{\infty v}$
$T_0 = 2210(25)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π		Deformation	140(25)	gas	PE	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C_3 a-stretch	1980(20)	gas	PE	1
	2	C_3 s-stretch	1320(20)	gas	PE	1
Π	5	Deformation	130T	gas	PE	1

Reference

[1] G. E. Davico, R. L. Schwartz, and W. C. Lineberger, J. Chem. Phys. **115**, 1789 (2001).

cyc-SiC_3 (prolate)

$\tilde{X}$ C_{2v} Structure: MW[1,2]
$A=1.266$; $B=0.210$; $C=0.180$ MW[1,2]

References

[1] M. C. McCarthy, A. J. Apponi, and P. Thaddeus, J. Chem. Phys. **110**, 10645 (1999).
[2] A. J. Apponi, M. C. McCarthy, C. A. Gottlieb, and P. Thaddeus, J. Chem. Phys. **111**, 3911 (1999).

cyc-SiC_3 (oblate)

$\tilde{X}$ C_{2v} Structure: MW[1]
$A=0.416$; $B=0.378$; $C=0.198$ MW[1]

Reference

[1] M. C. McCarthy, A. J. Apponi, and P. Thaddeus, J. Chem. Phys. **111**, 7175 (1999).

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}
$T_0=15570(160)$ gas PE[2,8]TPE[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1		450(20)	gas	PE,TPE	2,4,8

$^3B_{1g}$ D_{2h}
$T_0=13800(160)$ gas PE[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1		355(20)	gas	PE	8

^3B_g C_{2h}
$T_0=12100T$ gas PE[8]

$^1B_{3u}$ D_{2h}
$T_0=11050(80)$ gas PE[2,8]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,PE	4,8
			300(6)	Ne	AB	7

$^3B_{3u}$ D_{2h}
$T_0=6580(80)$ gas PE[2,8]TPE[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2		312	gas	PE,TPE	2,4,8

$\tilde{X}$ ^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		380(20)	gas	PE	2,8
			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 (London) **366**, 42 (1993).
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[8] C. Xu, T. R. Taylor, G. R. Burton, and D. M. Neumark, J. Chem. Phys. **108**, 1395 (1998).

PtNNN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		N_3 a-stretch	2104.4	N_2	IR	1
		N_3 s-stretch	1389.5	N_2	IR	1

Reference

[1] A. Citra, X. Wang, W. D. Bare, and L. Andrews, J. Phys. Chem. A **105**, 7799 (2001).

NNPtN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NN stretch	2280.0	N_2	IR	1
		PtN stretch	854.7	N_2	IR	1

Reference

[1] A. Citra, X. Wang, W. D. Bare, and L. Andrews, J. Phys. Chem. A **105**, 7799 (2001).

$OScCO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	2221.8	Ar	IR	1
		ScO stretch	965.5	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Am. Chem. Soc. **120**, 13230 (1998).

$OScOC^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OC stretch	2068.1	Ar	IR	1
		OSc stretch	974.1	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Am. Chem. Soc. **120**, 13230 (1998).

$ScOCO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	2105.7	Ar	IR	1
		ScO stretch	976.4	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Am. Chem. Soc. **120**, 13230 (1998).

$OYCO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	2206.0 2203.3	Ar	IR	1
		YO stretch	857.2	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Am. Chem. Soc. **120**, 13230 (1998).

$OYOC^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OC stretch	2078.0	Ar	IR	1
		OY stretch	869.1	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Am. Chem. Soc. **120**, 13230 (1998).

$YOCO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	2106.0	Ar	IR	1
		YO stretch	871.9	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Am. Chem. Soc. **120**, 13230 (1998).

$OTiCO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	2190.4 2185.5	Ar	IR	1
		TiO stretch	1004.3 1003.0	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 2066 (1999).

$OTiOC^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	2065.2	Ar	IR	1
		TiO stretch	1012.9	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 2066 (1999).

$OVCO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	2205.4 2203.3	Ar	IR	1
		VO stretch	1020.0	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 2066 (1999).

$OVOC^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	2059.3	Ar	IR	1
		VO stretch	1029.6	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 2066 (1999).

$OCrCO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	2175.5	Ar	IR	1

Reference

[1] M. Zhou, B. Liang, and L. Andrews, J. Phys. Chem. A **103**, 2013 (1999).

$OMnCO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	2173.0	Ar	IR	1
		MnO stretch	851.9	Ar	IR	1

Reference

[1] M. Zhou, B. Liang, and L. Andrews, J. Phys. Chem. A **103**, 2013 (1999).

$OThCO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	2009.9	Ne	IR	1
		ThO stretch	896.4	Ne	IR	1

Reference

[1] L. Andrews, M. Zhou, B. Liang, J. Li, and B. E. Bursten, J. Am. Chem. Soc. **122**, 11440 (2000).

$OUCO^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	2073.0	Ne	IR	1
		UO stretch	881.2	Ne	IR	1

Reference

[1] L. Andrews, M. Zhou, B. Liang, J. Li, and B. E. Bursten, J. Am. Chem. Soc. **122**, 11440 (2000).

$Al_2P_2^-$

Threshold for electron detachment from ground-state $Al_2P_2^- = 17350(800)$ gas PE[1]

Reference

[1] H. Gómez, T. R. Taylor, and D. M. Neumark, J. Phys. Chem. A **105**, 6886 (2001).

C_4^-

Threshold for electron detachment from ground-state $C_4^- = 31320(80)$ gas PE[1,2,7]

(3) $^2\Pi_u$ $D_{\infty h}$

$T_0 = 28717$ gas MPD[10] (3) $^2\Pi_u$–$\tilde{X}$ 336–348 nm

28868 Ne AB[6] (3) $^2\Pi_u$–$\tilde{X}$ 335–347 nm

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

$T_0 = 25989$ gas MPD[10] (2) $^2\Pi_u - \tilde{X}$ 347–385 nm
26069(14) Ne AB[6] (2) $^2\Pi_u - \tilde{X}$ 372–384 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		2056	gas	MPD	10
	2		710	gas	MPD	10
			755(20)	Ne	AB	6
Π_g	4		374H	gas	MPD	10
			349(10)H	Ne	AB	6
Π_u	5		268H	gas	MPD	10
			271(10)H	Ne	AB	6

$\tilde{C}\,^2\Pi_u$ $D_{\infty h}$

$T_0 = 21871.53$ gas PD[4]MPD[10] $\tilde{C} - \tilde{X}$ 379–460 nm
21896(5) Ne AB[3]LF[5] $\tilde{C} - \tilde{X}$ 410–527 nm
21720 Ar AB[8] $\tilde{C} - \tilde{X}$ 416–461 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		1729H	gas	MPD	10
	2		752.4	gas	PD	4
			759(5)	Ne	AB	3
			763	Ar	AB	8
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
Σ_u^+	3	Asym. stretch	1699.8	Ar	IR	9
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).
[2] D. W. Arnold, S. E. Bradforth, T. N. Kitsopoulos, and D. M. Neumark, J. Chem. Phys. **95**, 8753 (1991).
[3] P. Freivogel, J. Fulara, M. Jakobi, D. Forney, and J. P. Maier, J. Chem. Phys. **103**, 54 (1995).
[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).
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[7] C. Xu, G. R. Burton, T. R. Taylor, and D. M. Neumark, J. Chem. Phys. **107**, 3428 (1997).
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[9] J. Szczepanski, M. Vala, L. N. Shen, P. A. Withey, and W. R. M. Graham, J. Phys. Chem. A **101**, 8788 (1997).
[10] M. Tulej, D. A. Kirkwood, G. Maccaferri, O. Dopfer, and J. P. Maier, Chem. Phys. **228**, 293 (1998).

SiC_3^-

Threshold for electron detachment from ground-state linear SiC_3^- = 22810(60) gas PE[1]

Reference

[1] G. E. Davico, R. L. Schwartz, and W. C. Lineberger, J. Chem. Phys. **115**, 1789 (2001).

Si_4^-

Threshold for electron detachment from ground-state Si_4^- = 17180(80) gas PE[1,4]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).
[4] C. Xu, T. R. Taylor, G. R. Burton, and D. M. Neumark, J. Chem. Phys. **108**, 1395 (1998).

Ge_4^-

Threshold for electron detachment from ground-state $Ge_4^- = 15650(80)$ gas PE[1]

Reference

[1] G. R. Burton, C. Xu, C. C. Arnold, and D. M. Neumark, J. Chem. Phys. **104**, 2757 (1996).

Sn_4^-

Threshold for electron detachment from ground-state $Sn_4^- = 16460(80)$ gas PE[1]

Reference

[1] V. D. Moravec, S. A. Klopcic, and C. C. Jarrold, J. Chem. Phys. **110**, 5079 (1999).

OScCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CO stretch	1873.4	Ar	IR	1
		ScO stretch	894.1	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Am. Chem. Soc. **120**, 13230 (1998).

cyc-(ScOC)O

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OCO a-stretch	1763.4	Ar	IR	1
		Ring stretch	778.0	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Am. Chem. Soc. **120**, 13230 (1998).

cyc-(COSc)O

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CO stretch	1613.9	Ar	IR	1
		ScO stretch	909.6	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Am. Chem. Soc. **120**, 13230 (1998).

OYCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CO stretch	1861.5	Ar	IR	1
		YO stretch	796.5	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Am. Chem. Soc. **120**, 13230 (1998).

cyc-(YOC)O

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OCO a-stretch	1773.1	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Am. Chem. Soc. **120**, 13230 (1998).

cyc-(COY)O

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CO stretch	1614.5	Ar	IR	1
		YO stretch	804.4	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Am. Chem. Soc. **120**, 13230 (1998).

OTiCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1884.0	Ne	IR	2
			1866.7	Ar	IR	1,2
		TiO stretch	973.1	Ne	IR	2
			952.8	Ar	IR	1,2

References

[1] G. V. Chertihin and L. Andrews, J. Am. Chem. Soc. **117**, 1595 (1995).
[2] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 2066 (1999).

cyc-(COTi)O

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1539.0	Ne	IR	1
			1532.3	Ar	IR	1
		TiO stretch	990.6	Ne	IR	1
			965.0	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 2066 (1999).

OZrCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CO stretch	1837.8	Ar	IR	1
	2	ZrO stretch	878.9	Ar	IR	1

Reference

[1] L. Zhang, X. Wang, M. Chen, and Q.-Z. Qin, Chem. Phys. **254**, 231 (2000).

OVCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1881.1	Ar	IR	1
		VO stretch	974.8	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 2066 (1999).

cyc-(COV)O

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1516.1	Ar	IR	1
		VO stretch	990.0	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 2066 (1999).

ONbCO (I)

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CO stretch	1902.6	Ar	IR	1
	2	NbO stretch	960.1	Ar	IR	1

Reference

[1] M. Chen, X. Wang, L. Zhang, and Q. Qin, J. Phys. Chem. A **104**, 7010 (2000).

ONbCO (II)

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CO stretch	1821.6	Ar	IR	1
	2	NbO stretch	915.6	Ar	IR	1

Reference

[1] M. Chen, X. Wang, L. Zhang, and Q. Qin, J. Phys. Chem. A **104**, 7010 (2000).

OTaCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CO stretch	1887.3	Ar	IR	1
	2	TaO stretch	967.3	Ar	IR	1

Reference

[1] X.-F. Wang, M.-H. Chen, L.-N. Zhang, and Q.-Z. Qin, J. Phys. Chem. A **104**, 758 (2000).

OCrCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CO stretch	2014.4	Ar	IR	1
	2	CrO stretch	866.3	Ar	IR	1

Reference

[1] P. F. Souter and L. Andrews, J. Am. Chem. Soc. **119**, 7350 (1997).

CrOCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OCO a-stretch	1735.6	Ar	IR	1
		CrO stretch	721.0	Ar	IR	1
			716.1			

Reference

[1] P. F. Souter and L. Andrews, J. Am. Chem. Soc. **119**, 7350 (1997).

OMoCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CO stretch	1847.0	Ar	IR	1
	2	MoO stretch	951.8	Ar	IR	1

Reference

[1] P. F. Souter and L. Andrews, J. Am. Chem. Soc. **119**, 7350 (1997).

OWCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CO stretch	1879.0	Ar	IR	1
	2	WO stretch	969.6	Ar	IR	1
			483.8	Ar	IR	1

Reference

[1] P. F. Souter and L. Andrews, J. Am. Chem. Soc. **119**, 7350 (1997).

OMnCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	2082.5	Ar	IR	1
		MnO stretch	869.9	Ar	IR	1

Reference

[1] M. Zhou, B. Liang, and L. Andrews, J. Phys. Chem. A **103**, 2013 (1999).

OFeCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	2037.1	Ar	IR	1
		FeO stretch	872.8	Ar	IR	1

Reference

[1] M. Zhou, B. Liang, and L. Andrews, J. Phys. Chem. A **103**, 2013 (1999).

OCoCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	2026.6	Ar	IR	1
		CoO stretch	783.8	Ar	IR	1

Reference

[1] M. Zhou, B. Liang, and L. Andrews, J. Phys. Chem. A **103**, 2013 (1999).

ONiCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	2086.6	Ar	IR	1

Reference

[1] M. Zhou, B. Liang, and L. Andrews, J. Phys. Chem. A **103**, 2013 (1999).

OThCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1778.4	Ne	IR	1

Reference

[1] L. Andrews, M. Zhou, B. Liang, J. Li, and B. E. Bursten, J. Am. Chem. Soc. **122**, 11440 (2000).

OUCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	1806.9	Ne	IR	2
			1799.6	Ar	IR	1
	2	UO stretch	823.2	Ne	IR	2
			804.4	Ar	IR	1

References

[1] T. J. Tague, Jr., L. Andrews, and R. D. Hunt, J. Phys. Chem. **97**, 10920 (1993).
[2] L. Andrews, M. Zhou, B. Liang, J. Li, and B. E. Bursten, J. Am. Chem. Soc. **122**, 11440 (2000).

NNBN

$\tilde{A}$

$T_0 = 26350$ Ar AB[4] $\tilde{A}-\tilde{X}$ 348–380 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Deformation	480	Ar	AB	4

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NN stretch	2091.7	Ar	IR	2
			2100(2) N_2	Ar	IR	3
			2124.8	N_2	IR	1
	2	BN stretch	1802.0	Ar	IR	2
			1803(2) N_2	Ar	IR	3
			1806.1	N_2	IR	1
	3	N_2–BN stretch	760.3w	Ar	IR	2
			750.4	N_2	IR	1

References

[1] P. Hassanzadeh and L. Andrews, J. Phys. Chem. **96**, 9177 (1992).
[2] L. Andrews, P. Hassanzadeh, T. R. Burkholder, and J. M. L. Martin, J. Chem. Phys. **98**, 922 (1993).
[3] I. A. Al-Jihad, B. Liu, C. J. Linnen, and J. V. Gilbert, J. Phys. Chem. A **102**, 6220 (1998).
[4] M. J. Travers and J. V. Gilbert, J. Phys. Chem. A **104**, 3780 (2000).

AlNNN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	N_3 a-stretch	2144.0	N_2	IR	1
	2	N_3 s-stretch	1386.0	N_2	IR	1
	3	AlN stretch	509.7	N_2	IR	1

Reference

[1] L. Andrews, M. Zhou, G. V. Chertihin, W. D. Bare, and Y. Hannachi, J. Phys. Chem. A **104**, 1656 (2000).

GaNNN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	N_3 a-stretch	2096.8	N_2	IR	1
	2	N_3 s-stretch	1328.3	N_2	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 1648 (2000).

InNNN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	N_3 a-stretch	2074.5	N_2	IR	1
	2	N_3 s-stretch	1323.9	N_2	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 1648 (2000).

TlNNN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	N_3 a-stretch	2048.8	N_2	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 1648 (2000).

TlOTlO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		TlO stretch	726.9	Ar	IR	1
		TlO stretch	655.9	Ar	IR	1

Reference

[1] L. Andrews, G. P. Kushto, J. T. Yustein, E. Archibong, R. Sullivan, and J. Leszczynski, J. Phys. Chem. A **101**, 9077 (1997).

cyc-TlO_2Tl

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			422	Ar	IR	1,2
			422.7	N_2	IR	1

References

[1] B. J. Kelsall and K. D. Carlson, J. Phys. Chem. **84**, 951 (1980).
[2] L. Andrews, G. P. Kushto, J. T. Yustein, E. Archibong, R. Sullivan, and J. Leszczynski, J. Phys. Chem. A **101**, 9077 (1997).

NCCP

$\tilde{X}$ $C_{\infty v}$ Structure: MW[1]
$B_0 = 0.090$ MW[1]

Reference

[1] L. Bizzocchi, C. Degli Esposti, and P. Botschwina, J. Chem. Phys. **113**, 1465 (2000).

CCCO

$\tilde{X}$ $C_{\infty v}$ Structure: MW[4,7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1		2257.22	gas	IR	8
			2243vs	Ar	IR	1,5–7,10
			2237.2	Xe	IR	9
	2		1907.0m	Ar	IR	5,7
			1904.4	Xe	IR	9
	3		939.1vw	Ar	IR	7
Π	4		580m	Ar	IR	5,7
			571.9	Xe	IR	9

$B_0 = 0.160$ MW[2–4]IR[8]

References

[1] R. L. DeKock and W. Weltner, Jr., J. Am. Chem. Soc. **93**, 7106 (1971).
[2] R. D. Brown, F. W. Eastwood, P. S. Elmes, and P. D. Godfrey, J. Am. Chem. Soc. **105**, 6496 (1983).
[3] T. B. Tang, H. Inokuchi, S. Saito, C. Yamada, and E. Hirota, Chem. Phys. Lett. **116**, 83 (1985).
[4] R. D. Brown, P. D. Godfrey, P. S. Elmes, M. Rodler, and L. M. Tack, J. Am. Chem. Soc. **107**, 4112 (1985).
[5] R. D. Brown, D. E. Pullin, E. H. N. Rice, and M. Rodler, J. Am. Chem. Soc. **107**, 7877 (1985).
[6] B. J. Ortman, R. H. Hauge, J. L. Margrave, and Z. H. Kafafi, J. Phys. Chem. **94**, 7973 (1990).
[7] P. Botschwina and H. P. Reisenauer, Chem. Phys. Lett. **183**, 217 (1991).
[8] D. McNaughton, D. McGilvery, and F. Shanks, J. Mol. Spectrosc. **149**, 458 (1991).
[9] G. Maier and C. Lautz, Eur. J. Org. Chem. **1998**, 769.
[10] M. Dibben, J. Szczepanski, C. Wehlburg, and M. Vala, J. Phys. Chem. A **104**, 3584 (2000).

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
			2047.6vs	Ar	IR	2,6
	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).
[6] J. Szczepanski, R. Hodyss, J. Fuller, and M. Vala, J. Phys. Chem. A **103**, 2975 (1999).

SiNNSi

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SiN stretch	1153.3	N_2	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, and J. Glatthaar, Organomet. **19**, 4775 (2000).

cyc-$(SiN)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2		SiN stretch	900.9	N_2	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, and J. Glatthaar, Organomet. **19**, 4775 (2000).

SiNSiN

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		NSi stretch	1374.7	N_2	IR	1
		SiN stretch	1164.4	N_2	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, and J. Glatthaar, Organomet. **19**, 4775 (2000).

$OTaCO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1838.1	Ar	IR	1

Reference

[1] X.-F. Wang, M.-H. Chen, L.-N. Zhang, and Q.-Z. Qin, J. Phys. Chem. A **104**, 758 (2000).

$OCrCO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1831.1	Ar	IR	1
		CrO stretch	825.5	Ar	IR	1

Reference

[1] M. Zhou, B. Liang, and L. Andrews, J. Phys. Chem. A **103**, 2013 (1999).

$OMnCO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1810.0	Ar	IR	1
		MnO stretch	810.1	Ar	IR	1

Reference

[1] M. Zhou, B. Liang, and L. Andrews, J. Phys. Chem. A **103**, 2013 (1999).

$OFeCO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1806.3	Ar	IR	1
		FeO stretch	814.8	Ar	IR	1

Reference

[1] M. Zhou, B. Liang, and L. Andrews, J. Phys. Chem. A **103**, 2013 (1999).

$OCoCO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1849.2	Ar	IR	1
		CoO stretch	807.9	Ar	IR	1

Reference

[1] M. Zhou, B. Liang, and L. Andrews, J. Phys. Chem. A **103**, 2013 (1999).

$CoCO_2^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO_2 a-stretch	1693.5	Ar	IR	1
		CO_2 s-stretch	1228.4	Ar	IR	1
		CO_2 deform.	721.9	Ar	IR	1

Reference

[1] M. Zhou, B. Liang, and L. Andrews, J. Phys. Chem. A **103**, 2013 (1999).

$ONiCO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1881.4	Ar	IR	1

Reference

[1] M. Zhou, B. Liang, and L. Andrews, J. Phys. Chem. A **103**, 2013 (1999).

$NiCO_2^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO_2 a-stretch	1684.8	Ar	IR	1
		CO_2 s-stretch	1226.1	Ar	IR	1
		CO_2 deform.	723.9	Ar	IR	1

Reference

[1] M. Zhou, B. Liang, and L. Andrews, J. Phys. Chem. A **103**, 2013 (1999).

$OCuCO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1943.4	Ar	IR	1

Reference

[1] M. Zhou, B. Liang, and L. Andrews, J. Phys. Chem. A **103**, 2013 (1999).

$CuCO_2^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO_2 a-stretch	1713.4	Ar	IR	1
		CO_2 s-stretch	1234.2	Ar	IR	1
		CO_2 deform.	697.0	Ar	IR	1

Reference

[1] M. Zhou, B. Liang, and L. Andrews, J. Phys. Chem. A **103**, 2013 (1999).

$OZnCO^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	2084.4	Ar	IR	1

Reference

[1] M. Zhou, B. Liang, and L. Andrews, J. Phys. Chem. A **103**, 2013 (1999).

t-$OCCO^+$

$\tilde{B}$

gas PD[2] $\tilde{B}-\tilde{X}$ 270–330 nm

Superposed on continuum.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g			475(20)	gas	PD	2

$\tilde{X}\,^2B_u$ C_{2h} Structure: ESR, MO[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	CO s-stretch	2076T[a]	Ne	IR	4
			526(30)T	gas	PD	2
b_u	5	CO a-stretch	2056.6	Ne	IR	3–5

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

References

[1] L. B. Knight, Jr., J. Steadman, P. K. Miller, D. E. Bowman, E. R. Davidson, and D. Feller, J. Chem. Phys. **80**, 4593 (1984).
[2] S. C. Ostrander, L. Sanders, and J. C. Weisshaar, J. Chem. Phys. **84**, 529 (1986).
[3] M. E. Jacox and W. E. Thompson, Res. Chem. Intermed. **12**, 33 (1989).
[4] W. E. Thompson and M. E. Jacox, J. Chem. Phys. **95**, 735 (1991).
[5] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 2964 (1999).

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[7,8]

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	7,8
			2237.6	Ne	IR	5,6

$B_0 = 0.112$ DL[7,8]

[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).
[8] T. Speck, T. Ruchti, H. Linnartz, and J. P. Maier, J. Mol. Spectrosc. **185**, 425 (1997).

cyc-$(O_2Sc)O$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	1109.5w	Ar	IR	1
			922.0w	Ar	IR	1
		ScO stretch	909.0s	Ar	IR	1,2
			466.3w	Ar	IR	1,2

References

[1] G. V. Chertihin, L. Andrews, M. Rosi, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **101**, 9085 (1997).

[2] C. W. Bauschlicher, Jr., M. Zhou, L. Andrews, J. R. Tobias Johnson, I. Panas, A. Snis, and B. O. Roos, J. Phys. Chem. A **103**, 5463 (1999).

VO_3

$\tilde{B}\,^2B_2$ C_{2v}
$T_0 = 6370(400)$ gas PE[1]

$\tilde{A}\,^2A_1$ C_{2v}
$T_0 = 4760(400)$ gas PE[1]

Reference

[1] H. Wu and L.-S. Wang, J. Chem. Phys. **108**, 5310 (1998).

CrO_3

$\tilde{B}$
$T^a = 14280(230)$ gas PE[3]

$\tilde{A}$
$T^a = 8390(230)$ gas PE[3]

$\tilde{a}$
$T^a = 7660(230)$ gas PE[3]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CrO_3 s-stretch	890(60)	gas	PE	3
	3	CrO stretch	991.3	Ne	IR	2
			968.4	Ar	IR	1

[a] From vertical electron detachment energies.

References

[1] G. V. Chertihin, W. D. Bare, and L. Andrews, J. Chem. Phys. **107**, 2798 (1997).
[2] M. Zhou and L. Andrews, J. Chem. Phys. **111**, 4230 (1999).
[3] G. L. Gutsev, P. Jena, H.-J. Zhai, and L.-S. Wang, J. Chem. Phys. **115**, 7935 (2001).

MoO_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	MoO stretch	976T	Ne	IR	1
e	3	MoO stretch	923.4	Ne	IR	1,3
			915.8	Ar	IR	2

References

[1] W. D. Hewett, Jr., J. H. Newton, and W. Weltner, Jr., J. Phys. Chem. **79**, 2640 (1975).
[2] W. D. Bare, P. F. Souter, and L. Andrews, J. Phys. Chem. A **102**, 8279 (1998).
[3] M. Zhou and L. Andrews, J. Chem. Phys. **111**, 4230 (1999).

WO_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	WO stretch	924.3	Ne	IR	4
			918.3	Ar	IR	1–3
			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).
[3] W. D. Bare, P. F. Souter, and L. Andrews, J. Phys. Chem. A **102**, 8279 (1998).
[4] M. Zhou and L. Andrews, J. Chem. Phys. **111**, 4230 (1999).

(*cyc*-O_2Mn)O

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OO stretch	1092.2	Ar	IR	1
		MnO stretch	886.9	Ar	IR	1

Reference

[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. A **101**, 8547 (1997).

ReO_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	ReO_3 stretch	962.0	Ne	IR	1
			953.4	Ar	IR	1

Reference

[1] M. Zhou, A. Citra, B. Liang, and L. Andrews, J. Phys. Chem. A **104**, 3457 (2000).

FeO_3

$\tilde{A}$

$T_0 = 4440(160)$ gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			850(50)	gas	PE	2

$\tilde{X}$ 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); J. Am. Chem. Soc. **118**, 7434 (1996).

RuO_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	3	RuO_3 stretch	901.1	Ne	IR	2
			893.3	Ar	IR	1,2

References

[1] J. G. Kay, D. W. Green, K. Duca, and G. L. Zimmerman, J. Mol. Spectrosc. **138**, 49 (1989).
[2] M. Zhou, A. Citra, B. Liang, and L. Andrews, J. Phys. Chem. A **104**, 3457 (2000).

OsO_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	3	OsO_3 stretch	966.1	Ne	IR	1
			959.1	Ar	IR	1

Reference

[1] M. Zhou, A. Citra, B. Liang, and L. Andrews, J. Phys. Chem. A **104**, 3457 (2000).

OCoOO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	1331.5T	Ar	IR	1

Reference

[1] G. V. Chertihin, A. Citra, L. Andrews, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **101**, 8793 (1997).

cyc-$(O_2Co)O$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	1090.0	Ar	IR	1
			783.0	Ar	IR	1

Reference

[1] G. V. Chertihin, A. Citra, L. Andrews, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **101**, 8793 (1997).

ORhOO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	1367.3	Ar	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **103**, 4845 (1999).

PtO_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	3	OPtO a-stretch	833.4T	Ar	IR	1

Reference

[1] W. D. Bare, A. Citra, G. V. Chertihin, and L. Andrews, J. Phys. Chem. A **103**, 5456 (1999).

cyc-$(O_2Pt)O$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OO stretch	1174.2	Ar	IR	1

Reference

[1] W. D. Bare, A. Citra, G. V. Chertihin, and L. Andrews, J. Phys. Chem. A **103**, 5456 (1999).

OOPtO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	1402.1	Ar	IR	1

Reference

[1] W. D. Bare, A. Citra, G. V. Chertihin, and L. Andrews, J. Phys. Chem. A **103**, 5456 (1999).

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	760.3	Ne	IR	5
			745.6	Ar	IR	1–5
			740.7	Kr	IR	1
b_2	5	UO_2 a-stretch	865.3	Ne	IR	5
			852.6	Ar	IR	1–5
			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).
[4] K. Sankaran, K. Sundararajan, and K. S. Viswanathan, Bull. Mater. Sci. **22**, 785 (1999).
[5] M. Zhou, L. Andrews, N. Ismail, and C. Marsden, J. Phys. Chem. A **104**, 5495 (2000).

(*cyc*-NNB)Cl

In an argon matrix, a broad absorption with maximum at 24510 (408 nm) has been tentatively assigned[2] to (*cyc*-NNB)Cl.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Ring breathing	1677	Ar	IR	1

References

[1] M. J. Travers, E. L. Eldenburg, and J. V. Gilbert, J. Phys. Chem. A **103**, 9661 (1999).
[2] M. J. Travers and J. V. Gilbert, J. Phys. Chem. A **104**, 3780 (2000).

OCCS

In an argon matrix, a structured absorption between 280 and 320 nm with a maximum at 32680 (306 nm) has been assigned[1] to OCCS.

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	OCC stretch	2156.0vs	Ar	IR	1
	2	OCCS stretch	1505.2m	Ar	IR	1
	3	OCCS stretch	685T	Ar	IR	1
Π	4	Bend	452.2wm	Ar	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, and R. Ruppel, Angew. Chem. **109**, 1972 (1997); Angew. Chem. Int. Ed. Engl. **36**, 1862 (1997).

Ge_2O_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1		692.5	Ar	Ra	4
	2	Ge–Ge breathing	400(60)	gas	PE	3
			328.0	Ar	Ra	4
b_{1g}	3		469.0	Ar	Ra	4
b_{1u}	4		173T	Ar	Ra	4
b_{2u}	5	GeO stretch	667.7	Ar	IR	1,2,4
			667	N_2	IR	1
b_{3u}	6	GeO stretch	601.7	Ar	IR	1,2,4
			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).
[4] A. Zumbusch and H. Schnöckel, J. Chem. Phys. **108**, 8092 (1998).

NOCN

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CN stretch	2086.0vw	Ar	IR	1
	2	NO stretch	1836.9vs	Ar	IR	1
	3	Bend	485.4w	Ar	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, J. Eckwert, M. Naumann, and M. De Marco, Angew. Chem. **109**, 1795 (1997); Angew. Chem. Int. Ed. Engl. **36**, 1707 (1997).

CNNO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CN stretch	1997.5m[a]	Ar	IR	1
			1967.1m[a]			
	2	NO stretch	1681.0vs	Ar	IR	1
	3	Deformation	723.4m	Ar	IR	1
	4	NN stretch	261.0ms	Ar	IR	1

[a]In Fermi resonance with $(\nu_2+\nu_4)$.

Reference

[1] G. Maier, H. P. Reisenauer, J. Eckwert, M. Naumann, and M. De Marco, Angew. Chem. **109**, 1795 (1997); Angew. Chem. Int. Ed. Engl. **36**, 1707 (1997).

NCNO

An absorption maximum has been reported[3,9] at 216 nm, with absorption extending beyond 200 nm.

A weaker absorption maximum occurs near 270 nm, with a long wavelength threshold near 400 nm.[9]

$\tilde{A}\ ^1A''$ C_s Structure: PF[11]

$T_0=11339$ gas $AB^{1,3,7}PF^{11}$ $\tilde{A}-\tilde{X}$ 540–971 nm Threshold for photodissociation into CN and NO at 17085.[9,10] Extensively perturbed by interaction with high vibrational levels of the ground state.[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	C≡N stretch	1956	gas	PF	11
	2	N=O stretch	1485	gas	PF	11
	3	C–N stretch	918	gas	PF	11
	4	NCN bend	543	gas	AB,PF	7,11
	5	CNO bend	212.5	gas	AB,PF	7,11
a''	6	Torsion	411	gas	PF	11

$\tau_{rad}\cong 14\ \mu s$ gas $LF^{8,12}$
$\tau_{fluor}>40\ \mu s$ for all levels below D_0 (17085) LF^{12}
$A=4.76(2)$; $B=0.167(3)$ PF^{11}

$\tilde{X}$ C_s Structure: $MW^{2,4}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	C≡N stretch	2170.0	gas	IR	6
			2163.0s	Ar	IR	13
	2	N=O stretch	1501.0	gas	IR	6
			1498.5vs	Ar	IR	13
	3	C–N stretch	820.0	gas	IR	3,6
			809.5s	Ar	IR	13
	4	NCN bend	588.5	gas	IR	6
			576.1	Ar	IR	13
	5	CNO bend	212.0(2)	gas	IR	5
a''	6	Torsion	264.2	gas	IR	5

$A_0=2.709$; $B_0=0.180$; $C_0=0.168$ $MW^{2,4}IR^5$

References

[1] P. Horsewood and G. W. Kirby, Chem. Commun. 1139 (1971).
[2] R. Dickinson, G. W. Kirby, J. G. Sweeny, and J. K. Tyler, Chem. Commun. 241 (1973).
[3] E. A. Dorko and L. Buelow, J. Chem. Phys. **62**, 1869 (1975).
[4] R. Dickinson, G. W. Kirby, J. G. Sweeny, and J. K. Tyler, J. Chem. Soc., Faraday Trans. 2 **74**, 1393 (1978).
[5] F. M. Nicolaisen and O. J. Nielsen, J. Mol. Struct. **49**, 97 (1978).
[6] B. Bak, F. M. Nicolaisen, O. J. Nielsen, and S. Skaarup, J. Mol. Struct. **51**, 17 (1979).
[7] J. Pfab, Chem. Phys. Lett. **99**, 465 (1983).
[8] I. Nadler, J. Pfab, G. Radhakrishnan, H. Reisler, and C. Wittig, J. Chem. Phys. **79**, 2088 (1983).
[9] I. Nadler, J. Pfab, H. Reisler, and C. Wittig, J. Chem. Phys. **81**, 653 (1984).
[10] I. Nadler, H. Reisler, M. Noble, and C. Wittig, Chem. Phys. Lett. **108**, 115 (1984).
[11] M. Noble, I. Nadler, H. Reisler, and C. Wittig, J. Chem. Phys. **81**, 4333 (1984).
[12] C. X. W. Qian, H. Reisler, and C. Wittig, Chem. Phys. Lett. **139**, 175 (1987).
[13] G. Maier, H. P. Reisenauer, J. Eckwert, M. Naumann, and M. De Marco, Angew. Chem. **109**, 1795 (1997); Angew. Chem. Int. Ed. Engl. **36**, 1707 (1997).

NCPO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CN stretch	2165	gas	IR	1
	2	PO stretch	1385	gas	IR	1

Reference

[1] A. W. Allaf, M. Kassem, M. Alibrahim, and I. Boustani, J. Mol. Struct. **478**, 193 (1999).

ClCNC

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NC stretch	1943.6vs	Ar	IR	1,2
	2	CN stretch	1023.7m	Ar	IR	1,2
	3	CNC deform.	769.5wm	Ar	IR	2

References

[1] D. E. Milligan, M. E. Jacox, and A. M. Bass, J. Chem. Phys. **43**, 3149 (1965).
[2] G. Maier, A. Bothur, J. Eckwert, and H. P. Reisenauer, Chem. Eur. J. **4**, 1964 (1998).

ClCCN

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CN stretch	2114sT	Ar	IR	1,2
			995msT	Ar	IR	1,2

References

[1] D. E. Milligan, M. E. Jacox, and A. M. Bass, J. Chem. Phys. **43**, 3149 (1965).
[2] G. Maier, A. Bothur, J. Eckwert, and H. P. Reisenauer, Chem. Eur. J. **4**, 1964 (1998).

BrCNC

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NC stretch	1922.3vs	Ar	IR	1,2
			1925.7	N_2	IR	2
	2	CN stretch	1034.3m	Ar	IR	1,2
			1038.5	N_2	IR	2
	3	CNC deform.	672.4wm	Ar	IR	2

References

[1] D. E. Milligan, M. E. Jacox, and A. M. Bass, J. Chem. Phys. **43**, 3149 (1965).
[2] G. Maier, A. Bothur, J. Eckwert, and H. P. Reisenauer, Chem. Eur. J. **4**, 1964 (1998).

BrCCN

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CN stretch	2101.1mT	Ar	IR	1,2
			984.5vsT	Ar	IR	1,2

References

[1] D. E. Milligan, M. E. Jacox, and A. M. Bass, J. Chem. Phys. **43**, 3149 (1965).
[2] G. Maier, A. Bothur, J. Eckwert, and H. P. Reisenauer, Chem. Eur. J. **4**, 1964 (1998).

N_4

$\tilde{X}$ T_d

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
f_2	3		936.7T	N_2	IR	1

Reference

[1] J. P. Zheng, J. Waluk, J. Spanget-Larsen, D. M. Blake, and J. G. Radziszewski, Chem. Phys. Lett. **328**, 227 (2000).

P_4

$\tilde{X}\,^1A_1$ T_d Structure: IR[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1		600.5	gas	Ra	2,4,5
e	2		360.8	gas	Ra	2–5
f_2	3		466.29	gas	IR,Ra	1,2,4–6
			465.8	Ar	IR	7

$B_0 = 0.113$ IR[6]

References

[1] H. Gutowsky and C. Hoffman, J. Am. Chem. Soc. **72**, 5751 (1950).
[2] Y. M. Bosworth, R. J. H. Clark, and D. M. Rippon, J. Mol. Spectrosc. **46**, 240 (1970).
[3] N. J. Brassington, H. G. M. Edwards, and D. A. Long, J. Raman Spectrosc. **11**, 346 (1981).
[4] H. G. M. Edwards, J. Mol. Struct. **295**, 95 (1993).
[5] B. Persson, R. Taylor, and T. Lee, J. Chem. Phys. **107**, 5051 (1997).
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YO_3^-

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	YO_3 stretch	530.8	Ar	IR	1

Reference

[1] L. Andrews, M. Zhou, G. V. Chertihin, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **103**, 6525 (1999).

VO_3^-

Threshold for electron detachment from ground-state $VO_3^- = 35180(400)$ gas PE[1]

Reference

[1] H. Wu and L.-S. Wang, J. Chem. Phys. **108**, 5310 (1998).

NbO_3^-

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	NbO_3 stretch	817.1	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 8251 (1998).

TaO_3^-

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	TaO_3 stretch	807.0	Ar	IR	1,2

References

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 8251 (1998).
[2] M. Chen, X. Wang, L. Zhang, M. Yu, and Q. Qin, Chem. Phys. **242**, 81 (1999).

CrO_3^-

Threshold for electron detachment from ground-state $CrO_3^- = 29530(160)$ gas PE[2]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CrO_3 stretch	943.9	Ne	IR	1

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[1] M. Zhou and L. Andrews, J. Chem. Phys. **111**, 4230 (1999).
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ReO_3^-

Threshold for electron detachment from ground-state $ReO_3^- = 29000(800)$ gas PE[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e′	3	ReO_3 stretch	923.7	Ne	IR	1

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PrO_3^-

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	PrO_3 stretch	585.3	Ne	IR	1
			573.9	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 3171 (1999).

GdO_3^-

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		GdO stretch	566.1	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 3171 (1999).

TbO_3^-

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		TbO stretch	596.1T	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **103**, 6972 (1999).

UO_2F

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		UO_2 a-stretch	871.7	Ar	IR	1
			867.8			

Reference

[1] P. F. Souter and L. Andrews, J. Mol. Struct. **412**, 161 (1997).

t-OCCO$^-$

In solid neon, threshold for electron detachment <18000.[1,2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	3	Bend	524[a]	Ne	IR	2
b_u	5	CO a-stretch	1517.7	Ne	IR	1,2,5
			1515.5	Ar	IR	3,4

[a]$(\nu_3+\nu_5)-\nu_5$. Tentative assignment of combination band.

References

[1] M. E. Jacox and W. E. Thompson, Res. Chem. Intermed. **12**, 33 (1989).
[2] W. E. Thompson and M. E. Jacox, J. Chem. Phys. **95**, 735 (1991).
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ClCNO$^+$

$\tilde{A}\,^2\Pi$ $C_{\infty v}$
$T^a=28400(800)$ gas PE[1]

[a]From vertical ionization potentials.

Reference

[1] T. Pasinszki and N. P. C. Westwood, J. Phys. Chem. A **102**, 4939 (1998).

ONNO$^+$ [a]

In a neon matrix, photoisomerizes to the higher energy isomer or is promoted to a metastable state which has its ν_5 absorption[10,13,15] at 1424.1 when the deposit is exposed to 540–580 nm mercury-arc radiation.[15] The reverse conversion occurs on slight warming of the deposit or on exposure of the deposit to tungsten-lamp radiation of wavelength longer than 780 nm.[15]

In the gas phase, dissociates into $NO+NO^+$, with onset at 10700(1000) and maximum at 16400(1000). AB[2–5,7]PE[8]

$\tilde{X}$ $C_{2h}(C_{2v})$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
$a_g(a_1)$	1	NO s-stretch	2090.8	gas	PI,PE	6,8
					TPE	11,12,16
			2064.7[b]	Ne	IR	10,13,15
			2054.2[b]	Ar	IR	14
	2		317.4	gas	TPE	16
	3		118.5	gas	TPE	11,12,16
$a_u(a_2)$	4	Torsion	131.5	gas	TPE	16
$b_u(b_2)$	5	NO a-stretch	1618.2	gas	TPE	12,16
			1619.2	Ne	IR	10,12,13,15
			1593.3	Ar	IR	1,9,14
	6	Deformation	327.2	gas	TPE	11,16

[a]It is uncertain whether the *cis*- or the *trans*- isomer is the lower energy structure. *Ab initio* calculations suggest that the energy separation between the two isomers is small. The observation of the ν_1 absorption only for the noncentrosymmetric isotopomers[10,13] is consistent with the selection rules for the *trans*- but not the *cis*- conformation. However, a possible exception has been discussed by Ref. 15.
[b]$(\nu_1+\nu_5)-\nu_5$.

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ClBNCl

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BN stretch	2034	Ar	IR	1

Reference

[1] L. A. Johnson, S. A. Sturgis, I. A. Al-Jihad, B. Liu, and J. V. Gilbert, J. Phys. Chem. A **103**, 686 (1999).

$FAlO_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1		1077.3	Ar	IR	1
b_2	5		781.8	Ar	IR	1

Reference

[1] J. Bahlo, H.-J. Himmel, and H. Schnöckel, Angew. Chem. Int. Ed. **40**, 4696 (2001).

$F_2C=C$:

In an argon matrix, absorption maxima at 43860 (228 nm) and 39370 (254 nm) have been assigned[2] to $F_2C=C$:.

$\tilde{a}\,^3A_2$ C_{2v}
$T_0 = 7455(70)$ gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	C=C stretch	1670(25)	gas	PE	1
			1672m	Ar	IR	2
	2	CF_2 s-stretch	905(25)	gas	PE	1
			918m	Ar	IR	2
	3	CF_2 scissors	510(25)	gas	PE	1
			511w	Ar	IR	2
b_1	4	OPLA	551w	Ar	IR	2
b_2	5	CF_2 a-stretch	1267vs	Ar	IR	2
	6	CF_2 rock	334T	Ar	IR	2

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ClCNO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CNO a-stretch	2219	gas	IR	2
			2281.4	Ar	IR	1
			2261.7			
	2	CNO s-stretch	1343T	gas	IR	2
			1326.3	Ar	IR	1

Barrier to linearity = 167.[3]

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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. Pasinski and N. P. C. Westwood, J. Phys. Chem. A **102**, 4939 (1998).
[3] H. Lichau, C. W. Gillies, J. Z. Gillies, S. C. Ross, B. P. Winnewisser, and M. Winnewisser, J. Phys. Chem. A **105**, 10065 (2001).

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

Barrier to linearity = 131.[3]

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[1] G. Maier and J. H. Teles, Angew Chem. **99**, 152 (1987); Angew. Chem. Int. Ed. Engl. **26**, 155 (1987).
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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,Ra	3,13,15,24,26
			1867.2	Ne	IR	14,16,17,27
			1863.4m	Ar	IR	1,21
			1867.0	N_2	IR	2,17,23
			1862m	CO_2	IR,Ra	1,8
			1866	NO	IR,Ra	5,6,10
	2	N··N stretch	239.36	gas	IR,Ra	22,25,26
			242.8	Ar	IR	21
			244.5	N_2	IR	23
			262	CO_2	Ra	8
			266	NO	IR,Ra	5,6,10
	3	NNO s-bend	134.50	gas	IR,Ra	22,25,26
			175.5T	Ar	IR	21
a_2	4	Torsion	117T	gas	IR	22
			97T	NO	IR,Ra	5,6,10
b_2	5	NO a-stretch	1789.09	gas	IR,DL	3,11,12 13,18,19
			1780.6	Ne	IR	14,16,17,27
			1778.7			
			1776.3s	Ar	IR	1,21
			1779.9	N_2	IR	2,17,23
			1768s	CO_2	IR	1
			1762	NO	IR,Ra	6,10
	6	NNO a-bend	429.14vw	gas	IR	22,25

$A_0 = 0.862$; $B_0 = 0.187$; $C_0 = 0.154$ MW[9,20]IR[15]

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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	3,7
			1760.6			
			1747.1	Ar	IR	5
			1760.0	N_2	IR	2,4,5,6
			1740	CO_2	IR	1

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[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).
[5] L. Krim and N. Lacome, J. Phys. Chem. A **102**, 2289 (1998).
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[7] L. Andrews and M. Zhou, J. Chem. Phys. **111**, 6036 (1999).

BF_3^+

$\tilde{E}\,^2A_1'$ D_{3h}
$T_0 \cong 47800$ gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	BF stretch	800T	gas	PE	3

$\tau = 10$ ns gas EM[5]

$\tilde{D}\,^2E'$ D_{3h}
$T_0 = 34860(160)$ gas PE[1,4,7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	BF stretch	760(20)	gas	PE	1,4,7

Additional structure reported by Ref. 4 has been attributed to vibronic coupling.

$\tilde{C}\,^2A_2''$ D_{3h}
$T_0 = 27110(80)$ gas PE[1,2,4,7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	BF stretch	775(20)	gas	PE	2,4,7

$\tilde{B}\,^2E'$ D_{3h}
$T_0 = 10890(240)$ gas PE[1,2,4,7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	BF stretch	770(60)	gas	PE	1,4,7

$\tilde{A}\,^2E''$ D_{3h}
$T_0 = 5890(240)$ gas PE[1,4,7]

$\tilde{X}\,^2A_2'$ 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

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BCl_3^+

$\tilde{E}\,^2A_1'$ D_{3h}
$T_0 = 49200(120)$ gas PE[1,8]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	1,6,8

$\tilde{D}\,^2E'$ D_{3h}
$T_0 = 29700(120)$ gas PE[1,8]TPE[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	BCl stretch	420(20)	gas	PE	8

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]
$\tau=8.9(2)$ ns gas EM[9]

$\tilde{C}\,^2A_2''$ D_{3h}
$T_0=21780(120)$ gas PE[1,8]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	1,6,8

$\tilde{B}\,^2E'$ D_{3h}
$T^a=9280(120)$ gas PE[1,8]TPE[6]
$A=800$T gas TPE[6]

$\tilde{A}\,^2E''$ D_{3h}
$T_0=5080(120)$ gas PE[1,8]TPE[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	4	Deformation	320T	gas	PE	8

$\tilde{X}\,^2A_2'$ 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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BBr_3^+

$\tilde{F}$
$T\cong 53500(480)$ gas PE[1]

$\tilde{E}\,^2A_1'$ D_{3h}
$T_0=49380(560)$ gas PE[1,4]

$\tilde{D}\,^2E'$ D_{3h}
$T_0^a=25500(400)$ gas PE[1,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	BBr stretch	250(20)	gas	PE	4

Emission between 240 and 390 nm, with a lifetime $\leqslant$16 ns, which is observed when gas-phase BBr_3 is excited by radiation of wavelength shorter than 89 nm has been assigned[3] to the $\tilde{D}-\tilde{X}$ transition of BBr_3^+.

A broad absorption with maximum at 355 nm (28200) which appears on argon-resonance photolysis of BBr_3 isolated in an argon matrix and which can be destroyed by prolonged exposure of the sample to 340–600 nm radiation has been assigned[2] to the $\tilde{D}-\tilde{X}$ transition of BBr_3^+.

$A=2300(160)$ gas PE[1,4]

$\tilde{C}\,^2A_2''$ D_{3h}
$T_0=18440(480)$ gas PE[1,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	BBr stretch	260(20)	gas	PE	4

$\tilde{B}\,^2E'$ D_{3h}
$T^b=9680(480)$ gas PE[1,4]

$\tilde{A}\,^2E''$ D_{3h}
$T_0^a=5000(400)$ gas PE[1,4]
$A\cong 1130$ gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	3	BBr stretch	930	Ar	IR	2

[a]Onset of transition.
[b]From vertical ionization potential.

References

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BI_3^+

$\tilde{E}\,^2A_1'$ D_{3h}
$T_0 = 47200(400)$ gas PE[1,2]

$\tilde{D}\,^2E'$ D_{3h}
$T_0^a = 24450(480)$ gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	BI stretch	160(20)	gas	PE	2

$A = 4030(80)$ gas PE[1,2]

$\tilde{C}\,^2A_2''$ D_{3h}
$T_0 = 17840(400)$ gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	BI stretch	180(20)	gas	PE	2

$\tilde{B}\,^2E''$ D_{3h}
$T_0^a = 8310(400)$ gas PE[1,2]
$A = 810(160)$ gas PE[1]

$\tilde{A}\,^2E'$ D_{3h}
$T_0^a = 4840(400)$ gas PE[1,2]
$A = 1450(160)$ gas PE[1]

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

[a]Onset of transition.

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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	4,7
			1205.5m	Ar	IR	1,3

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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 $NO + NO^-$. Maximum in the photoelectron spectrum at 23640(400), or 2.93(5) eV gas PE[3]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_u	5	Asym. stretch	1227.5	Ne	IR	4,6
			1221.0	Ar	IR	2,5

References

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[6] L. Andrews and M. Zhou, J. Chem. Phys. **111**, 6036 (1999).

c-$(NO)_2^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NO s-stretch	1300.3	Ar	IR	1
b_2	5	NO a-stretch	1225.1	Ne	IR	3
			1222.7	Ar	IR	1,2
	6	NNO deform.	884.4	Ar	IR	1

References

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[3] L. Andrews and M. Zhou, J. Chem. Phys. **111**, 6036 (1999).

NO_3

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

$T_0=15089$ gas $AB^{1,2,4-7}LF^{8,9,17,21}$ $\tilde{B}-\tilde{X}$ 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

$\tau_0=340(20)$ μs gas LF^{10}

$\tilde{A}\,^2E''$ D_{3h} Structure: DL^{22}

$T_0=7061(8)$ gas $PE^{14}IR^{23}$

A high resolution diode laser study has been reported[22] for a band at 7602.58, contributed by excitation to the $^2A_1''$ vibronic component of $\nu_4=1$ in the $\tilde{A}$ state.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	804(4)T	gas	PE	14
a_2''	2	OPLA	683(8)T	gas	IR	23
e'	4	Deformation	541(8)T	gas	PE	14

$B_{0001}=0.433$; $C_{0001}=0.216$ DL^{22}

$\tilde{X}\,^2A_2'$ D_{3h} Structure: DL^{11}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	1050	gas	LF,PE	8,9,14,17
a_2''	2	OPLA	762.33	gas	IR,LF	12,17
e'	3	NO stretch[a]	1492.39	gas	LF,DL	8,9,11,17
					IR	12
	4	Deformation[b]	360	gas	LF,PE	8,9,14,17

$B_0=0.459$ $DL^{11,13}IR^{12,23}$

[a]Anomalous structure appears in the high resolution spectrum of this band because of the 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.[15,18,23] 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 υ_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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c-OSNO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO stretch	1450.8	Ar	IR	1
			1454.4	N_2	IR	1
	2	SO stretch	1154.9	Ar	IR	1
			1156.1	N_2	IR	1

Reference

[1] M. Bahou and Y.-P. Lee, J. Chem. Phys. **115**, 10694 (2001).

t-OSNO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO stretch	1456.0	Ar	IR	1
			1459.0	N_2	IR	1
	2	SO stretch	1181.2	Ar	IR	1
			1178.0	N_2	IR	1

Reference

[1] M. Bahou and Y.-P. Lee, J. Chem. Phys. **115**, 10694 (2001).

PO_3

$\tilde{C}\,^2E'$[a] D_{3h}
$T_0=14378$T Ar AB[1,3] $\tilde{B}-\tilde{X}$ 589–696 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	PO_3 s-stretch	913(10)	Ar	IR	1
e'	4	Deformation	525(10)	Ar	IR	1

$\tilde{B}\,^2A_2$ D_{3h}[b]
T[c]$=8790(680)$ gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	4	Deformation	500(80)	gas	PE	2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	1000(100)	gas	PE	2

[a]Tentative assignment, by analogy with NO_3.
[b]Upper component of $^2E''$ state, which is split by Jahn–Teller interaction.
[c]From vertical ionization potential.

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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	4,5
b_u	5	O=O a-stretch	1164.4	Ne	IR	4,5
			1118.6	Ar	IR	5

[a]$(\nu_1+\nu_5)-\nu_5$.

References

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cyc-O_4^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	O=O s-stretch	1628.3[a]	Ne	IR	1–3
b_{1u}	5	O=O a-stretch	1320.3	Ne	IR	1–3
			1331.4	Ar	IR	3
			1328.9			

[a]$(\nu_1+\nu_5)-\nu_5$.

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[1] W. E. Thompson and M. E. Jacox, J. Chem. Phys. **91**, 3826 (1989).
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CCl_3^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	3	CCl stretch	1045.9	Ne	IR	4
			1037	Ar	IR	1–3

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Cl_2SiO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Si=O stretch	1240s	Ar	IR	1,2
	2	SiCl s-stretch	501.1m	Ar	IR	1,2
b_1	4	OPLA	280ms	Ar	IR	1
b_2	5	SiCl a-stretch	637.5vs	Ar	IR	1,2
	6	$SiCl_2$ rock	269m	Ar	IR	1

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F_2SiS

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiF_2 s-stretch	996vs	Ar	IR	1
	2	SiS stretch	638vw	Ar	IR	1
	3	SiF_2 scissors	337wm	Ar	IR	1
b_1	4	OPLA	296m	Ar	IR	1
b_2	5	SiF_2 a-stretch	969s	Ar	IR	1
	6	FSiS deform.	247w	Ar	IR	1

Reference

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c-$OONO^-$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	N=O stretch	1458.3	Ar	IR	1
	3		806.1	Ar	IR	1

Reference

[1] B. Liang and L. Andrews, J. Am. Chem. Soc. **123**, 9848 (2001).

t-$OONO^-$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	N=O stretch	1433.3	Ar	IR	1
	2		983.2	Ar	IR	1

Reference

[1] B. Liang and L. Andrews, J. Am. Chem. Soc. **123**, 9848 (2001).

$BrNO_2$

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	1294.40	gas	IR	3–5,8
			1291.0vs	Ar	IR	1,2,5,7
			1291	O_2	IR	4
	2	NO_2 deform.	787	gas	IR	3–5
			782.7s	Ar	IR	2,5,7
			784	O_2	IR	4
	3	NBr stretch	281.8w	Ar	IR	5,7
			280.7w			
b_1	4	OPLA	605	gas	IR	5
			605.7	Ar	IR	5,7
b_2	5	NO_2 a-stretch	1666.98	gas	IR	3–6
			1659.6vs	Ar	IR	2,5,7
			1655	O_2	IR	4
	6	NO_2 wag	290Tsh	Ar	IR	5

$A_0 = 0.443$; $B_0 = 0.102$; $C_0 = 0.083$ IR[6,8]

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c-BrONO

In the gas phase, *c*-BrONO has unstructured absorption maxima at 43860 (228 nm) and 31650 (316 nm).[2]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	N=O stretch	1650.7vs	Ar	IR	1
	2	ONO deform.	862.6w	Ar	IR	1
	3	BrO stretch	573.5m	Ar	IR	1
	4	O–N stretch	420.2wm	Ar	IR	1
a''	6	Torsion	368.2w	Ar	IR	1

References

[1] D. Scheffler and H. Willner, Inorg. Chem. **37**, 4500 (1998).
[2] J. B. Burkholder and J. J. Orlando, Chem. Phys. Lett. **317**, 603 (2000).

t-BrONO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	N=O stretch	1723.4vs	Ar	IR	1–4
	2	ONO deform.	835.9m	Ar	IR	2–4
	3	BrO stretch	586.9vs	Ar	IR	1–4
	4	O–N stretch	391.2wm	Ar	IR	2–4
a''	6	Torsion	150HT	Ar	IR	3,4

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).
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PO_3^-

Threshold for electron detachment from ground-state PO_3^- = 39940(480) gas PE[2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	480.3	Ar	IR	1,3
e'	3	PO_3 stretch	1273.3	Ar	IR	1,3

References

[1] R. Withnall and L. Andrews, J. Phys. Chem. **92**, 4610 (1988).
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PO_2Cl

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PO_2 s-stretch	1122	Ar	IR	1
	2	PCl stretch	586	Ar	IR	1
b_2	5	PO_2 a-stretch	1429	Ar	IR	1

$A_0 = 0.296$; $B_0 = 0.141$; $C_0 = 0.095$ MW[2]

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[2] B. Brupbacher-Gatehouse, J. Am. Chem. Soc. **122**, 4171 (2000).

F_2PO^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PO stretch	1473.2wmT	Ne	IR	1
b_2	5	PF stretch	1135.5wT	Ne	IR	1

Reference

[1] C. L. Lugez, K. K. Irikura, and M. E. Jacox, J. Chem. Phys. **108**, 8381 (1998).

CCl_3

$\tilde{M}\,^2E'(4d)$[a] D_{3h}
$T_0 = 57733(10)$ gas MPI[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	542(3)	gas	MPI	9

$\tilde{L}\,^2A_2''(4p)$ D_{3h}
$T_0 = 56409(10)$ gas MPI[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	533(15)	gas	MPI	9

$\tilde{K}\,^2E'(4p)$ D_{3h}
$T_0 = 56236(10)$ gas MPI[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	526(16)	gas	MPI	9

$\tilde{J}\,^2A_1'(4s)$ D_{3h}
$T_0 = 53471(10)$ gas MPI[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	530(20)	gas	MPI	9

$\tilde{G}\,^2E'(3d)$[a] D_{3h}
$T_0 = 51218(10)$ gas MPI[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	520(17)	gas	MPI	9

$\tilde{F}\,^2A_2''(3p)$ D_{3h}
$T_0 = 47868(10)$ gas MPI[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	528(3)	gas	MPI	9

$\tilde{E}\,^2E'(3p)$ D_{3h}
$T_0=47170(10)$ gas MPI[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	544(6)	gas	MPI	9
a_2''	2	OPLA	509(21)	gas	MPI	9

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

$\tilde{C}\,^2A_1'(3s)$ D_{3h}
gas AB[8,11] $\tilde{C}-\tilde{X}$ 265–195 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	569(63)	gas	AB	11

Photodissociation of CCl_3 in a pulsed supersonic beam to produce CCl_2+Cl has been observed[10] at 308 nm.

A broad emission observed in radiofrequency discharges between 420 and 700 nm, with a maximum near 490 nm, has been attributed[7] to a transition between two electronically excited states of CCl_3.

$\tilde{X}\,^2A_1$ C_{3v} Structure: ESR[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2	2	Umbrella	290[b]	gas	MPI	9
			251			
e	3	CCl stretch	908.5	Ne	IR	12
			898vs	Ar	IR	1–4,6

[a]Tentative symmetry assignment.
[b]Inversion doublet. Barrier to inversion=460(40) gas MPI[9]

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[1] L. Andrews, J. Phys. Chem. **71**, 2761 (1967).
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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[4,8] 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. The lifetime for the emission between 380 and 650 nm has been found to be 3.9(7) ns.[8] 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} Structure: MW[9]

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

$B_0=0.250$ MW[9]

References

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F_2NO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO stretch	1573	Ar	IR	1
	2	NF_2 s-stretch	761	Ar	IR	1
	3	NF_2 scissors	705	Ar	IR	1
a''	5	NF_2 a-stretch	813	Ar	IR	1
	6	NF_2 deform.	553	Ar	IR	1

Reference

[1] E. Ya. Misochko, A. V. Akimov, I. U. Goldschleger, and C. A. Wight, J. Am. Chem. Soc. **120**, 11520 (1998).

PF_3^+

$\tilde{E}\,^2E$ C_{3v}
$T_0^a \geqslant 61500(200)$ gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PF stretch	660(30)	gas	PE	2
	2	Umbrella	360(30)	gas	PE	2

$\tilde{D}\,^2A_1$ C_{3v}
$T_0^a \geqslant 55000(200)$ gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PF stretch	690(30)	gas	PE	2
	2	Umbrella	395(30)	gas	PE	2

$\tilde{C}\,^2E$ C_{3v}
$T_0^a \geqslant 45500(200)$ gas PE[1,2]

$\tilde{B}\,^2E$ C_{3v}
$T^{ab} \geqslant 39300(600)$ gas PE[1,2]

$\tilde{A}\,^2A_2$ C_{3v}
$T_0^a \geqslant 31220(500)$ gas PE[1,2]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PF stretch	940.0ms	Ne	IR	5
	2	Umbrella	475(30)	gas	PE	1,2
			465.1ms	Ne	IR	5
e	3	PF stretch	1097.5s	Ne	IR	5

[a]In accord with recent photoionization studies,[3,4] the first ionization potential of PF_3 is taken to be $\leqslant 11.44$ eV.
[b]From vertical ionization potential.

References

[1] P. J. Bassett and D. R. Lloyd, J. Chem. Soc., Dalton Trans. 248 (1972).
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PCl_3^+

$\tilde{F}\,^2A_1$ C_{3v}
$T^a = 67050(320)$ gas PE[1,3]

$\tilde{E}\,^2E$ C_{3v}
$T^a = 37840(320)$ gas PE[1–3]
In the gas phase, an emission which results on vacuum ultraviolet excitation of PCl_3 which has its maximum near 550 nm, has been attributed[4] to the $\tilde{E}-\tilde{C}$ transition of PCl_3^+. Emission between 320 and 450 nm is attributed[4] to the $\tilde{E}-\tilde{B}$ and $\tilde{E}-\tilde{A}$ transitions.

$\tilde{D}\,^2A_1$ C_{3v}
$T^a = 30010(320)$ gas PE[1–3]

$\tilde{C}\,^2E$ C_{3v}
$T^a = 19850(320)$ gas PE[1–3]

$\tilde{B}\,^2E$ C_{3v}
$T^a = 12020(320)$ gas PE[1–3]

$\tilde{A}\,^2A_2$ C_{3v}
$T^a = 9600(320)$ gas PE[1–3]

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

[a]From vertical ionization potentials.

References

[1] P. A. Cox, S. Evans, A. F. Orchard, N. V. Richardson, and P. J. Roberts, Faraday Discuss. Chem. Soc. **54**, 26 (1972).
[2] J. L. Berkosky, F. O. Ellison, T. H. Lee, and J. W. Rabalais, J. Chem. Phys. **59**, 5342 (1973).
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PBr_3^+

$\tilde{E}\,^2E$ C_{3v}
$T^a = 33560(320)$ gas PE[1–3]

Unstructured emission between 500 and 600 nm which appears on vacuum ultraviolet excitation of gas-phase PBr_3 has been attributed[4] to the $\tilde{E}-\tilde{C}$ transition of PBr_3^+. Emission between 320 and 450 nm has been attributed[4] to the $\tilde{E}-\tilde{B}$ and $\tilde{E}-\tilde{A}$ transitions.

$\tilde{D}\,^2A_1$ C_{3v}
$T^a = 25580(320)$ gas PE[1–3]

$\tilde{C}\,^2E$ C_{3v}
$T^a = 14760(320)$ gas PE[1–3]

$\tilde{B}\,^2E$ C_{3v}
$T^a = 8390(320)$ gas PE[1–3]
$A = 2660(320)$ gas PE[1–3]

$\tilde{A}\,^2A_2$ C_{3v}
$T^a = 5240(320)$ gas PE[1–3]

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

[a]From vertical ionization potentials.

References

[1] P. A. Cox, S. Evans, A. F. Orchard, N. V. Richardson, and P. J. Roberts, Faraday Discuss. Chem. Soc. **54**, 26 (1972).
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cyc-O_4^-

An unstructured absorption which appears near 270 nm in Ar:O_2 samples in which an alkali metal is also present and which grows on controlled warmup of the sample has been attributed[6] to $M^+O_4^-$.

Threshold for photodestruction near 900 nm, and increasing cross section for photodestruction, probably by photodetachment, in the 850–400 nm spectral region.[7] Photoelectron studies[8] suggest that both photodetachment and photodissociation occur at 532 and 355 nm.

$\tilde{X}$ D_{2h} Structure: IR[11]MO[12]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	O=O stretch	1292 K	Ar	IR	9
	2	O···O stretch	287 Cs	Ar	Ra	5
			298 Rb	Ar	Ra	5
			305 K	Ar	Ra	4
b_{1u}	5	O=O a-stretch	973.1	Ne	IR	10
			953.8	Ar	IR	11
			1001 Cs	Ar	IR	3
			992 Rb	Ar	IR	2
			993 K	Ar	IR	2,9
			1001 Na	Ar	IR	1,3
			991 Na			
			990.8	N_2	IR	11
b_{2u}	6	Asym. bend	131 K	Ar	IR	9

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[12] A. J. A. Aquino, P. R. Taylor, and S. P. Walch, J. Chem. Phys. **114**, 3010 (2001).

$ClSO_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SO_2 s-stretch	1098.2s	Ar	IR	1
			1098.5s	Kr	IR	1
	2	OSO bend	497.7ms	Ar	IR	1
			497.0ms	Kr	IR	1
	3	Umbrella	456.1m	Ar	IR	1
			454.2m	Kr	IR	1
a''	5	SO_2 a-stretch	1309.6vs	Ar	IR	1
			1309.5vs	Kr	IR	1

Reference

[1] M. Bahou, S.-F. Chen, and Y.-P. Lee, J. Phys. Chem. A **104**, 3613 (2000).

F_2SO^+

$\tilde{E}$ C_s
$T_0 = 47120(320)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	SF_2 stretch	705(40)	gas	PE	1
	4	SF_2 scissors	390(40)	gas	PE	1

$\tilde{D}\ ^2A'$ C_s
$T^a = 38570(320)$ gas PE[1,2]

$\tilde{C}\ ^2A''$ C_s
$T^a = 34800(1000)$ gas PE[1,2]

$\tilde{B}\ ^2A''$ C_s
$T_0 = 18960(320)$ gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SO stretch	1180(40)	gas	PE	1,2
	2	SF_2 s-stretch	790(40)	gas	PE	1,2
	4	SF_2 scissors	350(40)	gas	PE	1,2

$\tilde{A}\ ^2A''$ C_s
$T^a = 15330(500)$ gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SO stretch	1000T	gas	PE	2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	FSO s-deform.	420(40)	gas	PE	1,2
			455.6	Ne	IR	3

[a] From vertical ionization potential.

References

[1] G. W. Mines, R. K. Thomas, and H. Thompson, Proc. R. Soc. London, Ser. A **329**, 275 (1972).
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[3] C. L. Lugez, M. E. Jacox, R. A. King, and H. F. Schaefer III, J. Chem. Phys. **108**, 9639 (1998).

F_2PO^-

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	PO stretch	1148.8wmT	Ne	IR	1
	2	PF stretch	685.7wT	Ne	IR	1

Reference

[1] C. L. Lugez, K. K. Irikura, and M. E. Jacox, J. Chem. Phys. **108**, 8381 (1998).

ClO_3^-

Threshold for electron detachment from ground-state ClO_3^- = 34290(800) gas PE[1]

Reference

[1] X.-B. Wang and L.-S. Wang, J. Chem. Phys. **113**, 10928 (2000).

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	4,9
			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	4,9
			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]

References

[1] R. A. Cox and G. D. Hayman, Nature (London) **332**, 796 (1988).
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[9] A. S. Brust, F. Zabel, and K. H. Becker, Geophys. Res. Lett. **24**, 1395 (1997).

$ClClO_2$

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[6,7]

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[6,7]

References

[1] H. S. P. Müller and H. Willner, Proc. 1st European Workshop on Polar Stratospheric Ozone, Schliersee, Germany, 1990 (Air Pollution Research Report 34, CEC and BMFT, J. A. Pyle and N. R. P. Harris, Eds.).
[2] H. S. P. Müller and H. Willner, Ber. Bunsenges. Phys. Chem. **96**, 427 (1992).
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SF_3^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SF stretch	944.2	Ne	IR	1
	2	Deformation	540.7T	Ne	IR	1
e	3	SF stretch	969.0	Ne	IR	1

Reference

[1] C. L. Lugez, M. E. Jacox, R. A. King, and H. F. Schaefer III, J. Chem. Phys. **108**, 9639 (1998).

PF_3^-

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	5	PF stretch	470.9	Ne	IR	1

Reference

[1] C. L. Lugez, K. K. Irikura, and M. E. Jacox, J. Chem. Phys. **108**, 8381 (1998).

8.8. Five-Atomic Tetra- and Trihydrides

$Pd(H_2)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	4	HH stretch	3038	Ar	IR	1
	5	PdH stretch	792.4	Ne	IR	1
			778.0	Ar	IR	1

$Pd(D_2)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	4	DD stretch	2160	Ar	IR	1
	5	PdD stretch	597.5	Ne	IR	1
			585.7	Ar	IR	1

Reference

[1] L. Andrews, X. Wang, M. E. Alikhani, and L. Manceron, J. Phys. Chem. A **105**, 3052 (2001).

CeH_4

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Sym. stretch	1500.5	Ar	IR	1
		Asym. stretch	1441.8	Ar	IR	1

CeD_4

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Sym. stretch	1070.2	Ar	IR	1
		Asym. stretch	1032.1	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **104**, 1640 (2000).

NdH_4

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Sym. stretch	1384.6	Ar	IR	1
		Asym. stretch	1304.3	Ar	IR	1
			1300.7			

NdD_4

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Sym. stretch	986.3	Ar	IR	1
		Asym. stretch	935.5	Ar	IR	1
			931.6			

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **104**, 1640 (2000).

SmH_4

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Asym. stretch	1331.4	Ar	IR	1
			1328.7			

SmD_4

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Asym. stretch	954.1	Ar	IR	1
			952.1			

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **104**, 1640 (2000).

DyH_4

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Asym. stretch	1386.6	Ar	IR	1

DyD_4

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Asym. stretch	992.9	Ar	IR	1

Reference

[1] S. P. Willson and L. Andrews, J. Phys. Chem. A **104**, 1640 (2000).

CH_4^+

$\tilde{C}\,^2A_1$ T_d
$T_0 = 78870(160)$[a] gas PE[3,6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	2190(80)	gas	PE	6

$\tilde{B}$[b] C_s?
T[c] $\cong 19240$ gas PE[1–3,5,6]

$\tilde{A}$[b] C_s?
$T_0 \leqslant 13350$[a] gas PE[1–3,5,6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1300(100)	gas	PE	5

$\tilde{X}\,^2B_2$[b] C_{2v} Structure: ESR[7]MO[8,10]TPE[11–13]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1700(100)[d]	gas	PE	5
			1200(100)	gas	PE	3,5

Evidence has been obtained[11] for the occurrence of pseudorotation.

CD_4^+

$\tilde{C}\,^2A_1$ T_d
$T_0 = 79400(200)$ gas PE[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD stretch	1460(80)	gas	PE	3,6

$\tilde{X}\,^2B_2$[b] C_{2v}
$A_0 = 3.368(59)$; $B_0 = 2.640(108)$; $C_0 = 1.967(54)$ TPE[13]

[a] Based on adiabatic ionization potential of 12.615(10) eV for CH_4[4,5] and of 12.658(15) eV for CD_4.[9]
[b] Resulting from Jahn–Teller distortion of the ground $^2F_2$ state of CH_4^+.
[c] From vertical ionization potential.
[d] Two progressions, with onset near 3670.

References

[1] A. D. Baker, C. Baker, C. R. Brundle, and D. W. Turner, Int. J. Mass Spectrom. Ion Phys. **1**, 285 (1968).
[2] B. P. Pullen, T. A. Carlson, W. E. Moddeman, G. K. Schweitzer, W. E. Bull, and F. Grimm, J. Chem. Phys. **53**, 768 (1970).
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[10] R. F. Frey and E. R. Davidson, J. Chem. Phys. **88**, 1775 (1988).
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[13] R. Signorell and F. Merkt, Faraday Discuss. Chem. Soc. **115**, 205 (2000).

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 EM[1,2] TPE[8] $3p^2F_2 - 3s^2A_1$ 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.
$B_0 = 2.937$ gas TPE[8]

$3s\ ^2A_1$ T_d

gas EM[1,2,4,7] $3p^2F_2 - 3s^2A_1$ 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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$LiCH_3$

$\tilde{X}\ ^1A_1$ C_{3v} Structure: MW[2–4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 s-stretch	2780	Ar	IR	1
	2	CH_3 umbrella	1158	Ar	IR	1
	3	CLi stretch	530T	Ar	IR	1
e	4	CH_3 a-stretch	2820	Ar	IR	1
	5	CH_3 deformation	1387	Ar	IR	1
	6	HCLi deformation	408.5	Ar	IR	1

$B_0 = 0.765$ MW[2,3]

$LiCD_3$

$\tilde{X}\ ^1A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_3 s-stretch	2030	Ar	IR	1
	2	CD_3 umbrella	883	Ar	IR	1
	3	CLi stretch	510	Ar	IR	1
e	5	CD_3 deformation	1027	Ar	IR	1
	6	DCLi deformation	319	Ar	IR	1

$B_0 = 0.643$ MW[2,3]

References

[1] L. Andrews, J. Chem. Phys. **47**, 4834 (1967).
[2] D. B. Grotjahn, T. C. Pesch, J. Xin, and L. M. Ziurys, J. Am. Chem. Soc. **119**, 12368 (1997).
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$NaCH_3$

$\tilde{X}\ ^1A_1$ C_{3v} Structure: MW[2,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 s-stretch	2760s	N_2	IR	1
	2	CH_3 s-deform.	1092w	N_2	IR	1
	3	CNa stretch	298s	N_2	IR	1
e	4	CH_3 a-stretch	2805s	N_2	IR	1
	5	CH_3 a-deform.	1384w	N_2	IR	1
	6	HCNa bend	362s	N_2	IR	1

$B_0 = 0.316$ MW[2,3]

$NaCD_3$

$\tilde{X}\ ^1A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_3 s-stretch	2019m	N_2	IR	1
	2	CD_3 s-deform.	836m	N_2	IR	1
	3	CNa stretch	278m	N_2	IR	1
e	4	CD_3 a-stretch	2123m	N_2	IR	1
	5	CD_3 a-deform.	972w	N_2	IR	1
	6	DCNa bend	285s	N_2	IR	1

$B_0 = 0.266$ MW[2,3]

References

[1] K. Burczyk and A. J. Downs, J. Chem. Soc., Dalton Trans. 2351 (1990).
[2] B.-Z. Li, J. Xin, and L. M. Ziurys, Chem. Phys. Lett. **280**, 513 (1997).
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KCH_3

$\tilde{X}$ C_{3v} Structure: MW[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 s-stretch	2732s	N_2	IR	1
	2	CH_3 s-deform.	1053w	N_2	IR	1
	3	CK stretch	280	N_2	IR	1
e	4	CH_3 a-stretch	2775s	N_2	IR	1
	5	CH_3 a-deform.	1384w	N_2	IR	1
	6	HCK bend	307m	N_2	IR	1

$B_0 = 0.205$ MW[2]

KCD_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_3 s-stretch	1994m	N_2	IR	1
	2	CD_3 s-deform.	807m	N_2	IR	1
	3	CK stretch	259s	N_2	IR	1
e	4	CD_3 a-stretch	2101m	N_2	IR	1
	5	CD_3 a-deform.	967w	N_2	IR	1
	6	DCK bend	237m	N_2	IR	1

$B_0 = 0.170$ MW^2

References

[1] K. Burczyk and A. J. Downs, J. Chem. Soc., Dalton Trans. 2351 (1990).
[2] D. B. Grotjahn, T. C. Pesch, M. A. Brewster, and L. M. Ziurys, J. Am. Chem. Soc. **122**, 4735 (2000).

$MgCH_3^+$

$\tilde{X}\,^1A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 umbrella	1020	gas	TPE	1
	3	MgC stretch	516	gas	TPE	1
e	6	HCMg deform.	673	gas	TPE	1

Reference

[1] T. A. Barckholtz, D. E. Powers, T. A. Miller, and B. E. Bursten, J. Am. Chem. Soc. **121**, 2576 (1999).

$ZnCH_3^+$

$\tilde{X}\,^1A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 umbrella	1109	gas	TPE	1
	3	ZnC stretch	482	gas	TPE	1
e	6	HCZn deform.	760	gas	TPE	1

Reference

[1] T. A. Barckholtz, D. E. Powers, T. A. Miller, and B. E. Bursten, J. Am. Chem. Soc. **121**, 2576 (1999).

$CdCH_3^+$

$\tilde{X}\,^1A_1$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 deformation	1089(2)	gas	TPE	1
	3	CdC stretch	422(2)	gas	TPE	1
e	5	CH_3 deformation	1386(2)	gas	TPE	1
	6	Deformation	752(2)	gas	TPE	1

Reference

[1] S. I. Panov, D. E. Powers, and T. A. Miller, J. Chem. Phys. **108**, 1335 (1998).

$BeCH_3$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 s-deform.	1180.6 1178.9	Ar	IR	1
	3	BeC stretch	851.7	Ar	IR	1

$BeCD_3$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_3 s-deform.	962.1	Ar	IR	1
	3	BeC stretch	765.6	Ar	IR	1

Reference

[1] T. M. Greene, D. V. Lanzisera, L. Andrews, and A. J. Downs, J. Am. Chem. Soc. **120**, 6097 (1998).

CH_2BeH

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	BeH stretch	2071.9	Ar	IR	1
	3	CH_2 scissors	1388.5	Ar	IR	1
b_1	5	H_2CBe OPLA	660.0	Ar	IR	1
b_2	9	HCBe deform.	577.6T	Ar	IR	1

CD_2BeD

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	BeD stretch	1578.2	Ar	IR	1
b_1	5	D_2CBe OPLA	541.8	Ar	IR	1
b_2	8	CD_2 deform.	577.4	Ar	IR	1

Reference

[1] T. M. Greene, D. V. Lanzisera, L. Andrews, and A. J. Downs, J. Am. Chem. Soc. **120**, 6097 (1998).

$BaCH_3$

$\tilde{X}\,^2A_1$ C_{3v} Structure: MW[1]
$B_0 = 0.174$ MW[1]

Reference

[1] J. Xin, J. S. Robinson, A. J. Apponi, and L. M. Ziurys, J. Chem. Phys. **108**, 2703 (1998).

$MgCH_3$

$\tilde{A}\,^2E$ C_{3v} Structure: LF[1]
$T_0 = 20030.296(2)$ gas LF[1,3]MPI[4] $\tilde{A}-\tilde{X}$ 463–557 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 umbrella	997.5	gas	LF,MPI	3,4
	3	MgC stretch	464	gas	MPI	4
e	6		669.1(2)	gas	LF,MPI	3,4

$\tau_0 = 60(20)$ ns gas LF[3]
$A = 28.591$ gas LF[3]
$A_0 = 4.992$; $B_0 = 0.365$ LF[1]

$\tilde{X}\,^2A_1$ C_{3v} Structure: LF[1]MW[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		509	gas	LF	3
e	6		1072	gas	LF	3

$A_0 = 5.222$; $B_0 = 0.367$ LF[1,3]MW[2]

References

[1] R. Rubino, J. M. Williamson, and T. A. Miller, J. Chem. Phys. **103**, 5964 (1995).
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[4] T. A. Barckholtz, D. E. Powers, T. A. Miller, and B. E. Bursten, J. Am. Chem. Soc. **121**, 2576 (1999).

$CaCH_3$

$\tilde{B}\,^2A_1$ 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]DR[5]

[a] Predissociated above ~16200.[1]

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[1] C. R. Brazier and P. F. Bernath, J. Chem. Phys. **86**, 5918 (1987).
[2] C. R. Brazier and P. F. Bernath, J. Chem. Phys. **91**, 4548 (1989).
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[5] K. C. Namiki and T. C. Steimle, J. Chem. Phys. **110**, 11309 (1999).

$ZnCH_3$

$\tilde{C}\,^2A_1$[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]MPI[7] $\tilde{A}-\tilde{X}$ 379–437 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 deform.	1060	gas	AB,LF MPI	1,4,5,7
	3	ZnC stretch	467	gas	LF,MPI	5,7
e	6	HCZn deform.	749	gas	MPI	7

$\tau = 40(3)$ 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.

References

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

$\tilde{A}\,^2E_{1/2}$ C_{3v} Structure: LF[8]
$T_0 = 22514$ gas AB[1]EM[2–5]LF[6–9]MPI[10]FD[11] $\tilde{A}-\tilde{X}$ 400–458 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 deform.	1019(3)	gas	LF,MPI FD	7,8,10,11
	3	CdC stretch	400(3)	gas	LF,MPI FD	6–8,10,11
e	6	Deformation	638(2)	gas	MPI,FD	10,11

$\tau = 70(4)$ ns gas EM[2,4]LF[7]
$A = 1008$ gas FD[11]
$A_0 = 4.87$; $B_0 = 0.245$ LF[8]MPI[10]

$\tilde{X}\,^2A_1$ 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]

References

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[10] S. I. Panov, D. E. Powers, and T. A. Miller, J. Chem. Phys. **108**, 1335 (1998).
[11] M. B. Pushkarsky, T. A. Barckholtz, and T. A. Miller, J. Chem. Phys. **110**, 2016 (1999).

$GaCH_3$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 stretch	2986.9	Ar	IR	1,2
	2	CH_3 umbrella	1147.9	Ar	IR	1–3
	3	GaC stretch	476.2s	Ar	IR	1–3
e	5	CH_3 deform.	1403.9	Ar	IR	1,3

$GaCD_3$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_3 stretch	2200.4	Ar	IR	1,2
	2	CD_3 umbrella	902.8	Ar	IR	1,2
e	5	CD_3 deform.	1025.4	Ar	IR	1,2

References

[1] H.-J. Himmel, A. J. Downs, T. M. Greene, and L. Andrews, Chem. Commun. 2243 (1999).
[2] H.-J. Himmel, A. J. Downs, T. M. Greene, and L. Andrews, Organomet. **19**, 1060 (2000).
[3] J. Müller, H. Sternkicker, U. Bergmann, and B. Atakan, J. Phys. Chem. A **104**, 3627 (2000).

$InCH_3$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 stretch	2905.2	Ar	IR	1,2
	2	CH_3 umbrella	1115.3	Ar	IR	1,2
	3	InC stretch	422.1	Ar	IR	1,2
e	4	CH_3 stretch	2976.2	Ar	IR	1,2
	5	CH_3 deform.	1424.0	Ar	IR	1,2

$InCD_3$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_3 umbrella	868.1	Ar	IR	1,2

References

[1] H.-J. Himmel, A. J. Downs, T. M. Greene, and L. Andrews, Chem. Commun. 2243 (1999).
[2] H.-J. Himmel, A. J. Downs, T. M. Greene, and L. Andrews, Organomet. **19**, 1060 (2000).

$AlNH_3^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	AlN stretch	333	gas	TPE	1
e	6	Deformation	557	gas	TPE	1

$AlND_3^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	AlN stretch	325(5)	gas	MPI	2

References

[1] D.-S. Yang and J. Miyawaki, Chem. Phys. Lett. **313**, 514 (1999).
[2] Z. J. Jakubek and B. Simard, J. Chem. Phys. **112**, 1733 (2000).

$GaNH_3^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	GaN stretch	266	gas	TPE	1

Reference

[1] S. Li, G. K. Rothschopf, D. Pillai, B. R. Sohnlein, B. M. Wilson, and D.-S. Yang, J. Chem. Phys. **115**, 7968 (2001).

$InNH_3^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	InN stretch	234	gas	TPE	1

Reference

[1] G. K. Rothschopf, J. S. Perkins, S. Li, and D.-S. Yang, J. Phys. Chem. A **104**, 3178 (2000).

$AlNH_3$

In an argon matrix, an absorption maximum at 23360 (428 nm) can be assigned[3] to $AlNH_3$. Irradiation near this frequency leads to the formation of $HAlNH_2$.

$\tilde{X}\,^2E_{1/2}$ C_{3v} (C_s)[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH_3 a-stretch	3447.1	Ar	IR	3
	4	NH_3 umbrella	1131.4	Ar	IR	3
	6	AlN stretch	227	gas	TPE	1
a''	8	NH_3 a-deform.	1593.6	Ar	IR	3

$A = 58$ gas TPE[1]

$AlND_3$

$\tilde{C}\,^2E$ C_{3v}
$T_0 = 21185(5)$ gas MPI[2] $\tilde{C}-\tilde{X}$ 406–472 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	AlN stretch	428(2) (ω)	gas	MPI	2
e	6	Deformation	594(12)T (ω)	gas	MPI	2

$\tilde{B}\,^2A_1$ C_{3v}
$T_0 = 18532.5(7)$ gas MPI[2] $\tilde{B}-\tilde{X}$ 468–542 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	AlN stretch	316.0(8) (ω)	gas	MPI	2

$\tilde{X}\,^2E_{1/2}$ C_{3v} (C_s)[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	4	ND_3 umbrella	972.6	Ar	IR	3
	6	AlN stretch	325(5)	gas	MPI	2

$A = 55.8(7)$ gas MPI[2]

[a] Jahn–Teller interaction leads to a slight distortion of the molecule, with resultant C_s symmetry. Vibrational fundamentals are numbered appropriately for the distorted molecule.

References

[1] D.-S. Yang and J. Miyawaki, Chem. Phys. Lett. **313**, 514 (1999).
[2] Z. J. Jakubek and B. Simard, J. Chem. Phys. **112**, 1733 (2000).

[3] H.-J. Himmel, A. J. Downs, and T. M. Greene, J. Am. Chem. Soc. **122**, 9793 (2000).

$HAlNH_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH_2 s-stretch	3476.4	Ar	IR	2
	3	AlH stretch	1761.7	Ar	IR	1,2
	4	NH_2 scissors	1533.6	Ar	IR	1,2
	5	AlN stretch	778.7	Ar	IR	1,2
	6	NH_2 rock	705.2	Ar	IR	1,2
	7	AlH deform.	482.2	Ar	IR	2
a''	8	NH_2 OPLA	483.8	Ar	IR	2
	9	AlH OPLA	393.8	Ar	IR	2

$DAlND_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ND_2 s-stretch	2595.6	Ar	IR	2
	3	AlD stretch	1282.7	Ar	IR	1,2
	4	ND_2 scissors	1151.4	Ar	IR	1,2
	5	AlN stretch	748.3	Ar	IR	1,2
	6	ND_2 rock	549.8	Ar	IR	1,2
a''	8	ND_2 OPLA	346.5	Ar	IR	2
	9	AlD OPLA	304.6	Ar	IR	2

References

[1] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **101**, 5082 (1997).
[2] H.-J. Himmel, A. J. Downs, and T. M. Greene, J. Am. Chem. Soc. **122**, 9793 (2000).

$GaNH_3$

In an argon matrix, an absorption maximum at 22730 (440 nm) can be assigned[1,2] to $GaNH_3$. Irradiation near this frequency leads to the formation of $HGaNH_2$.

$\tilde{X}$ C_{3v} (C_s)[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH_3 a-stretch	3441.5	Ar	IR	2
	4	NH_3 umbrella	1104.2	Ar	IR	1,2
	6	GaN stretch	161	gas	TPE	3
a''	8	NH_3 a-deform.	1580.7	Ar	IR	2

$GaND_3$

$\tilde{X}$ C_{3v} (C_s)[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	4	ND_3 umbrella	824.9	Ar	IR	2

[a] Jahn–Teller interaction leads to a slight distortion of the molecule, with resultant C_s symmetry. Vibrational fundamentals are numbered appropriately for the distorted molecule.

References

[1] H.-J. Himmel, A. J. Downs, and T. M. Greene, Chem. Commun. 871 (2000).
[2] H.-J. Himmel, A. J. Downs, and T. M. Greene, J. Am. Chem. Soc. **122**, 9793 (2000).
[3] S. Li, G. K. Rothschopf, D. Pillai, B. R. Sohnlein, B. M. Wilson, and D.-S. Yang, J. Chem. Phys. **115**, 7968 (2001).

$HGaNH_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	GaH stretch	1721.8	Ar	IR	1,2
	4	NH_2 scissors	1528.7	Ar	IR	1,2
	5	NH_2 rock	746.2	Ar	IR	1,2
	6	GaN stretch	668.5	Ar	IR	1,2
a''	8	NH_2 OPLA	494.1	Ar	IR	1,2
	9	GaH OPLA	210.9	Ar	IR	1,2

$DGaND_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	GaD stretch	1249.5	Ar	IR	2
	4	ND_2 scissors	1145.0	Ar	IR	2
	5	GaN stretch	626.6	Ar	IR	2
	6	ND_2 rock	563.5	Ar	IR	2

References

[1] H.-J. Himmel, A. J. Downs, and T. M. Greene, Chem. Commun. 871 (2000).
[2] H.-J. Himmel, A. J. Downs, and T. M. Greene, J. Am. Chem. Soc. **122**, 9793 (2000).

$InNH_3$

In an argon matrix, an absorption maximum at 22990 (435 nm) can be assigned[1] to $InNH_3$. Irradiation near this frequency leads to the formation of $HInNH_2$.

$\tilde{X}$ C_{3v} (C_s)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH_3 s-stretch	3424.4	Ar	IR	1
	4	NH_3 umbrella	1082.9	Ar	IR	1
	6	InN stretch	141	gas	TPE	2

$InND_3$

$\tilde{X}$ C_{3v} (C_s)[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	4	ND_3 umbrella	816.0	Ar	IR	1

[a]Jahn–Teller interaction leads to a slight distortion of the molecule, with resultant C_s symmetry. Vibrational fundamentals are numbered appropriately for the distorted molecule.

References

[1] H.-J. Himmel, A. J. Downs, and T. M. Greene, J. Am. Chem. Soc. **122**, 9793 (2000).
[2] G. K. Rothschopf, J. S. Perkins, S. Li, and D.-S. Yang, J. Phys. Chem. A **104**, 8178 (2000).

$HInNH_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH_2 s-stretch	3463.5	Ar	IR	1
	3	InH stretch	1533.8	Ar	IR	1
	4	NH_2 scissors	1512.9	Ar	IR	1
	5	NH_2 rock	709.0	Ar	IR	1
	6	InN stretch	564.8	Ar	IR	1

$DInND_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	ND_2 scissors	1122.2	Ar	IR	1
	4	InD stretch	1108.8	Ar	IR	1
	5	InN stretch	528.8	Ar	IR	1
	6	ND_2 rock	522.9	Ar	IR	1

Reference

[1] H.-J. Himmel, A. J. Downs, and T. M. Greene, J. Am. Chem. Soc. **122**, 9793 (2000).

$AlPH_3$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	PH s-stretch	2285.5	Ar	IR	1
	3	PH_3 a-deform.	1101.2	Ar	IR	1
	4	PH_3 s-deform.	974.7	Ar	IR	1

$AlPD_3$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	PD s-stretch	1659.4	Ar	IR	1
	3	PD_3 a-deform.	793.7	Ar	IR	1
	4	PD_3 s-deform.	718.3	Ar	IR	1

Reference

[1] H.-J. Himmel, A. J. Downs, and T. M. Greene, Inorg. Chem. **40**, 396 (2001).

$HAlPH_2$

In argon-matrix experiments,[1] an absorption maximum at 18180 (550 nm) can be assigned to $HAlPH_2$.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	3	AlH stretch	1768.2	Ar	IR	1
	4	PH_2 scissors	1159.4	Ar	IR	1
	5	PH_2 wag	727.1	Ar	IR	1
	7	HAlP deform.	403.9	Ar	IR	1

$DAlPD_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	3	AlD stretch	1288.4	Ar	IR	1
	5	PD_2 wag	532.3	Ar	IR	1

Reference

[1] H.-J. Himmel, A. J. Downs, and T. M. Greene, Inorg. Chem. **40**, 396 (2001).

H_2AlPH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	AlH_2 a-stretch	1874.7	Ar	IR	1
	3	AlH_2 s-stretch	1866.1	Ar	IR	1
	4	AlH_2 bend	765.9	Ar	IR	1
	5	HPAl bend	606.3	Ar	IR	1
	6	AlH_2 wag	569.0	Ar	IR	1

D_2AlPD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	AlD_2 a-stretch	1373.5	Ar	IR	1
	3	AlD_2 s-stretch	1345.6	Ar	IR	1
	4	AlD_2 bend	564.5	Ar	IR	1
	5	DPAl bend	482.8	Ar	IR	1

Reference

[1] H.-J. Himmel, A. J. Downs, and T. M. Greene, Inorg. Chem. **40**, 396 (2001).

$GaPH_3$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	PH s-stretch	2280.8	Ar	IR	1
	3	PH_3 a-deform.	1108.2	Ar	IR	1
	4	PH_3 s-deform.	973.6	Ar	IR	1

$GaPD_3$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	PD s-stretch	1660.3	Ar	IR	1
	3	PD_3 a-deform.	795.9	Ar	IR	1
	4	PD_3 s-deform.	717.7	Ar	IR	1

Reference

[1] H.-J. Himmel, A. J. Downs, and T. M. Greene, Inorg. Chem. **40**, 396 (2001).

$HGaPH_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	3	GaH stretch	1721.4	Ar	IR	1
	4	PH_2 scissors	1060.9	Ar	IR	1
	7	HGaP deform.	428.2	Ar	IR	1

$DGaPD_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	3	GaD stretch	1244.7	Ar	IR	1

Reference

[1] H.-J. Himmel, A. J. Downs, and T. M. Greene, Inorg. Chem. **40**, 396 (2001).

H_2GaPH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	GaH_2 a-stretch	1897.5	Ar	IR	1
	3	GaH_2 s-stretch	1893.3	Ar	IR	1
	4	GaH_2 bend	738.9	Ar	IR	1
	5	HPGa bend	646.5 644.8	Ar	IR	1
	6	GaH_2 wag	454.8	Ar	IR	1

D_2GaPD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	GaD_2 a-stretch	1372.8	Ar	IR	1
	3	GaD_2 s-stretch	1360.1	Ar	IR	1
	4	GaD_2 bend	528.8	Ar	IR	1
	5	DPGa bend	486.4	Ar	IR	1

Reference

[1] H.-J. Himmel, A. J. Downs, and T. M. Greene, Inorg. Chem. **40**, 396 (2001).

$InPH_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	4	PH_3 a-deform.	1105.7	Ar	IR	1
	6	PH_3 s-deform.	974.4	Ar	IR	1

$InPD_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	6	PD_3 s-deform.	717.6	Ar	IR	1

Reference

[1] H.-J. Himmel, A. J. Downs, and T. M. Greene, Inorg. Chem. **40**, 396 (2001).

$HInPH_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	PH_2 a-stretch	2299.4	Ar	IR	1
	3	InH stretch	1546.4	Ar	IR	1

$DInPD_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	3	InD stretch	1114.9	Ar	IR	1

Reference

[1] H.-J. Himmel, A. J. Downs, and T. M. Greene, Inorg. Chem. **40**, 396 (2001).

H_2InPH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	5	HPIn bend	674.7	Ar	IR	1

Reference

[1] H.-J. Himmel, A. J. Downs, and T. M. Greene, Inorg. Chem. **40**, 396 (2001).

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

Unstructured gas-phase absorption starting near 42000 (238 nm) and continuously increasing to the 225 nm observation limit has been assigned[6] to an in-plane $\pi^*(2a'')-\pi(1a'')$ transition of C_2H_3.

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

$T_0 = 20042$ gas $AB^1CR^{7,8}PD^9$ $\tilde{A}-\tilde{X}$ 400–530 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	5	Mixed	1249(2)	gas	PD	9
	6	CC stretch	1183(2)	gas	AB,PD	1,9
	7	CCH bend	934(2)	gas	AB,PD	1,9
a''	8	Torsion	1168(2)	gas	PD	9
	9	OPLA	836(2)	gas	PD	9

$\tilde{X}$ C_s[a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	7		674(2)	gas	PD	9
a''	8	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''	8	Mixed OPLA	704	Ar	IR	2

[a] Rapid tunneling, giving effective C_{2v} symmetry.[4]

References

[1] H. E. Hunziker, H. Kneppe, A. D. McLean, P. Siegbahn, and H. R. Wendt, Can. J. Chem. **61**, 993 (1983).
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[8] K. Tonokura, S. Marui, and M. Koshi, Chem. Phys. Lett. **313**, 771 (1999).
[9] M. B. Pushkarsky, A. M. Mann, J. S. Yeston, and C. B. Moore, J. Chem. Phys. **115**, 10738 (2001).

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

$\tau_0 = 415(8)$ ns gas LF[9,10]

$A = -22.52$ gas EM[4,7]

$A_0 = 5.423$; $B_0 = 0.845$ EM[4,7]

$\tilde{a}\,^1E$ C_{3v}

$T_0 = 10905(90)$ gas PE[11]

$\tilde{X}\,^3A_2$ 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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CH_3O^+

$^1E, ^3E$ C_{3v}

$T^a = 35700T$ gas PE[2]

$\tilde{b}\,^1A_1$ C_{3v}

$T_0 = 23720(100)$ gas PE[2]

$\tilde{a}\,^1E$ C_{3v}

$T_0 = 13880(100)$ gas PE[2]

$\tilde{X}\,^3A_2$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CO stretch	1950(60)	gas	PE	2

CD_3O^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_3 s-stretch	2400T	gas	PI	1

[a]From vertical ionization potential.

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CH_3S^+

$T^a = 44100T$ gas PE[3]

$T^a = 35000T$ gas PE[3]

$^1E, ^3E$ C_{3v}
$T^a = 21460(100)$ gas PE[3]

$\tilde{b}\ ^1A_1$ C_{3v}
$T_0 = 8550(100)$ gas PE[3]

$\tilde{a}\ ^1E$ C_{3v}
$T_0 = 5240(100)$ gas PE[3]

$\tilde{X}\ ^3A_2$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		1100(60)	gas	PE	3
	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

[a]From vertical ionization potential.

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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

$\tau = 2.57(13)\ \mu s$ 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 (E) (A_1)	1465(10)	gas	PE	33,35
			914	gas	SEP	30
	6	HCO deform. (E) (A_1)	1210(10)	gas	PE	33,35
			651.5	gas	LF	19,26,27
					SEP,PE	30,33,35

$A = -61.97(7)$ 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}
$T_0 = 31557$ gas LF[6,19,34]EM[12]FD[34] $\tilde{A}$–$\tilde{X}$ 269–410 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_3 stretch	1889T	gas	LF	34
	2	CD_3 umbrella	970	gas	LF	19,34
	3	CO stretch	664	gas	EM,LF	12,19,34
e	4	CD_3 stretch	2325T	gas	LF	34
	5	CD_2 scissors	1047	gas	LF	19,34
	6	DCO deform.	697	gas	LF	34

$\tau_0 = 2.8\ \mu s$ gas LF[34]

$\tilde{X}\ ^2E$ 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 (E)	1174	gas	LF,EM	6,12,19,
					PE	33
	6	DCO deform. (E) (A_1)	920(15)	gas	PE	33,35
			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

$\tilde{B}\,^2A''$ (**3*p***) C_s
$T_0 = 41065(3)$ gas MPI[3,4,7,8]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

Predissociates, with lifetime of 0.5(1) ps gas MPI[8]

$\tilde{A}\,^2A'$ (**3*s***) 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

$\tilde{B}\,^2A''$ (**3*p***) 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

$\tilde{A}\,^2A'$ (**3*s***) 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

$\tilde{B}\,^2A_2$

$T_0 = 45620$ gas AB[1,11]PF[13]

Dissociates into $CH_3 + S$.[13]

$\tilde{A}\,^2A_1$ C_{3v} Structure: LF[8]

$T_0 = 26396.8$ gas EM[2]LF[6,8,10]PF[13] $\tilde{A}-\tilde{X}$ 315–530 nm

Predissociation threshold = 27324.[13] 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,PF	10,13
	3	CS stretch	401(2)	gas	EM,LF	2,6,8,10
					PF	13
e	6	HCS deform.	635(10)	gas	LF	10

$\tau_0 = 1090(55)$ ns gas LF[9,10,15]

$A_0 = 5.343(47)$; $B_0 = 0.346$ LF[8]

$\tilde{X}\,^2E$ C_{3v} Structure: MW[7]LF[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 stretch	2960(30)	gas	PE	14
	2	CH_3 umbrella	1313(5)	gas	PD,LF	4,6,10
	3	CS stretch	727(3)	gas	EM,PE	2–4,6
					PD,LF	10,14
e	4	CH_3 stretch	2706T	gas	LF	10
	5	CH_3 deform.	1496(6)	gas	LF	10
	6	HCS deform.	586T	gas	LF	10

$A = -259.1$ gas LF[8,10]TPE[12]PF[13]PE[14]

$A_0 = 5.68(4)$; $B_0 = 0.450$ MW[7]LF[8]

CD_3S

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

$T_0 = 26574$ gas LF[6]PF[13] $\tilde{A}-\tilde{X}$ 339–378 nm

Predissociation threshold = 28089 PF[13]

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,PF	6,13

$\tau_0 = 0.45(11)$ μs gas LF[6]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_3 umbrella	1100(50)	gas	PD	4
	3	CS stretch	667(1)	gas	PD,LF	4,6
e	5	DCS deform.	780(30)H	gas	PD	4

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CH_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,TPE	3,4,9
		CH_3 deform.	649.4wm	Ne	IR	8
			626.9wm			
		CCl stretch	654(50)	gas	PE,TPE	3,4,9

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

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[2] A. W. Potts, H. J. Lempka, D. G. Streets, and W. C. Price, Phil. Trans. Roy Soc. (London) **A268**, 59 (1970).

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CH_3I^+

$\tilde{C}\,^2A_2$ C_{3v}
T[a] = 81200(900) gas PE[1]

$\tilde{B}\,^2E$ C_{3v}
T_0 = 35180(900) gas PE[1–3]
A Jahn–Teller splitting of ~5600 is observed.[1–3] (Onset of the transition is given.)

$\tilde{A}\,^2A_1$ C_{3v}
T_0 = 16884 gas PE[1–3]PF[6–11]
A broad, unstructured absorption with onset near 420 nm (23800) and with maximum at 373 nm (26800) which appears on argon-resonance photolysis of CH_3I isolated in solid argon and which has a photodecomposition threshold between 500 and 650 nm has been assigned[5] to the $\tilde{A}$–$\tilde{X}$ transition of CH_3I^+.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 stretch	2810	gas	PF	7
	2	CH_3 umbrella	1192	gas	PF	9–11
	3	CI stretch	294.2	gas	PE,PF	3,9–11

A[b] = 5.07(5); B[b] = 0.185 PF[6,8]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 stretch	2930(5)	gas	TPE	12
	2	CH_3 umbrella	1254(5)[c]	gas	PF,TPE	1–3,9,12
	3	CI stretch	478(5)[d]	gas	PE,TPE	1,3,12
e	4	CH_3 stretch	3036(5)	gas	PE,TPE	3,4,12
	5	Deformation	1405H	gas	TPE	12
	6	CH_3 rock	860(5)[e]	gas	PE,TPE	3,12

A = 5050 gas PE[1–4]PF[9,11]TPE[12]

CD_3I^+

$\tilde{A}\,^2A_1$ C_{3v}
T_0 = 16982 gas PE,PF[7,9–11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_3 stretch	2100	gas	PF	9
	2	CD_3 umbrella	918	gas	PF	10,11
	3	CI stretch	276.3	gas	PF	10,11

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_3 stretch	2168T	gas	PF,TPE	11,12
	2	CD_3 umbrella	952(5)	gas	PF,TPE	7,12
	3	CI stretch	454(5)	gas	PF,TPE	11,12
e	4	CD_3 stretch	2189HT	gas	TPE	12
	5	Deformation	959HT	gas	TPE	12
	6	CD_3 rock	650(5)	gas	TPE	12

A = 5036 gas PF[11]TPE[12]

[a] From vertical ionization potential.
[b] From study of band at 16978 in $\tilde{A}$–$\tilde{X}\,^2E_{1/2}$ transition.
[c] 1245(5) in $\tilde{X}\,^2E_{1/2}$.
[d] 465(5) in $\tilde{X}\,^2E_{1/2}$.
[e] 830(5) in $\tilde{X}\,^2E_{1/2}$.

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CH_3O^-

Threshold for electron detachment from ground-state CH_3O^- = 12680(30) gas PE[1,3,4]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 umbrella	1075(100)	gas	PE	1

CD_3O^-

Threshold for electron detachment from ground-state CD_3O^- = 12580(30) gas PE[1–4]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_3 umbrella	950(120)	gas	PE	1,2

References

[1] P. C. Engelking, G. B. Ellison, and W. C. Lineberger, J. Chem. Phys. **69**, 1826 (1978).
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CH_3S^-

Threshold for electron detachment from ground-state $CH_3S^- = 15060(30)$ gas PD^2PE[1,3,4]

$\tilde{X}$ C_{3v} Structure: MO^2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CS stretch	410(30)	gas	PE	4

References

[1] P. C. Engelking, G. B. Ellison, and W. C. Lineberger, J. Chem. Phys. **69**, 1826 (1978).
[2] B. K. Janousek and J. I. Brauman, J. Chem. Phys. **72**, 694 (1980).
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PH_3O

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PH_3 stretch	2359.0[a]	Ar	IR	1
	2	PO stretch	1240.2	Ar	IR	1
	3	PH_3 umbrella	1143.5	Ar	IR	1
e	4	PH_3 stretch	2371.5	Ar	IR	1
	5	PH_3 deform.	1114.3	Ar	IR	1
	6	HPO deform.	853.0	Ar	IR	1

$B_0 = 0.581$ MW^2

PD_3O

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PD_3 stretch	1721.1	Ar	IR	1
	2	PO stretch	1217.3	Ar	IR	1
	3	PD_3 umbrella	843.6	Ar	IR	1
e	6	DPO deform.	655.9	Ar	IR	1

$B_0 = 0.487$ MW^2

[a] In Fermi resonance with $\nu_2 + \nu_3$.

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[1] R. Withnall and L. Andrews, J. Phys. Chem. **91**, 784 (1987).
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8.9. Five-Atomic Dihydrides

HMnOMnH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		MnH stretch	1638.5	Ar	IR	1,2
		MnOMn stretch	870.5	Ar	IR	1,2

DMnOMnD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		MnD stretch	1175.3	Ar	IR	1,2
		MnOMn stretch	870.3	Ar	IR	1,2

References

[1] J. W. Kauffman, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **89**, 3541 (1985).
[2] M. Zhou, L. Zhang, L. Shao, W. Wang, K. Fan, and Q. Qin, J. Phys. Chem. A **105**, 5801 (2001).

HFeOFeH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		FeH stretch	1708.2	Ar	IR	1,2
		FeO stretch	911.8	Ar	IR	1,2

DFeOFeD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		FeD stretch	1228.7	Ar	IR	1,2
		FeO stretch	911.7	Ar	IR	1,2

References

[1] J. W. Kauffman, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **89**, 3541 (1985).
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BH_2CN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C≡N stretch	2092.2	Ar	IR	1

Reference

[1] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **101**, 824 (1997).

CH_2NB

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1830.5	Ar	IR	1

Reference

[1] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **101**, 824 (1997).

cyc-C_3H_2

Photodecomposition threshold in an argon matrix near 360 nm; linear C_3H_2 formed.[1,6,7]

$\tilde{X}$[a] C_{2v} Structure: MW[4,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3		1277.37	gas	IR	8
			1278.6	Ar	IR	1,6,7
			1277.7			
	4		887.1[b]	Ar	IR	1,6,7
b_1	6		1063.6[b]	Ar	IR	1,6,7
b_2	8		787.8[b]	Ar	IR	1,6,7

$A_0 = 1.171$; $B_0 = 1.075$; $C_0 = 0.559$ MW[2–5,9]

cyc-C_3D_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3		1261.8	Ar	IR	7

[a] Assigned in accord with *ab initio* calculations of Ref. 10.
[b] Did not diminish in intensity on mercury-arc irradiation at wavelengths longer than 345 nm,[7] calling into question the assignment to *cyc*-C_3H_2.

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[1] H. P. Reisenauer, G. Maier, A. Riemann, and R. W. Hoffmann, Angew. Chem. **96**, 596 (1984); Angew. Chem. Int. Ed. Engl. **23**, 641 (1984).
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$H_2C{=}C{=}C$:

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

$\tilde{C}\,{}^1A_1$ C_{2v}
$T_0 = 39063$ Ne AB[9] $\tilde{C}-\tilde{X}$ 212–256 nm
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	1000T	Ne	AB	9
			900T	Ar	AB	8

$\tilde{B}\,{}^1B_1$ C_{2v}
$T_0 = 16426$ Ne AB[9] $\tilde{B}-\tilde{X}$ 403–609 nm
$T_0 \leqslant 18720(80)$ Ar AB[8] $\tilde{B}-\tilde{X}$ 382–535 nm

The spectral region near the origin of this transition is complicated by extensive vibronic interactions.[9]
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	2	C_3 a-stretch	2120	Ne	AB	9
			985	Ne	AB	9
			1000T	Ar	AB	8

$\tilde{A}\,{}^1A_2$ C_{2v}
$T_0 \leqslant 13975$ Ne AB[9] $\tilde{A}-\tilde{X}$ 619–716 nm
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	Ar	IR	1,2
			3049.5			
	2	C_3 a-stretch	1963.2	Ar	IR	1,2
			1952.2			
	3	CH_2 scissors	1449.3	Ar	IR	1,2
			1446.9			
b_1	5	H_2CC OPLA	1003.0	Ar	IR	1,2
			999.2			
b_2	8	CH_2 rock	1025.0	Ar	IR	1

$A_0 = 9.633$; $B_0 = 0.353$; $C_0 = 0.340$ MW[3,5]

$D_2C=C=C$:

$\tilde{X}\,^1A_1$ 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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CH_2MgF

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		MgF stretch	772.9	Ar	IR	1

CD_2MgF

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		MgF stretch	762.9	Ar	IR	1

Reference

[1] W. D. Bare, A. Citra, C. Trindle, and L. Andrews, Inorg. Chem. **39**, 1204 (2000).

CH_2MgCl

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		MgCl stretch	663.0	Ar	IR	1

Reference

[1] W. D. Bare, A. Citra, C. Trindle, and L. Andrews, Inorg. Chem. **39**, 1204 (2000).

CH_2MgBr

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			650.9	Ar	IR	1

CD_2MgBr

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			626.4	Ar	IR	1

Reference

[1] W. D. Bare, A. Citra, C. Trindle, and L. Andrews, Inorg. Chem. **39**, 1204 (2000).

CH_2BO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BCO a-stretch	1946.6	Ar	IR	1
		Deformation	663.6	Ar	IR	1

CD_2BO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BCO a-stretch	1945.2	Ar	IR	1
		Deformation	554.8	Ar	IR	1

Reference

[1] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **101**, 1482 (1997).

$H_2C=C=C:^-$

$\tilde{D}\,^2B_1$ C_{2v}
$T_0=27754(20)$ gas PD[5] $\tilde{D}-\tilde{X}$ 338–360 nm
(Feshbach resonance)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		1776(30)	gas	PD	5
	4		1309(30)	gas	PD	5

$\tilde{C}\,^2A_1$ C_{2v}
$T_0=20055(5)$ gas PD[5] $\tilde{C}-\tilde{X}$ 445–500 nm
(Feshbach resonance)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C_3 a-stretch	1860(25)	gas	PD	5
	4		1245(25)	gas	PD	5
b_1	6	H_2CC OPLA	400(12)	gas	PD	5

$\tilde{B}\,^2A''$ C_s
$T_0=18255(5)$ gas PD[5] $\tilde{B}-\tilde{X}$ 496–548 nm
(Feshbach resonance)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	C_3 a-stretch	1896(12)	gas	PD	5
	4		1089(12)	gas	PD	5
	5		677(12)	gas	PD	5
	6		527(12)	gas	PD	5
	8		883(12)	gas	PD	5
	9		375(7)	gas	PD	5

Threshold for electron detachment from ground-state $H_2C=C=C:^-$ =14470(65) gas PE[1,2]

$\tilde{A}\,^2A_1$ C_{2v}
(Dipole-Bound State)
$T_0=14284.420(5)$ gas PD[3] $\tilde{A}-\tilde{X}$ 615–700 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C_3 a-stretch	1956	gas	PD	4,5
	4	C_3 s-stretch	1111	gas	PD	4,5
b_1	6	H2CC OPLA	221.45	gas	PD	4,5
b_2	9		276.69	gas	PD	4

$A_0=9.651$; $1/2(B_0+C_0)=0.346$ 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]

$D_2C=C=C:^-$

$\tilde{C}\,^2A_1$ C_{2v}
$T_0=20090(20)$ gas PD[5] $\tilde{C}-\tilde{X}$ 456–500 nm
(Feshbach resonance)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C_3 a-stretch	1830(30)	gas	PD	5
	4		990(30)	gas	PD	5
b_1	6	D_2CC OPLA	340(30)	gas	PD	5

$\tilde{B}\,^2A''$ C_s
$T_0=18273(10)$ gas PD[5] $\tilde{B}-\tilde{X}$ 504–547 nm
(Feshbach resonance)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	4		990(15)	gas	PD	5
	5		609(15)	gas	PD	5
	6		505(15)	gas	PD	5
	8		847(15)	gas	PD	5
	9		323(15)	gas	PD	5

$\tilde{A}\,^2A_1$ C_{2v}
$T_0=14246(2)$ gas PD[5] $\tilde{A}-\tilde{X}$ 618–702 nm
(Dipole-bound state)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C_3 a-stretch	1920(10)	gas	PD	5
	4		936(3)	gas	PD	5
b_1	6	D_2CC OPLA	188(3)	gas	PD	5

References

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[2] M. S. Robinson, M. L. Polak, V. M. Bierbaum, C. H. DePuy, and W. C. Lineberger, J. Am. Chem. Soc. **117**, 6766 (1995).
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[4] K. Yokoyama, G. W. Leach, J. B. Kim, W. C. Lineberger, A. I. Boldyrev, and M. Gutowski, J. Chem. Phys. **105**, 10706 (1996).
[5] M. Tulej, F. Güthe, M. V. Pachkov, K. Tikhomirov, R. Xu, M. Jungen, and J. P. Maier, Phys. Chem. Chem. Phys. **3**, 4674 (2001).

H_2CCN

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

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

$A_0=9.506(4)$; $B_0=0.348$; $C_0=0.329$ MW[2,4]

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

$A_0=4.768$; $B_0=0.303$; $C_0=0.284$ MW[4]

[a]From computer fit.

References

[1] S. Moran, H. B. Ellis, Jr., D. J. DeFrees, A. D. McLean, and G. B. Ellison, J. Am. Chem. Soc. **109**, 5996 (1987).
[2] S. Saito, S. Yamamoto, W. M. Irvine, L. M. Ziurys, H. Suzuki, M. Ohishi, and N. Kaifu, Astrophys. J. **334**, L113 (1988).
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[4] S. Saito and S. Yamamoto, J. Chem. Phys. **107**, 1732 (1997).

H_2CCP

$\tilde{X}\,^2B_1$ C_{2v} Structure: MW,MO[1]
$A_0=9.634(3)$; $B_0=0.182$; $C_0=0.179$ MW[1]

Reference

[1] I. K. Ahmad, H. Ozeki, S. Saito, and P. Botschwina, J. Chem. Phys. **109**, 4252 (1998).

$Y(OH)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		YO_2 a-stretch	597.9	Ar	IR	1

$Y(OD)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		YO_2 a-stretch	578.0	Ar	IR	1

Reference

[1] L. Zhang, L. Shao, and M. Zhou, Chem. Phys. **272**, 27 (2001).

$La(OH)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		LaO_2 s-stretch	519.3	Ar	IR	1
		LaO_2 a-stretch	491.2	Ar	IR	1

$La(OD)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		LaO_2 s-stretch	517.3	Ar	IR	1
		LaO_2 a-stretch	488.2	Ar	IR	1

Reference

[1] L. Zhang, L. Shao, and M. Zhou, Chem. Phys. **272**, 27 (2001).

$Mn(OH)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		MnO_2 a-stretch	709.0	Ar	IR	1

$Mn(OD)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		MnO_2 a-stretch	693.6	Ar	IR	1

Reference

[1] M. Zhou, L. Zhang, L. Shao, W. Wang, K. Fan, and Q. Qin, J. Phys. Chem. A **105**, 5801 (2001).

$Fe(OH)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OFeO stretch	735.5	Ar	IR	1,2

$Fe(OD)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OFeO stretch	721.7	Ar	IR	1,2

References

[1] J. W. Kauffman, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **89**, 3541 (1985).
[2] L. Zhang, M. Zhou, L. Shao, W. Wang, K. Fan, and Q. Qin, J. Phys. Chem. A **105**, 6998 (2001).

H_2CBF

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s-stretch	3050.2	Ar	IR	1
	2		1762.2	Ar	IR	1
			917.4	Ar	IR	1
b_1			755.0	Ar	IR	1
b_2			589.5	Ar	IR	1

D_2CBF

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1741.5	Ar	IR	1
b_1			671.8	Ar	IR	1

Reference

[1] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **104**, 9295 (2000).

H_2CBCl

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BC stretch	1605.7	Ar	IR	1
		Deformation	686.9	Ar	IR	1

D_2CBCl

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD_2 stretch	2232.4	Ar	IR	1
		BC stretch	1570.3	Ar	IR	1
		Deformation	611.1	Ar	IR	1

Reference

[1] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **104**, 9295 (2000).

H_2CBBr

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_2 stretch	3045.1	Ar	IR	1
		BC stretch	1576.0	Ar	IR	1

D_2CBBr

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD_2 stretch	2224.7	Ar	IR	1
		BC stretch	1541.0	Ar	IR	1

Reference

[1] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **104**, 9295 (2000).

HN=C=NH

$\tilde{X}$ C_2 Structure: MW[6]

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

$A_0 = 7.055$; $B_0 = 0.303$; $C_0 = 0.302$ MW[6]

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

References

[1] S. T. King and J. H. Strope, J. Chem. Phys. **54**, 1289 (1971).
[2] M. Birk and M. Winnewisser, Chem. Phys. Lett. **123**, 386 (1986).
[3] M. Winnewisser and M. Birk, J. Chem. Soc., Faraday Trans. 2 **84**, 1341 (1988).
[4] M. Birk, M. Winnewisser, and E. A. Cohen, J. Mol. Spectrosc. **136**, 402 (1989).
[5] V. Wagener, M. Winnewisser, and M. Bellini, J. Mol. Spectrosc. **170**, 323 (1995).
[6] W. Jabs, M. Winnewisser, S. P. Belov, F. Lewen, F. Maiwald, and G. Winnewisser, Mol. Phys. **97**, 213 (1999).

cyc-H_2COC:

In an argon or a nitrogen matrix, a weak, unstructured absorption maximum[1] at 30860 (324 nm) is associated with the isomerization of this species (oxiranylidene) to ketene.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Ring deform.	1470.8m	N_2	IR	1
	3	CH_2 scissors	1375.1ms	N_2	IR	1
	4	CH_2 wag	1078.5w	N_2	IR	1
	5	Ring deform.	830.1vs	N_2	IR	1
	6	Ring deform.	778.1wm	N_2	IR	1

cyc-D_2COC:

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	Ring deform.	1419.4s[a]	N_2	IR	1
			1400.6s			
	3	CD_2 scissors	1050.2wm	N_2	IR	1
	4	CD_2 wag	960.3ms	N_2	IR	1
	5	Ring deform.	780.1vs	N_2	IR	1
	6	CD_2 wag	706.3vs	N_2	IR	1

[a]In Fermi resonance with $2\nu_6$.

Reference

[1]G. Maier, H. P. Reisenauer, and M. Cibulka, Angew. Chem. **111**, 110 (1999); Angew. Chem. Int. Ed. **38**, 105 (1999).

$CH_2=CF$

Isomerized to *c*-CHF=CH by 355 nm radiation.[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CH_2 stretch	2778wT	Ar	IR	1
	3	C=C stretch	1654vs	Ar	IR	1
	4	CH_2 scissors	1355w	Ar	IR	1
	5	CF stretch	1133s	Ar	IR	1
	6	CH_2 rock	930wm	Ar	IR	1
a''	8	OPLA	798m	Ar	IR	1

$CD_2=CF$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CD_2 stretch	2221w	Ar	IR	1
	3	C=C stretch	1625vs	Ar	IR	1
	4	CF stretch	1138s	Ar	IR	1
	5	CD_2 scissors	973wm	Ar	IR	1
	6	CD_2 rock	797wm	Ar	IR	1
a''	8	OPLA	630wm	Ar	IR	1

Reference

[1]I. U. Goldschleger, A. V. Akimov, E. Ya. Misochko, and C. A. Wight, J. Mol. Spectrosc. **205**, 269 (2001).

c-CHF=CH

Partially converted to $CH_2=CF$ by 532 nm radiation.[2]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	3193wm	Ar	IR	2
	2	CH stretch	3026w	Ar	IR	2
	3	C=C stretch	1631s	Ar	IR	2
			1623vs	Ar	IR	1
	4	HCF scissors	1263wm	Ar	IR	2
			1211wm	Ar	IR	1
	5	CF stretch	1068vs	Ar	IR	1,2
	6	C=CH deform.	698m	Ar	IR	2
			678s	Ar	IR	1
	7	C=CF deform.	462m	Ar	IR	1
a''	8	HFC=C OPLA	785s	Ar	IR	1,2
	9	Torsion	643m	Ar	IR	2
			631vs	Ar	IR	1

c-DCF=CD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CD stretch	2406wm	Ar	IR	2
	2	CD stretch	2248w	Ar	IR	2
	3	C=C stretch	1572vs	Ar	IR	2
			1564s	Ar	IR	1
	4	CF stretch	1068s	Ar	IR	1,2
	5	Mixed	935wm	Ar	IR	2
	6	C=CD deform.	633wm	Ar	IR	2
			624m	Ar	IR	1
a''	8	DFC=C OPLA	660w	Ar	IR	2
	9	Torsion	485m	Ar	IR	1

References

[1]M. E. Jacox, Chem. Phys. **53**, 307 (1980).
[2]I. U. Goldschleger, A. V. Akimov, E. Ya. Misochko, and C. A. Wight, J. Mol. Spectrosc. **205**, 269 (2001).

H_2NCO

In a xenon matrix,[1] the photodecomposition threshold lies between 365 and 405 nm.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH_2 a-stretch	3518.5	Xe	IR	1
	3	CO stretch	1811.8	Xe	IR	1
			1806.5			
			1796.6			
			1794.2			
	4		1555.8	Xe	IR	1
	5		1214.4	Xe	IR	1

D_2NCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ND_2 a-stretch	2634.4	Xe	IR	1
	3	CO stretch[a]	1800.2	Xe	IR	1
			1797.8			
			1796.3			
			1793.9			

[a]Absorption of HDNCO could not be distinguished from that of D_2NCO.

Reference

[1] M. Pettersson, L. Khriachtchev, S. Jolkkonen, and M. Räsänen, J. Phys. Chem. A **103**, 9154 (1999).

$HCOOH^+$

$\tilde{E}\,^2A'$ C_s
$T^a = 49700(320)$ gas PE[1,3]

$\tilde{D}\,^2A'$ C_s
$T_0 = 45500(320)$ gas PE[1,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CO stretch	1300(40)	gas	PE	1,2

$\tilde{C}\,^2A''$ C_s
$T_0 \cong 32800$ gas PE[1,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			940	gas	PE	1

$\tilde{B}\,^2A'$ C_s
$T_0 \cong 23200$ gas PE[1,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			940	gas	PE	1

$\tilde{A}\,^2A''$ C_s
$T_0 = 8495(25)$ gas PE[1,3,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1398(20)	gas	PE	4
			1029(20)	gas	PE	1,2,4
			574(20)	gas	PE	4

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CO stretch	1495(20)	gas	PE	1,2,4
	5		1196(20)	gas	PE	4
	7		510(20)	gas	PE	4

$DCOOD^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CO stretch	1210(40)	gas	PE	2
		COD bend ?	880(40)	gas	PE	2

$\tilde{A}\,^2A''$ C_s
$T_0 = 8430(25)$ gas PE[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1085(20)	gas	PE	2,4
			521(20)	gas	PE	4

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CO stretch	1472(20)	gas	PE	2,4
		COD bend	965(20)	gas	PE	2,4
			447(20)	gas	PE	4

[a]From vertical ionization potential.

References

[1] C. R. Brundle, D. W. Turner, M. B. Robin, and H. Basch, Chem. Phys. Lett. **3**, 292 (1969).
[2] I. Watanabe, Y. Yokoyama, and S. Ikeda, Chem. Phys. Lett. **19**, 406 (1973).
[3] K. Kimura, S. Katsumata, T. Yamazaki, and H. Wakabayashi, J. Electron Spectrosc. Relat. Phenom. **6**, 41 (1975).
[4] M. Schwell, S. Leach, K. Hottmann, H.-W. Jochims, and H. Baumgärtel, Chem. Phys. **272**, 77 (2001).

HInCl(OH)

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3649.3	Ar	IR	1
		InH stretch	1857.2	Ar	IR	1
			810.0	Ar	IR	1
			606.4	Ar	IR	1
			451.6	Ar	IR	1
			428.3	Ar	IR	1
			348.5	Ar	IR	1

Reference

[1] H.-J. Himmel, A. J. Downs, and T. M. Greene, J. Am. Chem. Soc. **122**, 922 (2000).

H_2CSS

In an argon matrix, there is a prominent absorption maximum at 28100 (356 nm).[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH_2 stretch	3126.3vw	Ar	IR	1
	2	CH_2 stretch	3010.4w	Ar	IR	1
	3	CH_2 scissors	1366.4m	Ar	IR	1
	4	CS stretch	970.9m	Ar	IR	1
	5	CH_2 rock	910.2m	Ar	IR	1
	6	SS stretch	622.8s	Ar	IR	1
a''	8	CH_2 wag	756.8s	Ar	IR	1

Reference

[1] G. Mlostoń, J. Romański, H. P. Reisenauer, and G. Maier, Angew. Chem. Int. Ed. **40**, 393 (2001).

cyc-H_2CS_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 stretch	2986.7m	Ar	IR	1
	2	CH_2 scissors	1412.0w	Ar	IR	1
b_1	7	CH_2 rock	928.3m	Ar	IR	1
b_2	8	CH_2 wag	1053.0m	Ar	IR	1
	9	Ring stretch	581.0s	Ar	IR	1

Reference

[1] G. Mlostoń, J. Romański, H. P. Reisenauer, and G. Maier, Angew. Chem. Int. Ed. **40**, 393 (2001).

H_2CCl-Cl

A broad absorption with maximum near 360 nm (28000) which appears[1–3] on vacuum ultraviolet photolysis of CH_2Cl_2 isolated in solid argon and a much weaker absorption near 620 nm (16000) have been attributed[3] to this product. Exposure of the sample to radiation in the spectral region of either of these absorptions leads to destruction of H_2Cl-Cl and to re-formation of CH_2Cl_2.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_2 stretch	3143.3w	Ar	IR	3,4
		CH_2 stretch	3023.5wm	Ar	IR	3,4
			3019	Kr	IR	4
		CH_2 scissors	1404.9wm	Ar	IR	3,4
			1405	Kr	IR	4
			1402	Xe	IR	4
			1193sT	Ar	IR	1,2
		CCl stretch	958.5wm	Ar	IR	3,4
			965	Kr	IR	4
			763.2vs	Ar	IR	1–4
			775	Kr	IR	4
			776	Xe	IR	4

D_2CCl-Cl

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD_2 stretch	2375.5vw	Ar	IR	3
		CD_2 stretch	2220.7wm	Ar	IR	3,4
			2220	Kr	IR	4
			2212	Xe	IR	4
		CD_2 scissors	1083.4ms	Ar	IR	2–4
			1082	Xe	IR	4
		CCl stretch	886.1m	Ar	IR	3,4
		CD_2 wag	603.1vs	Ar	IR	1–4
			613	Xe	IR	4

References

[1] L. Andrews, F. T. Prochaska, and B. S. Ault, J. Am. Chem. Soc. **101**, 9 (1979).
[2] B. J. Kelsall and L. Andrews, J. Mol. Spectrosc. **97**, 362 (1983).
[3] G. Maier, H. P. Reisenauer, J. Hu, L. J. Schaad, and B. A. Hess, Jr., J. Am. Chem. Soc. **112**, 5117 (1990).
[4] T. D. Fridgen, X. K. Zhang, J. M. Parnis, and R. E. March, J. Phys. Chem. A **104**, 3487 (2000).

H_2CCl-Br

A broad absorption with maximum near 382 nm (26200) which appears[1] on 230- or 240-nm irradiation of CH_2ClBr isolated in solid argon has been attributed[1] to this product. Exposure of the sample to 360 nm radiation or to radiation of wavelength longer than 570 nm leads to destruction of H_2CCl-Br and to re-formation of CH_2ClBr.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_2 stretch	3038.6w	Ar	IR	1
		CH_2 scissors	1388.3wm	Ar	IR	1,2
		CCl stretch	931.2wm	Ar	IR	1,2
		CH_2 wag	726.6vs	Ar	IR	1,2

D_2CCl-Br

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD_2 stretch	2232.3wm	Ar	IR	1
		CD_2 scissors	1069.6s	Ar	IR	1
		CCl stretch	868.8m	Ar	IR	1
		CD_2 wag	573.3vs	Ar	IR	1

References

[1] G. Maier, H. P. Reisenauer, J. Hu, L. J. Schaad, and B. A. Hess, Jr., J. Am. Chem. Soc. **112**, 5117 (1990).
[2] T. D. Fridgen, X. K. Zhang, J. M. Parnis, and R. E. March, J. Phys. Chem. A **104**, 3487 (2000).

H_2O_3

$\tilde{X}$ C_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	OH s-stretch	3529.6	Ar	IR	1
	2	HOO s-bend	1347.4	Ar	IR	1
	3	O_3 s-stretch	821.0	Ar	IR	1
	4	O_3 deform.	509.1	Ar	IR	1
	5	Sym. torsion	346.4	Ar	IR	1
b	6	OH a-stretch	3529.6	Ar	IR	1
	7	HOO a-bend	1359.1	Ar	IR	1
	8	O_3 a-stretch	776.3	Ar	IR	1
	9	Asym. torsion	387.0	Ar	IR	1

D_2O_3

$\tilde{X}$ C_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	OH s-stretch	2610.4	Ar	IR	1
	5	Sym. torsion	273.5	Ar	IR	1
b	6	OD a-stretch	2610.4	Ar	IR	1
	7	DOO a-bend	1007.3	Ar	IR	1
	8	O_3 a-stretch	762.6	Ar	IR	1
	9	Asym. torsion	301.6	Ar	IR	1

Reference

[1] A. Engdahl and B. Nelander, Science **295**, 482 (2002).

t-HSSSH

$\tilde{X}$ C_2 Structure: MW^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

$A_0 = 0.470$; $B_0 = 0.092$; $C_0 = 0.079$ $MW^{1,2}$

t-DSSSD

$\tilde{X}$ C_2
$A_0 = 0.426$; $B_0 = 0.087$; $C_0 = 0.076$ MW^2

References

[1] M. Liedtke, A. H. Saleck, K. M. T. Yamada, G. Winnewisser, D. Cremer, E. Kraka, A. Dolgner, J. Hahn, and S. Dobos, J. Phys. Chem. **97**, 11204 (1993).
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c-HSSSH

$\tilde{X}$ C_s Structure: MW^5
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

$A_0 = 0.470$; $B_0 = 0.092$; $C_0 = 0.079$ MW^{1-5}

c-DSSSD

$\tilde{X}$ C_s
$A_0 = 0.425$; $B_0 = 0.087$; $C_0 = 0.077$ MW^5

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[1] D. Mauer, G. Winnewisser, K. M. T. Yamada, J. Hahn, and K. Reinartz, Z. Naturforsch. **43A**, 617 (1988).
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[5] M. Liedtke, K. M. T. Yamada, G. Winnewisser, and J. Hahn, J. Mol. Struct. **413/414**, 265 (1997).

8.10. Five-Atomic Monohydrides

PdCCNH

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1800(200)	gas	PE	1

Reference

[1] V. D. Moravec and C. C. Jarrold, J. Chem. Phys. **112**, 792 (2000).

$PdCCNH^-$

Threshold for electron detachment from ground-state $PdCCNH^-$ = 17510(240) gas PE[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1600(200)	gas	PE	1

Reference

[1] V. D. Moravec and C. C. Jarrold, J. Chem. Phys. **112**, 792 (2000).

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.

$\tilde{B}\,^2\Pi$ $C_{\infty v}$
T_0 = 24033.432(6) gas LF[10] $\tilde{B}-\tilde{X}$ 400–417 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	5	HCC bend	344.2[a]	gas	LF	10
	6	CCC bend	189.3[b]	gas	LF	10

A_{SO} = −22.1 gas LF[10]
B_{eff} = 0.150 LF[10]

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.

$\tilde{A}\,^2\Pi$ $C_{\infty v}$
$T_0 \leqslant 468$ gas PE[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	C≡C stretch	2081T	gas	PE	11
Π	7	CCC bend	201T	gas	PE	11

$\tilde{X}\,^2\Sigma$ $C_{\infty v}$ 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	8,12
			2060.6ms	Ar	IR	1,7,12
	4	C−C stretch	960(50)	gas	PE	11
Π	7	CCC bend	131T	gas	MW	6
			226T		PE	11

B_0 = 0.165 MW[2–5]

C_4D

$\tilde{B}\,^2\Pi$ $C_{\infty v}$
T_0 = 24099.191(2) gas LF[10] $\tilde{B}-\tilde{X}$ 400–415 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	5	DCC bend	295.3(5)[a]	gas	LF	10
	6	CCC bend	183.4[b]	gas	LF	10

A_{SO} = −19.40(41) gas LF[10]
B_{eff} = 0.140 LF[10]

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.

$\tilde{A}\,^2\Pi$ $C_{\infty v}$
$T_0 \leqslant 468$ gas PE[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	C≡C stretch	2073L	gas	PE	11
Π	7	CCC bend	185T	gas	PE	11

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

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	8,12
			2049.6ms	Ar	IR	1,7,12
	4	C−C stretch	895(50)	gas	PE	11
Π	7	CCC bend	210T	gas	PE	11

[a] ω. ϵ = −0.6566 for C_4H and −0.6921(8) for C_4D.[10]
[b] ω. ϵ = −0.01578 for C_4H and −0.01877 for C_4D.[10]

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[2] M. Guélin, S. Green, and P. Thaddeus, Astrophys. J. **224**, L27 (1978).
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[12] L. Andrews, G. P. Kushto, M. Zhou, S. P. Willson, and P. F. Souter, J. Chem. Phys. **110**, 4457 (1999).

Si_4H

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			310(20)	gas	PE	1

Reference

[1] C. Xu, T. R. Taylor, G. R. Burton, and D. M. Neumark, J. Chem. Phys. **108**, 7645 (1998).

$HC{\equiv}C{-}C{\equiv}N^+$

$\tilde{C}$
$T_0 = 48570(160)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1320(40)	gas	PE	1

$\tilde{B}\,^2\Pi$ $C_{\infty v}$
$T_0 = 19600(160)$ gas PE[1]
19374(43) Ne AB[2] $\tilde{B}{-}\tilde{X}$ 474–516 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+			1940(40)	gas	PE	1
	4	C–C stretch	810(40)	gas	PE	1
			820(60)	Ne	AB	2

$\tilde{A}\,^2\Sigma^+$ $C_{\infty v}$
$T_0 = 15650(160)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	4	C–C stretch	860(40)	gas	PE	1

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3196.5m	Ne	IR	3
	2		2180(40)	gas	PE	1
			2175.8w	Ne	IR	3
	3		1852.8s	Ne	IR	3

$DC{\equiv}C{-}C{\equiv}N^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2499.9wm	Ne	IR	3
	2		2114.8wm	Ne	IR	3
	3		1795.6s	Ne	IR	3

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C_4H^-

Threshold for electron detachment from ground-state $C_4H^- = 28710(120)$ gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	7	Deformation	210(50)	gas	PE	1

C_4D^-

Threshold for electron detachment from ground-state $C_4D^- = 28660(120)$ gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	7	Deformation	169(50)	gas	PE	1

Reference

[1] T. R. Taylor, C. Xu, and D. M. Neumark, J. Chem. Phys. **108**, 10018 (1998).

Si_4H^-

Threshold for electron detachment from ground-state $Si_4H^- = 21620(80)$ gas PE[1]

Reference

[1] C. Xu, T. R. Taylor, G. R. Burton, and D. M. Neumark, J. Chem. Phys. **108**, 7645 (1998).

HC≡C-N≡C

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3338.96s	gas	IR	1,3
	2	N≡C stretch	2218.64s	gas	IR	1,3
	3	C≡C stretch	2036.66s	gas	IR	1,3
	4	C–C stretch	938.09w[a]	gas	IR	3
Π	5	HCC bend	620.63vs	gas	IR	1,3
	6		430T	gas	IR	3
	7		207T	gas	IR	3

$B_0 = 0.166$ MW[1,2,5]

DC≡C-N≡C

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2617.39s	gas	IR	3
	2	N≡C stretch	2157.58s	gas	IR	3
	3	C≡C stretch	1965.48s	gas	IR	3
	4	C–C stretch	923.58w[a]	gas	IR	3
Π	5	DCC bend	480.17	gas	IR	3
	6		425T	gas	IR	3

$B_0 = 0.153$ MW[1,4]IR[3]

[a]Deperturbed value.

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HNCCC

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH stretch	3562m	Ar	IR	2
	2	NC stretch	2205vs	Ar	IR	2
	3	Skel. stretch	1905w	Ar	IR	2

Quasilinear. $B_0 = 0.156$ MW[1]

DNCCC

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ND stretch	2611m	Ar	IR	2
	2	NC stretch	2162vs	Ar	IR	2
	3	Skel. stretch	1890vwT	Ar	IR	2

$B_0 = 0.147$ MW[1]

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[1] Y. Hirahara, Y. Ohshima, and Y. Endo, Astrophys. J. **403**, L83 (1993).
[2] R. Kolos and A. L. Sobolewski, Chem. Phys. Lett. **344**, 625 (2001).

$HNCCN^+$

$\tilde{X}$ $D_{\infty h}$ Structure: MW[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NH stretch	3448.27	gas	LD	1

$B_0 = 0.148$ LD[1]MW[2,5]

$DNCCN^+$

$\tilde{X}$ $D_{\infty h}$
$B_0 = 0.139$ MW[3]

References

[1] H. E. Warner and T. Amano, J. Mol. Spectrosc. **145**, 66 (1991).
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HClCCO

$\tilde{X}$ C_s Structure: MW[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CO stretch	2157.19	gas	DL	3
			2141.4vs	Xe	IR	2
	3	HCCl deform.	1293w	Xe	IR	2
	4	CC stretch	1107w	Xe	IR	2
	5	CCl stretch	842.2vw	Xe	IR	2
a''	8	HClCC OPLA	747	Xe	IR	2

$A_0 = 1.206$; $B_0 = 0.101$; $C_0 = 0.093$ MW[1]

DClCCO

$\tilde{X}$ C_s

$A_0 = 0.974$; $B_0 = 0.101$; $C_0 = 0.091$ MW[1]

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BF_2OH

$\tilde{X}$ C_s Structure: MW[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3712.5s	Ne	IR	2
	2	BF_2, BO stretch	1464.3vs	Ne	IR	2
	3	BF_2 a-stretch	1414.9vs	Ne	IR	2
	4	BOH deform.	959.1s	Ne	IR	2
	5	BF_2, BO stretch	879.3wm	Ne	IR	2
	7	Deformation	447.5m	Ne	IR	2
a''	8	OPLA	680.9ms	Ne	IR	2
	9	Torsion	520.8ms	Ne	IR	2

$A_0 = 0.344$; $B_0 = 0.337$; $C_0 = 0.170$ MW[1]

BF_2OD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2737.2m	Ne	IR	2
	2	BF_2, BO stretch	1456.8s	Ne	IR	2
	3	BF_2 a-stretch	1400.9	Ne	IR	2
	4	BF_2, BO stretch	879.3wm	Ne	IR	2
	5	BOD deform.	751.1wm	Ne	IR	2
	6	Deformation	481.5wm	Ne	IR	2
	7	Deformation	413.4	Ne	IR	2
a''	8	OPLA	680.4	Ne	IR	2

$A_0 = 0.343$; $B_0 = 0.314$; $C_0 = 0.164$ MW[1]

References

[1] H. Takeo and R. F. Curl, J. Chem. Phys. **56**, 4314 (1972).
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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, 47
			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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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	1–5
			3563.3[a]	Ar	IR	1–4
			3541.7	N_2	IR	1,2,5
	2	N=O stretch	1703.6s	Ar	IR	1–5
			1708.3[a]	Ar	IR	1–5
			1701.4	N_2	IR	1,2,5
	3	HOO bend	1364.4m	Ar	IR	1–5
			1372.7[a]	Ar	IR	1–5
			1394.9	N_2	IR	1,2,5
	4	OO stretch	952.0m	Ar	IR	1–5
			957.4[a]	Ar	IR	1–5
			960.5	N_2	IR	1,2,5
	5	ONO bend	772.8m	Ar	IR	1–5
			782.9[a]	Ar	IR	1–5
			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.

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[1] B.-M. Cheng, J.-W. Lee, and Y.-P. Lee, J. Phys. Chem. **95**, 2814 (1991).
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HXeNCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NCO a-stretch	2148.3	Xe	IR	1
	2	XeH stretch	1788.1	Xe	IR	1

DXeNCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NCO a-stretch	2145.4	Xe	IR	1
	2	XeD stretch	1298.8	Xe	IR	1

Reference

[1] M. Pettersson, L. Khriachtchev, J. Lundell, S. Jolkkonen, and M. Räsänen, J. Phys. Chem. A **104**, 3579 (2000).

HCF_3^+

$\tilde{F}\,^2A_1$ C_{3v}
$T^a = 85360(400)$ gas PE[1,3,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	2660(80)	gas	PE	4
	3	CF_3 stretch	1050(80)	gas	PE	4

$\tilde{D},\tilde{E}\,^2E,^2A_1$ C_{3v}
$T^a \cong 54400$ gas PE[1–4]
Broad emission bands between about 230 and 580 nm which appear on excitation of HCF_3 by synchrotron radiation in the 48–62 nm spectral region have been attributed[5,6,8] to transitions of HCF_3^+. A peak in this emission near 290 nm corresponds to the $\tilde{D}-\tilde{B}$ transition, and a shoulder qnear 430 nm to the $\tilde{D}-\tilde{C}$ transition.[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			480(80)	gas	PE	1

$\tau = 12.6(8)$ ns gas TPEFCO[7]

$\tilde{C}\,^2E$ C_{3v}
$T_0 = 26220(400)$ gas PE[1–4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF_3 stretch	1050(80)	gas	PE	1–4
	3	CF_3 umbrella	550(80)	gas	PE	1,3,4

$\tilde{B}\,^2E$ C_{3v}
$T^a = 18800(1000)$ gas PE[1–4]

$\tilde{A}\,^2A_2$ C_{3v}
$T^a = 13200(1000)$ gas PE[1–4]

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

DCF_3^+

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF_3 stretch	1050(80)	gas	PE	3
	3	CF_3 umbrella	500(80)	gas	PE	3

[a]From vertical ionization potential.

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8.11. Five-Atomic Nonhydrides

Ag_5

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			162	Ar	Ra	1
			136	Ar	Ra	1
			100	Ar	Ra	1
			68	Ar	Ra	1
b_1			174	Ar	Ra	1
			126	Ar	Ra	1
			80	Ar	Ra	1

Reference

[1] T. L. Haslett, K. A. Bosnick, and M. Moskovits, J. Chem. Phys. **108**, 3453 (1998).

$Y_3C_2^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	2	Y_3 stretch	228.8(4)	gas	TPE	1
e'	5	Y_3 deformation	86	gas	TPE	1

Reference

[1] D.-S. Yang, M. Z. Zgierski, and P. A. Hackett, J. Chem. Phys. **108**, 3591 (1998).

$Nb_3C_2^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	2	Nb_3 s-stretch	339.2(4)	gas	TPE	1
e'	5	Nb_3 deformation	258.8(4)	gas	TPE	1

Reference

[1] D.-S. Yang, M. Z. Zgierski, A. Bérces, P. A. Hackett, P.-N. Roy, A. Martinez, T. Carrington, Jr., D. R. Salahub, R. Fournier, T. Pang, and C. Chen, J. Chem. Phys. **105**, 10663 (1996).

Y_3C_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4	Y_3 deformation	82.4(4)	gas	TPE	1
b_1	7	Y_3 deformation	24.5(2)	gas	TPE	1

Reference

[1] D.-S. Yang, M. Z. Zgierski, and P. A. Hackett, J. Chem. Phys. **108**, 3591 (1998).

Nb_3C_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Nb_3 s-stretch	326.3(6)	gas	TPE	1
		Nb_3 deformation	237.6(3)	gas	TPE	1
		Nb_3 deformation	82.7(3)	gas	TPE	1

Reference

[1] D.-S. Yang, M. Z. Zgierski, A. Bérces, P. A. Hackett, P.-N. Roy, A. Martinez, T. Carrington, Jr., D. R. Salahub, R. Fournier, T. Pang, and C. Chen, J. Chem. Phys. **105**, 10663 (1996).

$Nb_3N_2^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		Nb_3 s-deformation	257	gas	TPE	1

Reference

[1] D.-S. Yang, M. Z. Zgierski, A. Bérces, P. A. Hackett, A. Martinez, and D. R. Salahub, Chem. Phys. Lett. **227**, 71 (1997).

Al_5

$\tilde{D}$
$T^a = 17710(650)$ gas PE[1]

$\tilde{C}$
$T^a = 14160(330)$ gas PE[1]

$\tilde{B}$
$T^a = 5240(180)$ gas PE[1]

$\tilde{A}$
$T^a = 2860(140)$ gas PE[1]

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

[a]From vertical ionization potentials.

Reference

[1] G. D. Geske, A. I. Boldyrev, X. Li, and L.-S. Wang, J. Chem. Phys. **113**, 5130 (2000).

Al_5^-

Threshold for electron detachment from ground-state $Al_5^- = 18440(80)$ gas PE[1]

Reference

[1] G. D. Geske, A. I. Boldyrev, X. Li, and L.-S. Wang, J. Chem. Phys. **113**, 5130 (2000).

Al_4C

$\tilde{C}$
$T^a = 5240(680)$ gas PE[1]

$\tilde{B}$
$T^a = 2820(680)$ gas PE[1]

$\tilde{A}$
$T^a = 1690(680)$ gas PE[1]

$\tilde{X}$ T_d

[a]From vertical electron detachment energies.

Reference

[1] X. Li, L.-S. Wang, A. I. Boldyrev, and J. Simons, J. Am. Chem. Soc. **121**, 6033 (1999).

Al_4Si

$\tilde{C}$ C_{2v}
$T_0 = 8380(290)$ gas PE[1]

$\tilde{B}$ C_{2v}
$T^a = 6280T$ gas PE[1]

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

$T_0 = 4270(290)$ gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			220T	gas	PE	1

[a]From vertical electron detachment energy.

Reference

[1] A. I. Boldyrev, X. Li, and L.-S. Wang, Angew. Chem. Int. Ed. **39**, 3307 (2000).

Al_4Ge

$\tilde{C}$ C_{2v}
$T_0 = 7960(290)$ gas PE[1]

$\tilde{B}$ C_{2v}
$T^a = 6340T$ gas PE[1]

$\tilde{A}$ C_{2v}
$T_0 = 4400(510)$ gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			160T	gas	PE	1

[a]From vertical electron detachment energy.

Reference

[1] A. I. Boldyrev, X. Li, and L.-S. Wang, Angew. Chem. Int. Ed. **39**, 3307 (2000).

Al_4C^-

Vertical electron detachment energy from ground-state $Al_4C^- = 21380(480)$ gas PE[1]

The slow onset of electron detachment is interpreted[1] as supporting a planar structure for the anion, contrasted with a tetrahedral structure for the uncharged species.

Reference

[1] X. Li, L.-S. Wang, A. I. Boldyrev, and J. Simons, J. Am. Chem. Soc. **121**, 6033 (1999).

Al_4Si^-

Threshold for electron detachment from ground-state $Al_4Si^- = 17110(160)$ gas PE[1]

Reference

[1] A. I. Boldyrev, X. Li, and L.-S. Wang, Angew. Chem. Int. Ed. **39**, 3307 (2000).

Al_4Ge^-

Threshold for electron detachment from ground-state Al_4Ge^- = 17060(160) gas PE[1]

Reference

[1] A. I. Boldyrev, X. Li, and L.-S. Wang, Angew. Chem. Int. Ed. **39**, 3307 (2000).

Al_4N

$\tilde{A}$ D_{4h}
T^a = 8800(350) gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			330T	gas	PE	1

The photoelectron spectrum[1] of Al_4N^- is consistent with the occurrence of an almost isoenergetic isomer of Al_4N that has C_{2v} symmetry.

$\tilde{X}$ D_{4h}

[a]From vertical electron photodetachment energy.

Reference

[1] S. K. Nayak, B. K. Rao, P. Jena, X. Li, and L.-S. Wang, Chem. Phys. Lett. **301**, 379 (1999).

CAl_3Si

$\tilde{C}$ C_{2v}
T^a = 10650(520) gas PE[1]

$\tilde{B}$ C_{2v}
T^a = 4920(470) gas PE[1]

$\tilde{A}$ C_{2v}
T^a = 1210(520) gas PE[1]

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

[a]From vertical electron detachment energies.

Reference

[1] L.-S. Wang, A. I. Boldyrev, X. Li, and J. Simons, J. Am. Chem. Soc. **122**, 7681 (2000).

CAl_3Ge

$\tilde{C}$ C_{2v}
T^a = 11700(460) gas PE[1]

$\tilde{B}$ C_{2v}
T^a = 5570(400) gas PE[1]

$\tilde{A}$ C_{2v}
T^a = 1610(460) gas PE[1]

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

[a]From vertical electron detachment energies.

Reference

[1] L.-S. Wang, A. I. Boldyrev, X. Li, and J. Simons, J. Am. Chem. Soc. **122**, 7681 (2000).

TiC_4

$\tilde{B}$
T_0 = 6050(360) gas PE[1]

$\tilde{A}$
T_0 = 1500(510) gas PE[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			440(40)	gas	PE	1

Reference

[1] X.-B. Wang, C.-F. Ding, and L.-S. Wang, J. Phys. Chem. A **101**, 7699 (1997).

TiC_4^-

Threshold for electron detachment from ground-state TiC_4^- = 12050(160) gas PE[1]

Reference

[1] X.-B. Wang, C.-F. Ding, and L.-S. Wang, J. Phys. Chem. A **101**, 7699 (1997).

Al_4N^- (D_{4h})

Threshold for electron detachment from Al_4N^- (singlet, D_{4h}) = 18720(240) gas PE[1]

Reference

[1] S. K. Nayak, B. K. Rao, P. Jena, X. Li, and L.-S. Wang, Chem. Phys. Lett. **301**, 379 (1999).

Al_4N^- (C_{2v})

Threshold for electron detachment from Al_4N^- (triplet, C_{2v}) = 13720(240) gas PE[1]

Reference

[1] S. K. Nayak, B. K. Rao, P. Jena, X. Li, and L.-S. Wang, Chem. Phys. Lett. **301**, 379 (1999).

CAl_3Si^-

Vertical electron detachment energy from ground-state CAl_3Si^- = 23240(400) gas PE[1]

Reference

[1] L.-S. Wang, A. I. Boldyrev, X. Li, and J. Simons, J. Am. Chem. Soc. **122**, 7681 (2000).

CAl_3Ge^-

Vertical electron detachment energy from ground-state CAl_3Ge^- = 22430(320) gas PE[1]

Reference

[1] L.-S. Wang, A. I. Boldyrev, X. Li, and J. Simons, J. Am. Chem. Soc. **122**, 7681 (2000).

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 = 19566.3(2) gas CR[18] $^1\Pi_u$–$\tilde{X}$ 493–411 nm
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.
			675	gas	CR	18
			697(10)	Ne	AB	13
Σ_g^+	2	Sym. stretch	530	gas	CR	18
			542(10)	Ne	AB	13
Π_u	7	Bend	139H	gas	CR	18
			143(5)H	Ne	AB	13

$\tilde{a}$ $D_{\infty h}$
T^a = 16060(80) gas PE[17]

$\tilde{X}\ ^1\Sigma_g^-$ $D_{\infty h}$ 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	1
Σ_u^+	3	Asym. stretch	2169.441	gas	IR,DL	4–7
			2166.4	Ne	IR	2,12,13,16
			2164	Ar	IR	1–3
			2157.0	Kr	IR	15
			2164.5	H_2	IR	14
	4	Asym. stretch	1444.3	Ne	IR	12,16
			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]

[a]From vertical ionization potentials.

References

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[17] M. Kohno, S. Suzuki, H. Shiromaru, and Y. Achiba, J. Chem. Phys. **110**, 3781 (1999).
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C_4Si

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

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[1,4]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).
[4] V. D. Gordon, E. S. Nathan, A. J. Apponi, M. C. McCarthy, and P. Thaddeus, J. Chem. Phys. **113**, 5311 (2000).

SiCCCSi

$\tilde{A}$
T_0 = 3870(100) gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			420(25)	gas	PE	3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C_3 s-stretch	1520(25)	gas	PE	3
	2	SiC s-stretch	490(25)	gas	PE	3
Σ_u^+	3	C_3 a-stretch	1968.19	gas	DL	2
			1955.2vs	Ar	IR	1
	4	SiC a-stretch	898.9w	Ar	IR	1

$B_0 = 0.0316$ DL^2

References

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[2] A. Van Orden, T. F. Giesen, R. A. Provencal, H. J. Hwang, and R. J. Saykally, J. Chem. Phys. **101**, 10237 (1994).
[3] X. Duan, L. W. Burggraf, D. E. Weeks, G. E. Davico, R. L. Schwartz, and W. C. Lineberger, J. Chem. Phys. **116**, 3601 (2002).

Si_5

$T_0 = 9360(400)$ gas PE[1]

$^3B_1$ C_{2v}
$T_0 = 4680(400)$ gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'			233(20)	gas	PE	1

Reference

[1] C. Xu, T. R. Taylor, G. R. Burton, and D. M. Neumark, J. Chem. Phys. **108**, 1395 (1998).

GeCCCGe

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u	3	C_3 a-stretch	1920.7	Ar	IR	1

Reference

[1] D. L. Robbins, C. M. L. Rittby, and W. R. M. Graham, J. Chem. Phys. **114**, 3570 (2001).

BeOBeNO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BeO stretch	1484.5 1483.0	Ar	IR	1

Reference

[1] G. P. Kushto, F. Ding, B. Liang, X. Wang, A. Citra, and L. Andrews, Chem. Phys. **257**, 223 (2000).

$Sc(CO)_2^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO a-stretch	1926.0	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 2964 (1999).

$Fe(CO)_2^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	2134.0	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Chem. Phys. **110**, 10370 (1999).

$Co(CO)_2^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	2168.9	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7773 (1999).

$Rh(CO)_2^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	2184.7	Ne	IR	1,2

References

[1] M. Zhou and L. Andrews, J. Am. Chem. Soc. **121**, 9171 (1999).
[2] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7773 (1999).

$Ir(CO)_2^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	2153.8	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7773 (1999).

$Ni(CO)_2^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO a-stretch	2205.3	Ne	IR	1

Reference

[1] B. Liang, M. Zhou, and L. Andrews, J. Phys. Chem. A **104**, 3905 (2000).

$Pd(CO)_2^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO a-stretch	2210.5	Ne	IR	1

Reference

[1] B. Liang, M. Zhou, and L. Andrews, J. Phys. Chem. A **104**, 3905 (2000).

$Pt(CO)_2^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO a-stretch	2210.3	Ne	IR	1

Reference

[1] B. Liang, M. Zhou, and L. Andrews, J. Phys. Chem. A **104**, 3905 (2000).

$Cu(CO)_2^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	2230.4	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Chem. Phys. **111**, 4548 (1999).

$Ag(CO)_2^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	2234.6	Ne	IR	1

Reference

[1] B. Liang and L. Andrews, J. Phys. Chem. A **104**, 9156 (2000).

$Au(CO)_2^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	2233.4	Ne	IR	1

Reference

[1] B. Liang and L. Andrews, J. Phys. Chem. A **104**, 9156 (2000).

Ga_2P_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'			213	gas	PE	1

Reference

[1] T. R. Taylor, H. Gómez, K. R. Asmis, and D. M. Neumark, J. Chem. Phys. **115**, 4620 (2001).

Ga_2As_3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'			193	gas	PE	1

Reference

[1] T. R. Taylor, H. Gómez, K. R. Asmis, and D. M. Neumark, J. Chem. Phys. **115**, 4620 (2001).

Al_3O_2

$\tilde{C}$

$T_0 = 23400(800)$ gas PE[1]

$\tilde{B}$

$T_0 = 19930(940)$ gas PE[1]

$\tilde{A}$

$T_0 = 10970(630)$ gas PE[1]

Reference

[1] H. Wu, X. Li, X.-B. Wang, C.-F. Ding, and L.-S. Wang, J. Chem. Phys. **109**, 449 (1998).

C_5^-

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

$T_0 = 27785(3)$ gas PD[9] $\tilde{C}-\tilde{X}$ 337–360 nm

27847(15) Ne AB[6] $\tilde{C}-\tilde{X}$ 311–360 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		1792(6)	gas	PD	9
			1756(20)	Ne	AB	6
	2		754(6)	gas	PD	9
			724(20)	Ne	AB	6
	7	Deformation	168H	gas	PD	9

$\tilde{B}$

$T_0 = 24563(3)$ gas PD[9] $\tilde{B}-\tilde{X}$ 372–407 nm

24540(20) Ne AB[9] $\tilde{B}-\tilde{X}$ 372–408 nm

Threshold for electron detachment from ground-state $C_5^- = 23020(10)$ gas TPE[1]PE[2]

$\tilde{A}\,^2\Pi_g$ $D_{\infty h}$

$T_0 = 20164$ gas MPD[3,7] $\tilde{A}-\tilde{X}$ 446–496 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		1649	gas	MPD	7
			1679(9)	Ne	AB	6
	2		729	gas	MPD	3,7
			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	4,8
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).
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[8] J. Szczepanski, R. Hodyss, and M. Vala, J. Phys. Chem. A **102**, 8300 (1998).
[9] N. M. Lakin, F. Güthe, M. Tulej, M. Pachkov, and J. P. Maier, Faraday Discuss. **115**, 383 (2000).

$SiCCCSi^-$

Threshold for electron detachment from ground-state $SiCCCSi^- = 14250(100)$ gas PE[1]

$\tilde{X}\,^2\Pi$ $D_{\infty h}$

$A = 60(30)$ PE[1]

Reference

[1] X. Duan, L. W. Burggraf, D. E. Weeks, G. E. Davico, R. L. Schwartz, and W. C. Lineberger, J. Chem. Phys. **116**, 3601 (2002).

Si_5^-

Threshold for electron detachment from ground-state $Si_5^- = 20900(160)$ gas PE[1]

Reference

[1] C. Xu, T. R. Taylor, G. R. Burton, and D. M. Neumark, J. Chem. Phys. **108**, 1395 (1998).

$Sc(CO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CO stretch	1851.4	Ar	IR	1
b_2		CO stretch	1716.3	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 2964 (1999).

$Ti(CO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO s-stretch	1893.1	Ne	IR	1
b_2		CO a-stretch	1799.3	Ne	IR	1

Reference

[1]M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 5259 (1999).

$Zr(CO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO stretch	1855.5	Ne	IR	1
b_2		CO stretch	1785.1	Ne	IR	1

Reference

[1]M. Zhou and L. Andrews, J. Am. Chem. Soc. **122**, 1531 (2000).

OZrCCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CCO a-stretch	2046.4	Ne	IR	1
		ZrO stretch	902.3	Ne	IR	1

Reference

[1]M. Zhou and L. Andrews, J. Am. Chem. Soc. **122**, 1531 (2000).

$Hf(CO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO stretch	1850.9	Ne	IR	1
b_2		CO stretch	1806.7	Ne	IR	1

Reference

[1]M. Zhou and L. Andrews, J. Am. Chem. Soc. **122**, 1531 (2000).

OHfCCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CCO a-stretch	2063.5	Ne	IR	1
		HfO stretch	897.2	Ne	IR	1

Reference

[1]M. Zhou and L. Andrews, J. Am. Chem. Soc. **122**, 1531 (2000).

$V(CO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO s-stretch	1944.0	Ne	IR	3
b_2		CO a-stretch	1844.2	Ne	IR	3
			1820	Ar	IR	1
			1816	Kr	IR	1
			1814	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).
[3]M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 5259 (1999).

$Nb(CO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1847.2	Ne	IR	1

Reference

[1]M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7785 (1999).

ONbCCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	2065.5	Ne	IR	1
		NbO stretch	950.9	Ne	IR	1

Reference

[1]M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7785 (1999).

$Ta(CO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1918.3	Ne	IR	1
		CO stretch	1838.6	Ne	IR	1

Reference

[1]M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7785 (1999).

OTaCCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	2087.5	Ne	IR	1
		TaO stretch	965.7	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7785 (1999).

$Mn(CO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO s-stretch	1972.8	Ne	IR	1
		CO a-stretch	1851.5	Ne	IR	1
			1832.5	Ar	IR	1

Reference

[1] L. Andrews, M. Zhou, X. Wang, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **104**, 8887 (2000).

$Re(CO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1905.4	Ne	IR	1
			1895.9	Ar	IR	1

Reference

[1] L. Andrews, M. Zhou, X. Wang, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **104**, 8887 (2000).

$Fe(CO)_2$

$^3B_2$[a] C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO stretch	1984.8w	Ar	IR	3
b_2		CO stretch	1879.2	Ar	IR	3

$\tilde{X}\ ^3\Sigma_g^-$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	CO a-stretch	1928.18	gas	IR,DL	1,2,5
			1917.1	Ne	IR	4

$B_0 = 0.0472$ DL[2,5]

[a]It has been proposed[3] that in an argon matrix this low-lying state occurs below the $^3\Sigma_g^-$ state.

References

[1] T. A. Seder, A. J. Ouderkirk, and E. Weitz, J. Chem. Phys. **85**, 1977 (1986).
[2] K. Tanaka, Y. Tachikawa, and T. Tanaka, Chem. Phys. Lett. **281**, 285 (1997).
[3] M. Zhou, G. V. Chertihin, and L. Andrews, J. Chem. Phys. **109**, 10893 (1998).
[4] M. Zhou and L. Andrews, J. Chem. Phys. **110**, 10370 (1999).
[5] K. Tanaka, Y. Tachikawa, K. Sakaguchi, T. Hikida, and T. Tanaka, J. Chem. Phys. **111**, 3970 (1999).

$Ru(CO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO a-stretch	1955.3	Ne	IR	1
			1915.3[a]	Ar	IR	1

[a]It is likely that for $Ru(CO)_2$, as for $Fe(CO)_2$, the ground electronic state of the molecule trapped in an argon matrix is not the same as that of the molecule trapped in a neon matrix.[1]

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 6956 (1999).

$Os(CO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO a-stretch	1975.2	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 6956 (1999).

$Co(CO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	7	CO stretch	1945.6	Ne	IR	3
			1920.8	Ar	IR	1,2

References

[1] L. A. Hanlan, H. Huber, E. P. Kundig, B. R. McGarvey, and G. A. Ozin, J. Am. Chem. Soc. **97**, 7054 (1975).
[2] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 10250 (1998).
[3] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7773 (1999).

$Rh(CO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	2031.0	Ne	IR	2,3
			2014.6	Ar	IR	1,3

References

[1] G. A. Ozin and A. J. L. Hanlan, Inorg. Chem. **18**, 2091 (1979).
[2] M. Zhou and L. Andrews, J. Am. Chem. Soc. **121**, 9171 (1999).
[3] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7773 (1999).

$Ir(CO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	2014.5	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7773 (1999).

$Ni(CO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO stretch	2100(80)	gas	PE	2
			2089.7	Ne	IR	5
			2071.5w	Ar	IR	1,4
	2		461.5Tvw	Ar	IR	4
	3		449.5Tvw	Ar	IR	4
b_1	6		398.9vw	Ar	IR	4
b_2	7	CO stretch	1978.9	Ne	IR	5
			1965.5vs	Ar	IR	1,3,4
	8	NiC stretch	515.5	Ar	IR	1,3,4
	9		335vw	Ar	IR	4

References

[1] R. L. DeKock, Inorg. Chem. **10**, 1205 (1971).
[2] A. E. Stevens, C. S. Feigerle, and W. C. Lineberger, J. Am. Chem. Soc. **104**, 5026 (1982).
[3] M. Zhou and L. Andrews, J. Am. Chem. Soc. **120**, 11499 (1998).
[4] L. Manceron and M. E. Alikhani, Chem. Phys. **244**, 215 (1999).
[5] B. Liang, M. Zhou, and L. Andrews, J. Phys. Chem. A **104**, 3905 (2000).

$Pd(CO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO a-stretch	2065.8	Ne	IR	2
			2051.6	Ar	IR	1

References

[1] B. Tremblay and L. Manceron, Chem. Phys. **250**, 187 (1999).
[2] B. Liang, M. Zhou, and L. Andrews, J. Phys. Chem. A **104**, 3950 (2000).

$Pt(CO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO a-stretch	2053.2	Ne	IR	2
			2039.8	Ar	IR	1
		PtCO deform.	801.9	Ar	IR	1
		PtC a-stretch	383.4	Ar	IR	1

References

[1] L. Manceron, B. Tremblay, and M. E. Alikhani, J. Phys. Chem. A **104**, 3750 (2000).
[2] B. Liang, M. Zhou, and L. Andrews, J. Phys. Chem. A **104**, 3950 (2000).

$Cu(CO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1904.4	Ne	IR	2
			1890.7	Ar	IR	1,2

References

[1] H. Huber, E. P. Kündig, M. Moskovits, and G. A. Ozin, J. Am. Chem. Soc. **97**, 2097 (1975).
[2] M. Zhou and L. Andrews, J. Chem. Phys. **111**, 4548 (1999).

$Ag(CO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1858.7	Ne	IR	2
			1842.0	Ar	IR	1
			1827.5			
			1798.8	Kr	IR	1
			1790.0			
			1802.0	Xe	IR	1
			1790.8			

References

[1] D. McIntosh and G. A. Ozin, J. Am. Chem. Soc. **98**, 3167 (1976).
[2] B. Liang and L. Andrews, J. Phys. Chem. A **104**, 9156 (2000).

$Au(CO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1943.7	Ne	IR	1

Reference

[1] B. Liang and L. Andrews, J. Phys. Chem. A **104**, 9156 (2000).

$Th(CO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO s-stretch	1827.7	Ne	IR	1
b_2		CO a-stretch	1775.6	Ne	IR	1

Reference

[1] J. Li, B. E. Bursten, M. Zhou, and L. Andrews, Inorg. Chem. **40**, 5448 (2001).

OThCCO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CO stretch	2048.6vs	Ne	IR	1
	2	CC stretch	1353.6vw	Ne	IR	1
		ThO stretch	822.5w	Ne	IR	1

Reference

[1] J. Li, B. E. Bursten, M. Zhou, and L. Andrews, Inorg. Chem. **40**, 5448 (2001).

$U(CO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO stretch	1840.2	Ne	IR	1
b_2	7	CO stretch	1790.8	Ne	IR	1

Reference

[1] M. Zhou, L. Andrews, J. Li, and B. E. Bursten, J. Am. Chem. Soc. **121**, 9712 (1999).

OUCCO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CO stretch	2051.5	Ne	IR	1
			1361.8	Ne	IR	1
		UO stretch	841.0	Ne	IR	1

Reference

[1] M. Zhou, L. Andrews, J. Li, and B. E. Bursten, J. Am. Chem. Soc. **121**, 9712 (1999).

NNPtNN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NN stretch	2206.9	Ne	IR	2
			2195.4	Ar	IR	1,2
			2205.7	N_2	IR	1,2

References

[1] D. W. Green, J. Thomas, and D. M. Gruen, J. Chem. Phys. **58**, 5453 (1973).
[2] A. Citra, X. Wang, W. D. Bare, and L. Andrews, J. Phys. Chem. A **105**, 7799 (2001).

NNThNN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NN stretch	1895.5	Ar	IR	1

Reference

[1] G. P. Kushto, P. F. Souter, and L. Andrews, J. Chem. Phys. **108**, 7121 (1998).

OVOVO

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1026.2	Ar	IR	1

Reference

[1] G. V. Chertihin, W. D. Bare, and L. Andrews, J. Phys. Chem. A **101**, 5090 (1997).

Co_2O_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			952.5T	Ar	IR	1

Reference

[1] G. V. Chertihin, A. Citra, L. Andrews, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **101**, 8793 (1997).

Ni_2O_3

$\tilde{X}$

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

Reference

[1] A. Citra, G. V. Chertihin, L. Andrews, and M. Neurock, J. Phys. Chem. A **101**, 3109 (1997).

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.
			995.3	Ar	IR	2
			640T	gas	PE	1

References

[1] L.-S. Wang, H. Wu, S. R. Desai, and L. Lou, Phys. Rev. B **53**, 8028 (1996).
[2] G. V. Chertihin, L. Andrews, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **101**, 4026 (1997).

$Ga_2P_3^-$

Threshold for electron detachment from ground-state $Ga_2P_3^- = 24130(20)$ gas PE[1]

Reference

[1] T. R. Taylor, H. Gómez, K. R. Asmis, and D. M. Neumark, J. Chem. Phys. **115**, 4620 (2001).

$Ga_2As_3^-$

Threshold for electron detachment from ground-state $Ga_2As_3^- = 22450(200)$ gas PE[1]

Reference

[1] T. R. Taylor, H. Gómez, K. R. Asmis, and D. M. Neumark, J. Chem. Phys. **115**, 4620 (2001).

$Al_3O_2^-$

Threshold for electron detachment from ground-state $Al_3O_2^- = 17590(480)$ gas PE[1]

Evidence for the participation of a second electronic state of $Al_3O_2^-$ in its photoelectron spectrum is presented by Ref. 2.

References

[1] H. Wu, X. Li, X.-B. Wang, C.-F. Ding, and L.-S. Wang, J. Chem. Phys. **109**, 449 (1998).
[2] T. K. Ghanty and E. R. Davidson, J. Phys. Chem. A **103**, 8985 (1999).

C_4S

$\tilde{B}$
$T_0 \cong 41700T$ Ar AB[1]

$\tilde{A}\,^3\Sigma^-$ $C_{\infty v}$
$T_0 = 22380(10)$ Ne AB[4] $\tilde{A}-\tilde{X}$ 400–447 nm
22220T Ar AB[1] $\tilde{A}-\tilde{X}$ 380–450 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1		2022(10)	Ne	AB	4
	2		1595(10)	Ne	AB	4
	3		1060(10)	Ne	AB	4
	4		584(10)	Ne	AB	4

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1746.8	Ar	IR	3

$B_0 = 0.051$ 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).
[3] J. Szczepanski, R. Hodyss, J. Fuller, and M. Vala, J. Phys. Chem. A **103**, 2975 (1999).
[4] E. Riaplov, M. Wyss, N. M. Lakin, and J. P. Maier, J. Phys. Chem. A **105**, 4894 (2001).

$Sn(CN)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		SnC stretch	370(60)	gas	PE	1

Reference

[1] V. D. Moravec and C. C. Jarrold, J. Chem. Phys. **113**, 1035 (2000).

$Ti(CO)_2^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO s-stretch	1742.1	Ne	IR	1
b_2		CO a-stretch	1677.5	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 5259 (1999).

$Zr(CO)_2^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO stretch	1745.9	Ne	IR	1
b_2		CO stretch	1682.2	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Am. Chem. Soc. **122**, 1531 (2000).

$Hf(CO)_2^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO stretch	1747.4	Ne	IR	1
b_2		CO stretch	1681.0	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Am. Chem. Soc. **122**, 1531 (2000).

$V(CO)_2^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO s-stretch	1777.9	Ne	IR	1
b_2		CO a-stretch	1670.6	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 5259 (1999).

$Nb(CO)_2^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO stretch	1768.6	Ne	IR	1
b_2	7	CO stretch	1656.7	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7785 (1999).

$Ta(CO)_2^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1773.6T	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7785 (1999).

$Mn(CO)_2^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1756.2	Ne	IR	1
			1754.9	Ar	IR	1

Reference

[1] L. Andrews, M. Zhou, X. Wang, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **104**, 8887 (2000).

$Re(CO)_2^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1788.7	Ne	IR	1

Reference

[1] L. Andrews, M. Zhou, X. Wang, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **104**, 8887 (2000).

$Fe(CO)_2^-$

$^2A_1$ [a] C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CO s-stretch	1815.0w	Ar	IR	1
b_2		CO a-stretch	1721.9	Ar	IR	1

$\tilde{X}\,^2\Pi_u$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+		CO a-stretch	1732.9	Ne	IR	2

[a] It has been proposed[2] that in an argon matrix this low-lying state occurs below the $^2\Pi_u$ state.

References

[1] M. Zhou, G. V. Chertihin, and L. Andrews, J. Chem. Phys. **109**, 10893 (1998).
[2] M. Zhou and L. Andrews, J. Chem. Phys. **110**, 10370 (1999).

$Ru(CO)_2^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO s-stretch	1830.6	Ne	IR	1
			1834.2	Ar	IR	1
b_2		CO a-stretch	1769.6	Ne	IR	1
			1756.9	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 6956 (1999).

$Os(CO)_2^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO s-stretch	1898.8	Ne	IR	1
b_2		CO a-stretch	1783.5	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 6956 (1999).

$Co(CO)_2^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO stretch	1847.1	Ne	IR	2
			1860.2	Ar	IR	1
b_2	7	CO stretch	1789.2	Ne	IR	2
			1768.9	Ar	IR	1

References

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 10250 (1998).
[2] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7773 (1999).

$Rh(CO)_2^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO stretch	1900.4	Ne	IR	1,2
b_2	7	CO stretch	1816.7	Ne	IR	1,2
			1799.4	Ar	IR	2

References

[1] M. Zhou and L. Andrews, J. Am. Chem. Soc. **121**, 9171 (1999).
[2] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7773 (1999).

$Ir(CO)_2^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1818.1	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 7773 (1999).

$Ni(CO)_2^-$

Threshold for electron detachment from ground-state $Ni(CO)_2^-$ = 5190(110) gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO a-stretch	1813.8	Ne	IR	3
			1801.7	Ar	IR	2

References

[1] A. E. Stevens, C. S. Feigerle, and W. C. Lineberger, J. Am. Chem. Soc. **104**, 5026 (1982).
[2] M. Zhou and L. Andrews, J. Am. Chem. Soc. **120**, 11499 (1998).
[3] B. Liang, M. Zhou, and L. Andrews, J. Phys. Chem. A **104**, 3905 (2000).

$Pd(CO)_2^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO a-stretch	1832.3	Ne	IR	1

Reference

[1] B. Liang, M. Zhou, and L. Andrews, J. Phys. Chem. A **104**, 3905 (2000).

$Pt(CO)_2^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO a-stretch	1844.0	Ne	IR	1

Reference

[1] B. Liang, M. Zhou, and L. Andrews, J. Phys. Chem. A **104**, 3905 (2000).

$Cu(CO)_2^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1793.9	Ne	IR	1
			1780.8	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Chem. Phys. **111**, 4548 (1999).

$Th(CO)_2^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1719.1	Ne	IR	1

Reference

[1] J. Li, B. E. Bursten, M. Zhou, and L. Andrews, Inorg. Chem. **40**, 5448 (2001).

$U(CO)_2^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1661.2	Ne	IR	1

Reference

[1] M. Zhou, L. Andrews, J. Li, and B. E. Bursten, J. Am. Chem. Soc. **121**, 9712 (1999).

$Pt(NN)_2^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NN stretch	1869.0	Ne	IR	1
			1862.5	N_2	IR	1

Reference

[1] A. Citra, X. Wang, W. D. Bare, and L. Andrews, J. Phys. Chem. A **105**, 7799 (2001).

$Al(CO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO s-stretch	1995.3m	Ar	IR	2–4
			1988.7			
			1988	Kr	IR	1
			2003.0	N_2	IR	3
			497.0w	Ar	IR	2
b_1		Wag	234.7vw	Ar	IR	2
b_2		CO a-stretch	1907.6vs	Ar	IR	2–4
			1891.0			
			1890	Kr	IR	1
			1912.8	N_2	IR	3
		AlCO deform.	281.0w	Ar	IR	2

References

[1] A. J. Hinchliffe, J. S. Ogden, and D. D. Oswald, J. Chem. Soc., Chem. Commun. 388 (1972).
[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).
[4] L. Zhang, J. Dong, M. Zhou, and Q. Qin, J. Chem. Phys. **113**, 10169 (2000).

$Ga(CO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO s-stretch	2016.8	Ar	IR	1,2
			2011.8			
			2009.2			
			2006.1	Kr	IR	2
			2040.2	N_2	IR	1
b_2		CO a-stretch	1933.6	Ar	IR	2
			1920.4			
			1912.4			
			1909.3	Kr	IR	2
			1938.7	N_2	IR	1

References

[1] A. Feltrin, M. Guido, and S. Nunziante Cesaro, Vib. Spectrosc. **8**, 175 (1995).
[2] H.-J. Himmel, A. J. Downs, J. C. Green, and T. M. Greene, J. Phys. Chem. A **104**, 3642 (2000).

$In(CO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO s-stretch	2029.2	Ar	IR	1
		CO a-stretch	1980.2	Ar	IR	1
			483w	Ar	IR	1

Reference

[1] H.-J. Himmel, A. J. Downs, J. C. Green, and T. M. Greene, J. Phys. Chem. A **104**, 3642 (2000).

$Sn(CN)_2^-$

Threshold for electron detachment from ground-state $Sn(CN)_2^-$ $=21160(32)$ gas PE[1]

Reference

[1] V. D. Moravec and C. C. Jarrold, J. Chem. Phys. **113**, 1035 (2000).

$Ni(NO)_2^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO a-stretch	1926.2	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 3915 (2000).

C_4O^-

$\tilde{B}\,^2\Pi$ $C_{\infty v}$
$T_0=22610(10)$ Ne AB[1] $\tilde{B}-\tilde{X}$ 417–443 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	4		676(10)	Ne	AB	1

$\tilde{A}\,^2\Sigma^+$ $C_{\infty v}$
$T_0=11434(3)$ Ne AB[1] $\tilde{A}-\tilde{X}$ 870–875 nm

Reference

[1] E. Riaplov, M. Wyss, N. M. Lakin, and J. P. Maier, J. Phys. Chem. A **105**, 4894 (2001).

$V(NO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NO s-stretch	1736.8	Ar	IR	1
b_2		NO a-stretch	1627.8	Ne	IR	2
			1614.5	Ar	IR	1

References

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 478 (1999).
[2] L. Andrews and X. Wang, J. Phys. Chem. A **106**, 1196 (2002).

$Nb(NO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO stretch	1583.6	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 10025 (1998).

$Ta(NO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO stretch	1574.8	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 10025 (1998).

$Cr(NO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO stretch	1628.8	Ne	IR	2
			1623.3	Ar	IR	1

References

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 7452 (1998).
[2] L. Andrews and X. Wang, J. Phys. Chem. A **106**, 1196 (2002).

$Mo(NO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO stretch	1642.7	Ar	IR	1

Reference

[1] L. Andrews and M. Zhou, J. Phys. Chem. A **103**, 4167 (1999).

$W(NO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO stretch	1639.2	Ar	IR	1

Reference

[1] L. Andrews and M. Zhou, J. Phys. Chem. A. **103**, 4167 (1999).

$Mn(NO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NO stretch	1744.7	Ar	IR	1
b_2		NO stretch	1706.2	Ne	IR	2
			1693.0	Ar	IR	1

References

[1] L. Andrews, M. Zhou, and D. W. Ball, J. Phys. Chem. A **102**, 10041 (1998).
[2] L. Andrews and X. Wang, J. Phys. Chem. A **106**, 1196 (2002).

$Re(NO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO stretch	1651.6	Ar	IR	1

Reference

[1] L. Andrews, M. Zhou, and D. W. Ball, J. Phys. Chem. A **102**, 10041 (1998).

$Fe(NO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO s-stretch	1810.8	Ne	IR	2
			1798.1	Ar	IR	2
		NO a-stretch	1744.6	Ne	IR	2
			1731.6	Ar	IR	1,2

References

[1] G. K. Ruschel, T. M. Nemetz, and D. W. Ball, J. Mol. Struct. **384**, 101 (1996).
[2] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 3915 (2000).

$Ru(NO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO s-stretch	1805.3	Ne	IR	1
		NO a-stretch	1721.4	Ne	IR	1
			1709.6	Ar	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 8689 (2000).

$Os(NO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO s-stretch	1834.7	Ne	IR	1
			1823.8			
			1815.8			
			1811.1			
		NO a-stretch	1726.9	Ne	IR	1
			1723.2	Ar	IR	1
			1717.9			
			1712.5			

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 8689 (2000).

$Co(NO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO s-stretch	1827.2	Ar	IR	1
		NO a-stretch	1749.1	Ne	IR	1
			1737.6	Ar	IR	1
		CoN stretch	581.5	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 3915 (2000).

$Rh(NO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO s-stretch	1801.8	Ar	IR	1
		NO a-stretch	1746.9	Ne	IR	1
			1736.5	Ar	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 11897 (2000).

$Ir(NO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO a-stretch	1743.2	Ar	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 11897 (2000).

$Ni(NO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	NO a-stretch	1762.0	Ne	IR	2
			1750.2vs	Ar	IR	1–3
	4	NiN a-stretch	524.4wm	Ar	IR	2,3
Π_u	6	Bend	623.9vw	Ar	IR	3

References

[1] G. K. Ruschel, T. M. Nemetz, and D. W. Ball, J. Mol. Struct. **384**, 101 (1996).
[2] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 3915 (2000).
[3] M. E. Alikhani, L. Krim, and L. Manceron, J. Phys. Chem. A **105**, 7817 (2001).

$Pd(NO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	NO a-stretch	1753.0	Ne	IR	1
			1739.0vs	Ar	IR	1,2
	4	PdN a-stretch	433.5w	Ar	IR	2
Π_u	6	Bend	494.5vw	Ar	IR	2

References

[1] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 8160 (2000).
[2] M. E. Alikhani, L. Krim, and L. Manceron, J. Phys. Chem. A **105**, 7817 (2001).

$Pt(NO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO a-stretch	1776.9T	Ne	IR	1
			1763.8	Ar	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 8160 (2000).

$Cu(NO)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO a-stretch	1637.2	Ne	IR	1
			1611.6	Ar	IR	1
		CuN a-stretch	615.1vw	Ne	IR	1
			608.6	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 2618 (2000).

$Al(CO)_2^-$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO s-stretch	1803.9	Ar	IR	1
b_2	7	CO a-stretch	1741.0	Ar	IR	1

Reference

[1] L. Zhang, J. Dong, M. Zhou, and Q. Qin, J. Chem. Phys. **113**, 10169 (2000).

$Si(CO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO s-stretch	1995.9w	Ar	IR	2
b_2	7	CO a-stretch	1928.3	Ar	IR	1,2

References

[1] R. R. Lembke, R. F. Ferrante, and W. Weltner, Jr., J. Am. Chem. Soc. **99**, 416 (1977).
[2] L. Zhang, J. Dong, and M. Zhou, J. Chem. Phys. **113**, 8700 (2000).

$Ge(CO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO s-stretch	2000.8	Ar	IR	1
b_2	7	CO a-stretch	1934.8	Ar	IR	1

Reference

[1] L. Zhang, J. Dong, and M. Zhou, J. Chem. Phys. **113**, 8700 (2000).

$Sn(CO)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO s-stretch	1996.6	Ar	IR	1
b_2	7	CO a-stretch	1904.3	Ar	IR	1

Reference

[1] L. Zhang, J. Dong, and M. Zhou, J. Chem. Phys. **113**, 8700 (2000).

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	80.52	gas	IR,MW	3,5

$B_0 = 0.077$ IR[2,5]MW[4,5]

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).
[5] H. Lichau, S. C. Ross, M. Lock, S. Albert, B. P. Winnewisser, M. Winnewisser, and F. C. De Lucia, J. Phys. Chem. A **105**, 10080 (2001).

$Cr(NO)_2^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO stretch	1463.1	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 7452 (1998).

$Co(NO)_2^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO a-stretch	1593.8	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 3915 (2000).

$Ni(NO)_2^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO a-stretch	1592.2	Ne	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 3915 (2000).

$Cu(NO)_2^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO a-stretch	1565.2	Ne	IR	1
			1551.2	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 2618 (2000).

$Si(N_2)_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NN s-stretch	2045.0	N_2	IR	1
b_2	7	NN a-stretch	1912.9	N_2	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, and J. Glatthaar, Organomet. **19**, 4775 (2000).

(*cyc*-$O_2V)O_2$

$\tilde{C}$
$T_0 = 16140(800)$ gas PE[2]

$\tilde{B}$
$T_0 = 11300(800)$ gas PE[2]

$\tilde{A}$
$T_0 = 8070(800)$ gas PE[2]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	1121.9	Ar	IR	1
			1126.4	N_2	IR	1
		OVO s-stretch	975.3	Ar	IR	1
		OVO a-stretch	974.1s	Ar	IR	1
			968.8	N_2	IR	1
			555.6	Ar	IR	1
			561.8	N_2	IR	1
			506.9	Ar	IR	1,3

References

[1] G. V. Chertihin, W. D. Bare, and L. Andrews, J. Phys. Chem. A **101**, 5090 (1997).
[2] H. Wu and L.-S. Wang, J. Chem. Phys. **108**, 5310 (1998).
[3] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 8251 (1998).

(*cyc*-$O_2Nb)O_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	1109.3	Ar	IR	1
		ONbO s-stretch	945.9	Ar	IR	1
			943.5			
		ONbO a-stretch	903.6	Ar	IR	1
			900.7			
			511.3	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 8251 (1998).

(*cyc*-$O_2Ta)O_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	1095.7	Ar	IR	1,2
		OTaO s-stretch	950.5	Ar	IR	1,2
			946.3			
		OTaO a-stretch	894.5	Ar	IR	1,2
			889.4			
			524.2	Ar	IR	1

References

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 8251 (1998).
[2] M. Chen, X. Wang, L. Zhang, M. Yu, and Q. Qin, Chem. Phys. **242**, 81 (1999).

(*cyc*-$O_2Mn)O_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	1130	Ar	IR	1
		OMnO a-stretch	974.9	Ar	IR	1

Reference

[1] G. V. Chertihin and L. Andrews, J. Phys. Chem. A **101**, 8547 (1997).

(*cyc*-$O_2Re)O_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OReO s-stretch	992.6	Ne	IR	1
			992.4	Ar	IR	1
		OReO a-stretch	969.8	Ne	IR	1
			964.3	Ar	IR	1
		OO stretch	878.6	Ne	IR	1
			882.4	Ar	IR	1

Reference

[1] M. Zhou, A. Citra, B. Liang, and L. Andrews, J. Phys. Chem. A **104**, 3457 (2000).

(*cyc*-$O_2Fe)O_2$

$\tilde{A}$

$T_0 = 4360(160)$ gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			850(50)	gas	PE	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
			920(50)	gas	PE	2
			968.9	Ar	IR	1
			970.2	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] H. Wu, S. R. Desai, and L.-S. Wang, J. Am. Chem. Soc. **118**, 5296 (1996); J. Am. Chem. Soc. **118**, 7434 (1996).

(*cyc*-$O_2Ru)O_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ORuO s-stretch	946.9	Ne	IR	1
			940.2	Ar	IR	1
		ORuO a-stretch	928.5	Ne	IR	1
			920.7	Ar	IR	1

Reference

[1] M. Zhou, A. Citra, B. Liang, and L. Andrews, J. Phys. Chem. A **104**, 3457 (2000).

RuO_4

$\tilde{X}$ T_d

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
f_2	3	RuO_4 stretch	922.2	Ne	IR	2
			916.6	Ar	IR	1,2

References

[1] D. W. Green, J. G. Kay, G. L. Zimmerman, and B. A. Balko, J. Mol. Spectrosc. **138**, 62 (1989).
[2] M. Zhou, A. Citra, B. Liang, and L. Andrews, J. Phys. Chem. A **104**, 3457 (2000).

(*cyc*-$O_2Os)O_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OOsO s-stretch	1004.8	Ar	IR	1
		OOsO a-stretch	970.0	Ar	IR	1
		OO stretch	898.1	Ar	IR	1

Reference

[1] M. Zhou, A. Citra, B. Liang, and L. Andrews, J. Phys. Chem. A **104**, 3457 (2000).

$OOCoO_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OCoO a-stretch	954.7	Ar	IR	1

Reference

[1] G. V. Chertihin, A. Citra, L. Andrews, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **101**, 8793 (1997).

(*cyc*-$O_2Co)O_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OCoO a-stretch	897.3	Ar	IR	1
		OCoO s-stretch	797.3	Ar	IR	1

Reference

[1] G. V. Chertihin, A. Citra, L. Andrews, and C. W. Bauschlicher, Jr., J. Phys. Chem. A **101**, 8793 (1997).

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	1048.4	Ar	IR	1,2
			1045	Xe	IR	1
			1038	O_2	IR	1

References

[1] A. J. L. Hanlan and G. A. Ozin, Inorg. Chem. **16**, 2848 (1977).
[2] A. Citra and L. Andrews, J. Phys. Chem. A **103**, 4845 (1999).

O_2PdO_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	1112.5	Ne	IR	3
			1110.8	Ar	IR	1,2
		PdO stretch	504w	Ar	IR	1

References

[1] H. Huber, W. Klotzbücher, G. A. Ozin, and A. Vander Voet, Can. J. Chem. **51**, 2722 (1973).
[2] W. D. Bare, A. Citra, G. V. Chertihin, and L. Andrews, J. Phys. Chem. A **103**, 5456 (1999).
[3] X. Wang and L. Andrews, J. Phys. Chem. A **105**, 5812 (2001).

O_2PtO_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	1056.0	Ne	IR	3
			1051.3	Ar	IR	1,2

References

[1] H. Huber, W. Klotzbücher, G. A. Ozin, and A. Vander Voet, Can. J. Chem. **51**, 2722 (1973).
[2] W. D. Bare, A. Citra, G. V. Chertihin, and L. Andrews, J. Phys. Chem. A **103**, 5456 (1999).
[3] X. Wang and L. Andrews, J. Phys. Chem. A **105**, 5812 (2001).

ReO_4^-

$\tilde{X}$ T_d

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
f_2	3	ReO_4 stretch	914.5	Ne	IR	1
			907.2	Ar	IR	1

Reference

[1] M. Zhou, A. Citra, B. Liang, and L. Andrews, J. Phys. Chem. A **104**, 3457 (2000).

FeO_4^-

Threshold for electron detachment from ground-state $FeO_4^- = 26620(320)$ gas PE[1]

Reference

[1] H. Wu, S. R. Desai, and L.-S. Wang, J. Am. Chem. Soc. **118**, 5296 (1996); J. Am. Chem. Soc. **118**, 7434 (1996).

$C_2O_3^-$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CO stretch	1793.7	Ar	IR	1
a''		CO_2 a-stretch	1701.7	Ar	IR	1

Reference

[1] M. Zhou, L. Zhang, M. Chen, and Q. Qin, J. Chem. Phys. **112**, 7089 (2000).

UO_2F_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		UO_2 a-stretch	940.5	Ar	IR	1

Reference

[1] P. F. Souter and L. Andrews, J. Mol. Struct. **412**, 161 (1997).

F_2CCO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CCO a-stretch	2161.6m	Ar	IR	1
	2	CCO s-stretch	1426.8vs	Ar	IR	1
b_2	7	CF_2 a-stretch	1274.4s	Ar	IR	1

Reference

[1] C. Kötting, W. Sander, M. Senzlober, and H. Bürger, Chem. Eur. J. **4**, 1611 (1998).

O_2CNO^-

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NO stretch	1495.8	Ar	IR	1
	2	CO_2 s-stretch	1310.4	Ar	IR	1
a''		CO_2 a-stretch	1713.6	Ar	IR	1

Reference

[1] M. Zhou, L. Zhang, and Q. Qin, J. Am. Chem. Soc. **122**, 4483 (2000).

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
			1831.5	Ar	IR	11,12
			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
			1630.1	Ar	IR	11,12
			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
			1296.2	Ar	IR	11,12
			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
			769.2	Ar	IR	11,12
			776wm	N_2	IR	4,11
			788	O_2	IR	2
			787	NO	IR,Ra	6
	5	NO wag	627	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	414	gas	IR	5
			420w	N_2	IR	4
			405	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^3IR[9,10]

References

[1] L. D'Or and P. Tarte, Bull. Soc. Roy. Sci. Liège **22**, 276 (1953).
[2] W. G. Fateley, H. A. Bent, and B. Crawford, Jr., J. Chem. Phys. **31**, 204 (1959).
[3] A. H. Brittain, A. P. Cox, and R. L. Kuczkowski, Trans. Faraday Soc. **65**, 1963 (1969).
[4] E. L. Varetti and G. C. Pimentel, J. Chem. Phys. **55**, 3813 (1971).
[5] C. H. Bibart and G. E. Ewing, J. Chem. Phys. **61**, 1293 (1974).
[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).
[12] C.-I Lee, Y.-P. Lee, X. Wang, and Q.-Z. Qin, J. Chem. Phys. **109**, 10446 (1998).

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	NON s-stretch	973.6m	Ne	IR	3
			971.0	Ar	IR	4,5
			969w	N_2	IR	1
			973m	NO	IR,Ra	2
	3	NON bend	366s	N_2	IR	1
			395	NO	Ra	2
a_2	5	Torsion	210	NO	Ra	2
b_1	6	Torsion	140	NO	Ra	2
b_2	7	N=O a-stretch	1697.2vs	Ne	IR	3
			1688.6	Ar	IR	4,5
			1690s	N_2	IR	1
			1687vs	NO	IR	2
			1661w	N_2	IR	1
	8	O=NO a-bend	704.6	Ar	IR	5
			704vw	N_2	IR	1
			705vw	NO	IR	2
	9	NON a-stretch	380	Ar	IR	5
			387m	N_2	IR	1,5

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).
[5] C.-I Lee, Y.-P. Lee, X. Wang, and Q.-Z. Zin, J. Chem. Phys. **109**, 10446 (1998).

t,c-ONONO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	*t*-N=O stretch	1704.5	Ar	IR	1,2
	2	*c*-N=O stretch	1665.7	Ar	IR	1,2
	3	ONO a-deform.	877.8	Ar	IR	1,2
	6	N··O stretch	243.0	Ar	IR	1,2

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OPOPO

$\tilde{X}$ C_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1253.4	Ar	IR	1,2
			1247.8	Ar	IR	1,2
			859.3	Ar	IR	1,2

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[1] M. McCluskey and L. Andrews, J. Phys. Chem. **95**, 2679 (1991).
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CO_4^-

The gas-phase photodestruction cross section of CO_4^- ($O_2C\cdot\cdot O_2^-$) is small over the 840–350 nm range.[1–4] In a neon matrix,[5] the onset of photodestruction occurs near 260 nm, with evidence for the detachment of O or O^-.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CO_2 a-stretch	1895.2vs	Ne	IR	5
			1891.5	Ar	IR	5,6
	2	CO_2 s-stretch	1256.5s	Ne	IR	5
			1257.0	Ar	IR	5,6
	4	CO_2 scissors	697.1m	Ne	IR	5
			691.2	Ar	IR	5,6

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c-FC(O)OO

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	C=O stretch	1913.2vs	Ne	IR	1
			1904.5vs	Ar	IR	1
	2	CF stretch	1202.1s	Ne	IR	1
			1196.7s	Ar	IR	1
	3	OO stretch	1078.1wm	Ne	IR	1
			1071.9wm	Ar	IR	1
	4	C–O stretch	867.1wm	Ne	IR	1
			863.6wm	Ar	IR	1
	5	OCO deform.	661.0w	Ne	IR	1
			659.2w	Ar	IR	1
	6	FCO deform.	552.7w	Ne	IR	1
			550.3vw	Ar	IR	1
	7	COO deform.	346.2vw	Ne	IR	1
a''	8	OPLA	708.7w	Ne	IR	1
			704.2w	Ar	IR	1

Reference

[1] S. Sander, H. Pernice, and H. Willner, Chem. Eur. J. **6**, 3645 (2000).

t-FC(O)OO

A gas-phase absorption between 200 and 285 nm, with maximum at 43100 (232 nm), has been assigned[1,2] to FC(O)OO. This absorption maximum has been observed[3] at 42550 (235 nm) in a neon matrix.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	C=O stretch	1925.9s	Ne	IR	3
			1919.2	Ar	IR	3
	2	CF stretch	1175.0vs	Ne	IR	3
			1168.3	Ar	IR	3
	3	OO stretch	1090.1m	Ne	IR	3
			1084.8	Ar	IR	3
	4	C–O stretch	900.8m	Ne	IR	3
			895.7	Ar	IR	3
	5	OCO deform.	680.2w	Ne	IR	3
			678.4	Ar	IR	3
	6	FCO deform.	520.9w	Ne	IR	3
			518.5	Ar	IR	3
	7	COO deform.	335.7vw	Ne	IR	3
a''	8	OPLA	712.0wm	Ne	IR	3
			707.4	Ar	IR	3

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CF_3N

^3E C_{3v}
$T_0=28250$ Ar AB[1] 342–354 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1160T	Ar	AB	1
			500T	Ar	AB	1

Reference

[1] N. P. Gritsan, I. Likhotvorik, Z. Zhu, and M. S. Platz, J. Phys. Chem. A **105**, 3039 (2001).

$ClONO_2$

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	1292.84vs	gas	IR,Ra	1,2,4,13
					DL	18,21,23
			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	1,2,4
					DL	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]DL[23]
Torsional barrier=1900(100) gas IR[6,8]

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SO_4

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		S=O stretch	1443s	Ar	IR	1,2
		S=O stretch	1273s	Ar	IR	1,2
		O–O stretch	925wm	Ar	IR	1
			777wm	Ar	IR	1
			611m	Ar	IR	1
			498sh	Ar	IR	1
			490sh	Ar	IR	1

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CF_3O

$\tilde{B}$
$T_0 \leqslant 34000$ Ne AB[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			495(10)	Ne	AB	8

$\tilde{A}\,^2A_1$ C_{3v} Structure: LF[6]
T_0=28531.26(2) gas LF[3–6] $\tilde{A}-\tilde{X}$ 330–400 nm
28517(3) Ne AB[8] $\tilde{A}-\tilde{X}$ 310–351 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		819(5)	Ne	AB	8
	3		635.0	gas	LF	5,6
			632(5)	Ne	AB	8
e	4	CF_3 a-stretch	1254(5)	Ne	AB	8
	5	CF_3 deform.	626.1	gas	LF	6
			632(5)	Ne	AB	8
	6	FCO deform.	426.3	gas	LF	3–6
			434(5)	Ne	AB	8

τ_0=30.1 ns gas LF[3]
A_0=0.191; B_0=0.195 LF[5,6]

$\tilde{X}\,^2E$[a] C_{3v} Structure: LF[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO stretch	1215 (ω)	gas	LF	3,4,7
			1273ms	Ne	IR	8
			1260ms	Ar	IR	8
	2	CF_3 s-stretch	977 (ω)	gas	LF	3,4,7
			891w	Ne	IR	8
			894w	Ar	IR	8
	3	CF_3 umbrella	527 (ω)	gas	LF	7
			621w	Ne	IR	8
			622w	Ar	IR	8
e	4	CF_3 a-stretch	1215s (a'')	Ne	IR	8
			1207vs (a')	Ne	IR	8
			1207s[b] (a'')	Ar	IR	8
			1199vs (a')	Ar	IR	8
	5	CF_3 deform.	600 (ω)	gas	LF	7
			666w (a')	Ne	IR	8
			663w (a')	Ar	IR	8
	6	FCO deform.	465 (ω)	gas	LF	3,4,7

$A=-41(5)$ gas LF[5]
B_0=0.198 LF[5]

[a] Significant Jahn–Teller interaction.[7] Reference 8 has proposed that the unusually large shifts in the vibrational fundamentals of CF_3O isolated in neon and argon matrices from their gas-phase positions may be a consequence of an interaction between CF_3O and Ne or Ar which increases the Jahn–Teller stabilization energy sufficiently to ''lock in'' the distorted structure.
[b] References 1 and 2 report 1221.6.

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CF_3S

$\tilde{A}\,^2A_1$ C_{3v} Structure: LF[3]
T_0=26393.16(2) gas LF[1–3]FD[1,2] $\tilde{A}-\tilde{X}$ 339–380 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF stretch	990.5	gas	LF,FD	2,3
	2	CF_3 umbrella	737.7	gas	LF,FD	2,3
	3	CS stretch	310.2	gas	LF,FD	1–3
e	5	CF_3 deformation	548	gas	LF,FD	2,3
	6	CF_3 rock	281.4	gas	LF,FD	2,3

τ_0=2.74(14) μs gas LF[1,2]
A_0=0.189; B_0=0.103 LF[3]

$\tilde{X}\,^2E$[a] C_{3v} Structure: LF[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF_3 s-stretch	1142(ω)	gas	LF	4
	2	CS stretch	765(ω)	gas	LF	4
	3	CF_3 umbrella	449(ω)	gas	LF	4
e	5	CF_3 deform.	536(ω)	gas	LF	4
	6	FCS deform.	320(ω)	gas	LF	4

$A_0 = -160$ gas LF[2]
$A_0 = 0.189$; $B_0 = 0.111$ LF[3]

[a]Significant Jahn–Teller interaction.[4]

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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

$\tau = 2.1(2)$ 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[10,16] 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]
$\tau = 9.0(9)$ ns gas EF[1]EM[9,11]TPEFCO[13,15]
$B_0 = 0.169$ 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. TPEPICO[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 $CF_3^+ + F$. TPEPICO[12]

$\tilde{X}\,^2F_1$
Direct dissociation into $CF_3^+ + F$. TPEPICO[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_3Cl^+

$\tilde{F}\,^2E$ C_{3v}
$T_0^a \leqslant 66130(400)$ gas PE[2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF_3 umbrella	589(80)	gas	PE	4
	3	CCl stretch	420(80)	gas	PE	4

$\tilde{E}\,^2A_1$ C_{3v}
$T_0^a = 60420(400)$ gas PE[2,4]
Broad emission bands in the 190–600 nm spectral region[8,9,11] which appear on excitation of CF_3Cl by synchrotron radiation with energy greater than 19 eV have been attributed[9,11] to transitions arising from the $\tilde{E}$ state of CF_3Cl^+. Discrete structure between 190 and 270 nm is contributed by the $B-X$ and $A-X$ transitions of CF.[11]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF_3 umbrella	637(80)	gas	PE	4

$\tau = 9.4(1.8)$ ns gas TPEFCO[10]

$\tilde{D}\,^2E$ C_{3v}
T_0 [a] $= 39720(400)$ gas PE[1,2,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF_3 umbrella	726(80)	gas	PE	4
	3	CCl stretch	387(80)	gas	PE	4
e	4	CF_3 stretch	1130(80)	gas	PE	4

$\tilde{C}\,^2E$ C_{3v}
$T^{ab} = 34610(400)$ gas PE[1,2,4]
Broad, unstructured absorption with onset near 400 nm (25000) and maximum at 295 nm (33900) which appears on argon-resonance photolysis of CF_3Cl isolated in solid argon and which has a photodecomposition threshold at a wavelength longer than 340 nm has been assigned[7] to the $\tilde{C}-\tilde{X}$ transition of CF_3Cl^+.

$\tilde{B}\,^2A_2$ C_{3v}
$T^{ab} = 26950(400)$ gas PE[1,2,4]

$\tilde{A}\,^2A_1$ C_{3v}
$T^{ab} = 22110(400)$ gas PE[1,2,4]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1299vs	Ar	IR	5,6
		CCl stretch	734wm	Ar	IR	5,6
		Deformation	460ms 451m	Ar	IR	5,6
		Deformation	416m	Ar	IR	5,6

[a]The first ionization potential of CF_3Cl is taken as 12.42(4) eV, the mean of the values reported in the photoionization studies of Refs. 2 and 3.
[b]From vertical ionization potential.

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SiF_4^+

$\tilde{D}\,^2A_1$ T_d Structure: PE,EF[9]
$T^{ab} = 50800(200)$ gas PE[2]TPE[13,15]EM[14]
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	7,13,15
e	2	Deformation	258(40)	gas	TPE	13
f_2	3	SiF stretch	1178(40)	gas	TPE	13
	4	Deformation	379(12)	gas	TPE	15

$\tau = 9.30(4)$ ns gas EF[7]EM[12,14]TPEFCO[13]
$B_0 = 0.136(1)$ [c] EF[9]

$\tilde{C}\,^2F_2$ T_d [d] Structure: PE,EF[9]
T_0 [a] $= 33130(100)$ gas PE[2,3,5]TPE[13,15]
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	TPE,EF	3,5,7,13,15
e	2	Deformation	159.0(5)	gas	EF	7
f_2	4	Deformation	431.0(5)	gas	TPE,EF	3,5,7,13,15

$A = +6.9(2)$ 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]TPE[15]

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]TPE[15]

$\tilde{X}\,^2F_1$ T_d

[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[8,11]
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
			339(12)	gas	TPE	11

$\tilde{C}\,^2F_2$
$T_0 = 26620(160)$ gas PE[1,2]TPE[8,11]
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[6,10] of $SiCl_4$, as well as TPEFCO measurements,[8] a radiative lifetime of 39(2) 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]TPE[11]

$\tilde{A}\,^2F_2$
$T_0 = 7750(160)$ gas PE[1,2]TPE[11]
Splitting between $G_{3/2}$ and $E_{5/2}$ spin-orbit components = 920(12) gas TPE[11]

$\tilde{X}\,^2F_1$

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).
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[11] L. Cooper, L. G. Shpinkova, D. M. P. Holland, and D. A. Shaw, Chem. Phys. **270**, 363 (2001).

$SiBr_4^+$

$\tilde{D}\,^2A_1$ T_d
$T^a = 52550(20)$ gas PE[1]TPE[3]

$\tilde{C}\,^2F_2$ T_d
$T^a = 25450(20)$ gas PE[1]TPE[3]
A broad, unstructured emission with maxima at 435 and 550 nm (23000 and 18200) has been assigned[2] to the $\tilde{C}-\tilde{X}$ and $\tilde{C}-\tilde{A}$ transitions, respectively, of gas-phase $SiBr_4^+$, excited by electron impact. Using pulsed synchrotron excitation of $SiBr_4$, a radiative lifetime of 47.6(3) ns has been determined[2] for the $\tilde{C}$ state of $SiBr_4^+$.
Splitting between $G_{3/2}$ and $E_{5/2}$ spin-orbit levels ~1570.[3]

$\tilde{B}\,^2E$ T_d
$T^a = 11560(80)$ gas PE[1]TPE[3]

$\tilde{A}\,^2F_2$ T_d
$T^a = 5740(20)$ gas PE[1]TPE[3]
Splitting between $G_{3/2}$ and $E_{5/2}$ spin-orbit levels ~3950.[3]

$\tilde{X}\,^2F_1$ T_d

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
f_2	2	SiBr stretch	444T	gas	TPE	3

Splitting between $E_{1/2}$ and $G_{3/2}$ spin-orbit levels ~2400, with superposed structure arising from Jahn–Teller interaction.[3]

[a]From vertical ionization potentials.

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] J. C. Creasey, I. R. Lambert, R. P. Tuckett, and A. Hopkirk, J. Chem. Soc., Faraday Trans. **86**, 2021 (1990).
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GeF_4^+

$\tilde{D}\,^2A_1$ T_d
$T^{ab}=45300(1000)$ gas PE[2,4]
EF[6] $\tilde{D}-\tilde{C}$ 390–420 nm

Broad, unstructured emission maxima at 290 and 255 nm (34500 and 39200) which appear on ion impact on GeF_4 have been interpreted as arising from the $\tilde{D}-\tilde{B}$ and $\tilde{D}-\tilde{A}$ transitions of GeF_4^+, respectively.[5] On 21.4 eV synchrotron excitation of GeF_4,[8] not only these two bands but also emission maxima at 400 and 230 nm (25000 and 43500), arising from the $\tilde{D}-\tilde{C}$ and $\tilde{D}-\tilde{X}$ transitions of GeF_4^+, respectively, appear.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	GeF stretch	644.3	gas	EF	6

$\tau=5.02(1)$ ns gas EM[8]

$\tilde{C}\,^2F_2$[c]
$T_0^a=20330(240)$ gas PE[1–4]
EF[6] $\tilde{D}-\tilde{C}$ 390–420 nm

$\tilde{D}-\tilde{C}$ band origin measured at 25064.0 in emission studies on a cooled beam.[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	GeF stretch	620.8	gas	EF	6
e	2	Deformation	82.8	gas	EF	6
f_2	4	Deformation	288.3	gas	EF	6

$A=-18.6$[d] EF[6]

$\tilde{B}\,^2E$
$T^{ab}=11210(320)$ gas PE[1–4]

$\tilde{A}\,^2F_2$
$T^{ab}=7020(320)$ gas PE[1–4]

$\tilde{X}\,^2F_1$

[a]First ionization potential taken to be 15.69(2) eV, as in Ref. 1.
[b]From vertical ionization potential.
[c]Distorted by Jahn–Teller interaction.
[d]Tentative value.

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$GeCl_4^+$

$\tilde{D}\,^2A_1$ 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[3,4,6] 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 65.9(1.4) ns has been determined[4,7] for the $\tilde{C}$ state of $GeCl_4^+$.

$\tilde{B}\,^2E$ T_d
$T_0=8880(1100)$ gas PE[1,2]TPE[5]

$\tilde{A}\,^2F_2$ T_d
$T_0=5650(1100)$ gas PE[1,2]TPE[5]

$\tilde{X}\,^2F_1$ T_d

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[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).
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SO_4^-

Threshold for electron detachment from ground-state $SO_4^-=41150(800)$ gas PE[1]

Reference

[1] X.-B. Wang, J. B. Nicholas, and L.-S. Wang, J. Phys. Chem. A **104**, 504 (2000).

$Cl_2CCl\text{-}Cl$

A strong, broad absorption with maximum near 415 nm (24000) which appears on argon-resonance photolysis of CCl_4 isolated in an argon matrix was originally assigned[2,3] to the $\tilde{C}-\tilde{X}$ transition of CCl_4^+. Subsequent argon-matrix studies[4] showed that this absorption can also be produced by 220 or 193 nm irradiation of the sample. Ab initio calculations are consistent with the alternate assignment of this band and of the associated infrared absorption pattern to $Cl_2CCl\text{-}Cl$. The product absorptions are destroyed, and the absorptions of ordinary CCl_4 are intensified, by exposure of the sample to radiation of wavelength longer than 360 nm.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CCl stretch	1018.2	Ne	IR	5
			1019.7m	Ar	IR	1,4
	2	CCl stretch	503.9	Ne	IR	5
			501.9m	Ar	IR	1,4
	3	Deformation	373.9wm	Ar	IR	1,4
	4	Deformation	291.2wm	Ar	IR	1,4
	5	Cl–Cl stretch	246.4wm	Ar	IR	4
a''	7	CCl stretch	931.6	Ne	IR	5
			929.1vs	Ar	IR	1,4

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PF_4^+

$\tilde{X}$ T_d

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
f_2	3	PF stretch	1174.4	Ne	IR	1

Reference

[1] C. L. Lugez, K. K. Irikura, and M. E. Jacox, J. Chem. Phys. **108**, 8381 (1998).

ClO_4^-

Threshold for electron detachment from ground-state $ClO_4^- = 42360(800)$ gas PE[1]

Reference

[1] X.-B. Wang and L.-S. Wang, J. Chem. Phys. **113**, 10928 (2000).

$Cl_2CCl\text{-}Cl^-$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CCl stretch	899.3	Ne	IR	2
a''	7	CCl stretch	848.3	Ne	IR	2
			851	Ar	IR	1

References

[1] A. Richter, H. Meyer, T. Muller, H. Specht, and A. Schweig, J. Mol. Struct. **436/437**, 359 (1997).
[2] C. L. Lugez, M. E. Jacox, and R. D. Johnson III, J. Chem. Phys. **109**, 7147 (1998).

CCl_4^-

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	4	CCl_3 stretch	757.9	Ne	IR	1

Reference

[1] C. L. Lugez, M. E. Jacox, and R. D. Johnson III, J. Chem. Phys. **109**, 7147 (1998).

F_3PO^-

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	PO stretch	1200.0mT	Ne	IR	1
	2	PF stretch	768.0m	Ne	IR	1
a''	7	PF stretch	614.7ms	Ne	IR	1

Reference

[1] C. L. Lugez, K. K. Irikura, and M. E. Jacox, J. Chem. Phys. **108**, 8381 (1998).

PF_4

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PF stretch	910.7mT	Ne	IR	1
b_1	6	PF stretch	948.2mT	Ne	IR	1
b_2	8	PF stretch	849.1sT	Ne	IR	1

Reference

[1] C. L. Lugez, K. K. Irikura, and M. E. Jacox, J. Chem. Phys. **108**, 8381 (1998).

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}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_1	6	SF stretch	975.4	Ne	IR	4
b_1	8	SF stretch	698.3	Ne	IR	4

[a]From vertical ionization potential. The adiabatic first ionization potential of SF_4 is estimated to be 11.90 eV.[3]

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[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).
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PF_4^-

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PF stretch	775.6wT	Ne	IR	1
b_1	6	PF stretch	517.0m	Ne	IR	1
b_2	8	PF stretch	730.0mT	Ne	IR	1

Reference

[1] C. L. Lugez, K. K. Irikura, and M. E. Jacox, J. Chem. Phys. **108**, 8381 (1998).

SF_4^-

$\tilde{X}$ C_{4v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	6		540.7	Ne	IR	1

Reference

[1] C. L. Lugez, M. E. Jacox, R. A. King, and H. F. Schaefer III, J. Chem. Phys. **108**, 9639 (1998).

8.12. Six-Atomic Molecules

CH_5^+

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		HH stretch	2950T	gas	LD	1

Reference

[1] E. T. White, J. Tang, and T. Oka, Science **284**, 135 (1999).

CH_3BeH

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	BeH stretch	2062.3 2059.4	Ar	IR	1
	3	CH_3 s-deform.	1205.4	Ar	IR	1
e	7	CH_3 rock	704.1	Ar	IR	1
	8	BeH deform.	443.0 435.4	Ar	IR	1

CD_3BeD

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	BeD stretch	1570.5 1568.0	Ar	IR	1
	3	CD_3 s-deform.	979.3	Ar	IR	1
	4	BeC stretch	748.0	Ar	IR	1
e	7	CD_3 rock	580.7 579.8	Ar	IR	1

Reference

[1] T. M. Greene, D. V. Lanzisera, L. Andrews, and A. J. Downs, J. Am. Chem. Soc. **120**, 6097 (1998).

CH_3MgH

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	MgH stretch	1560.3 1552.2	Ar	IR	1,2
	3	CH_3 s-deform.	1127.7	Ar	IR	1
e	7	CH_3 rock	547.9 545.4 542.8	Ar	IR	1

CD_3MgD

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	MgD stretch	1136.8	Ar	IR	1,2
	3	CD_3 s-deform.	877.1	Ar	IR	1
	4	CMg stretch	506.9	Ar	IR	1
e	7	CD_3 rock	423.8	Ar	IR	1
			422.9			
			421.1			

References

[1] T. M. Greene, D. V. Lanzisera, L. Andrews, and A. J. Downs, J. Am. Chem. Soc. **120**, 6097 (1998).
[2] W. D. Bare and L. Andrews, J. Am. Chem. Soc. **120**, 7293 (1998).

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
			1953.8	N_2	IR	3
	3	CH_3 deform.	1191.7vw	Ar	IR	1,2
	4	HgC stretch	534.0w	Ar	IR	1,2
			530.3	N_2	IR	3
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			
			778.4	N_2	IR	3
			777.4			
			774.3			
	8	CHgH deform.	526.5	Ar	IR	1,2
			527.2	N_2	IR	3
			525.2			

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
			1402.6	N_2	IR	3
	3	CD_3 deform.	1024.5vwT	Ar	IR	1
	4	HgC stretch	487.0	Ar	IR	2
			485.6	N_2	IR	3
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			
			592.8	N_2	IR	3
			589.3			
	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).
[3] N. Legay-Sommaire and F. Legay, Chem. Phys. **211**, 367 (1996).

SiH_3HgH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		HgH stretch	1888.5	Ar	IR	1
			1865.4	Kr	IR	1
			1873.7	N_2	IR	1
			867.8	Ar	IR	1
			864.4	Kr	IR	1
			867.8	N_2	IR	1

SiD_3HgD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		HgD stretch	1354.7	Ar	IR	1
			1338.2	Kr	IR	1
			1344.4	N_2	IR	1
			645.9	Ar	IR	1
			643.2	Kr	IR	1
			646.5	N_2	IR	1

Reference

[1] N. Legay-Sommaire and F. Legay, J. Phys. Chem. A **102**, 8759 (1998).

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	1–4
			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	1–4
			747.8	Kr	IR	2
		CH_3 rock	642	Ar	IR	1
		GaC stretch	528.6	Ar	IR	1–4
			520.0	Kr	IR	2
		Deformation	475.5	Ar	IR	3,4

CD_3GaD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD stretch	2223.9	Ar	IR	1,4
		CD stretch	2137	Ar	IR	1
		GaD stretch	1243.6	Ar	IR	1,2,4
			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	1,2,4
		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).
[3] H.-J. Himmel, A. J. Downs, T. M. Greene, and L. Andrews, Chem. Commun. 2243 (1999).
[4] H.-J. Himmel, A. J. Downs, T. M. Greene, and L. Andrews, Organomet. **19**, 1060 (2000).

CH_3InH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	InH stretch	1545.9	Ar	IR	1,2
	6	CH_3 rock	697.3	Ar	IR	1,2

CD_3InD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	6	InD stretch	1115.0	Ar	IR	2

References

[1] H.-J. Himmel, A. J. Downs, T. M. Greene, and L. Andrews, Chem. Commun. 2243 (1999).
[2] H.-J. Himmel, A. J. Downs, T. M. Greene, and L. Andrews, Organomet. **19**, 1060 (2000).

H_2AlNH_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NH_2 s-stretch	3499.7	Ar	IR	1,2
	2	AlH_2 s-stretch	1891.0	Ar	IR	1,2
	3	NH_2 scissors	1541.6	Ar	IR	1,2
	4	AlN stretch	818.7	Ar	IR	1,2
	5	AlH_2 scissors	755.0	Ar	IR	1,2
b_1	7	AlH_2 OPLA	608.7	Ar	IR	1,2
	8	NH_2 OPLA	518.3	Ar	IR	1,2
b_2	10	AlH_2 a-stretch	1899.3	Ar	IR	1,2
	11	NH_2 rock	769.8	Ar	IR	1,2

D_2AlND_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	ND_2 scissors	1159.5	Ar	IR	2
	5	AlD_2 scissors	548.4	Ar	IR	2
b_1	7	AlD_2 OPLA	450.4	Ar	IR	2
	8	ND_2 OPLA	397.7	Ar	IR	2
b_2	10	AlD_2 a-stretch	1384.2	Ar	IR	2
	11	ND_2 rock	611.0	Ar	IR	2

References

[1] H.-J. Himmel, A. J. Downs, and T. M. Greene, Chem. Commun. 871 (2000).
[2] H.-J. Himmel, A. J. Downs, and T. M. Greene, J. Am. Chem. Soc. **122**, 9793 (2000).

H_2GaNH_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NH_2 s-stretch	3413.4	Ar	IR	1,2
	2	GaH_2 s-stretch	1970.8T	Ar	IR	1,2
	3	NH_2 scissors	1530.4	Ar	IR	1,2
	4	GaH_2 scissors	779.6	Ar	IR	1,2
	5	GaN stretch	706.2	Ar	IR	1,2
b_1	7	GaH_2 OPLA	567.7	Ar	IR	1,2
	8	NH_2 OPLA	304.9	Ar	IR	1,2
b_2	9	NH_2 a-stretch	3510.7	Ar	IR	1,2
	10	GaH_2 a-stretch	1970.8T	Ar	IR	1,2
	11	NH_2 rock	782.8	Ar	IR	1,2

D_2GaND_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	GaD_2 s-stretch	1407.7	Ar	IR	2
	3	ND_2 scissors	1150.9	Ar	IR	2
	4	GaN stretch	667.8	Ar	IR	2
	5	GaD_2 scissors	568.8	Ar	IR	2
b_1	7	GaD_2 OPLA	405.9	Ar	IR	2
b_2	10	GaD_2 a-stretch	1419.1	Ar	IR	2
	11	ND_2 rock	605.1	Ar	IR	2

References

[1] H.-J. Himmel, A. J. Downs, and T. M. Greene, Chem. Commun. 871 (2000).
[2] H.-J. Himmel, A. J. Downs, and T. M. Greene, J. Am. Chem. Soc. **122**, 9793 (2000).

H_2InNH_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	NH_2 scissors	1506.6	Ar	IR	1,2
	4	InN stretch	616.3	Ar	IR	1,2
b_2	10	InH_2 a-stretch	1805.9	Ar	IR	1,2
	11	NH_2 rock	733.3	Ar	IR	1,2

D_2InND_2

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4	InD_2 scissors	474.6	Ar	IR	2
b_2	10	InD_2 a-stretch	1299.0	Ar	IR	2

References

[1] H.-J. Himmel, A. J. Downs, and T. M. Greene, Chem. Commun. 871 (2000).
[2] H.-J. Himmel, A. J. Downs, and T. M. Greene, J. Am. Chem. Soc. **122**, 9793 (2000).

$CH_2{=}SiH_2$

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]

$\tilde{X}$[a] 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]

$\tilde{X}$[a] 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
		SiD_2 wag	396w	Ar	IR	1,3
			396	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

[a]Assigned using density functional theory calculations of Ref. 6.

References

[1] G. Maier, G. Mihm, and H. P. Reisenauer, Angew. Chem. **93**, 615 (1981); Angew. Chem. Int. Ed. Engl. **20**, 597 (1981).
[2] H. P. Reisenauer, G. Mihm, and G. Maier, Angew. Chem. **94**, 864 (1982); Angew. Chem. Int. Ed. Engl. **21**, 854 (1982).
[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).
[6] V. N. Khabashesku, K. N. Kudin, and J. L. Margrave, J. Mol. Struct. **443,** 175 (1998).

CH_3GeH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	GeH stretch	1798.6	Ar	IR	1
	5	CH_3 rock	1201.2	Ar	IR	1
	6	Deformation	868.8	Ar	IR	1
a''	8	CH stretch	2891.6	Ar	IR	1
	11	GeC stretch	535.6	Ar	IR	1

Reference

[1] V. N. Khabashesku, K. N. Kudin, J. Tamás, S. E. Boganov, J. L. Margrave, and O. M. Nefedov, J. Am. Chem. Soc. **120**, 5005 (1998).

CH_3SH^+

$\tilde{C}\,^2A''$ C_s
$T^a = 49820(160)$ gas PE[1–3]

$\tilde{B}\,^2A'$ C_s
$T^a = 34000(160)$ gas PE[1–3]

$\tilde{A}\,^2A'$ C_s
$T^a = 21170(160)$ gas PE[1–3]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CH_3 umbrella	1250(80)	gas	PE	2
		SH bend	782(3)T	gas	TPE	6
		CS stretch	687(3)	gas	TPE,PI	1,2,4–6
a''		Torsion	178(3)T	gas	TPE	6

[a]From vertical ionization potential. The first ionization potential of CH_3SH is taken as 9.553 eV, as in the two-photon pulsed field ionization photoelectron spectroscopic study of Ref. 6.

References

[1] S. Cradock and R. A. Whiteford, J. Chem. Soc., Faraday Trans. 2 **68**, 281 (1972).
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CH_2NH_2

$\tilde{C}\,(3p)$ C_s
$T_0 = 31300$ gas AB[1] $\tilde{C}-\tilde{X}$ 270–320 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		NH_2 scissors	1700	gas	AB	1
		Deformation	850	gas	AB	1
		Deformation	600	gas	AB	1

$\tilde{B}\,(3p)$ C_s
$T_0 = 27130$ gas AB[1] $\tilde{B}-\tilde{X}$ 320–368 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			830T	gas	AB	1

Reference

[1] T. la Cour Jansen, I. Trabjerg, S. Rettrup, P. Pagsberg, and A. Sillesen, Acta Chem. Scand. **53**, 1054 (1999).

cyc-$(CH)_2BH$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	BH stretch	2639.6	Ar	IR	1,2
	4	Ring deform.	1175.3	Ar	IR	1,2
b_1	7	Deformation	832.5	Ar	IR	1,2
	8		653.0	Ar	IR	1,2
b_2	10		1169.5	Ar	IR	1,2

cyc-$(CD)_2BD$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	BD stretch	2006.1	Ar	IR	1,2
	4	Ring deform.	1126.0	Ar	IR	1,2
b_1	8	Deformation	481.6	Ar	IR	1,2

References

[1] D. V. Lanzisera, P. Hassanzadeh, Y. Hannachi, and L. Andrews, J. Am. Chem. Soc. **119**, 12402 (1997).
[2] L. Andrews, D. V. Lanzisera, P. Hassanzadeh, and Y. Hannachi, J. Phys. Chem. A **102**, 3259 (1998).

H_2BCCH

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	C≡C stretch	2058.1	Ar	IR	1
b_2	9	BH_2 a-stretch	2593.3	Ar	IR	1

D_2BCCD

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1832.5	Ar	IR	1
b_2	9	BD_2 a-stretch	1945.9	Ar	IR	1

Reference

[1] L. Andrews, D. V. Lanzisera, P. Hassanzadeh, and Y. Hannachi, J. Phys. Chem. A **102**, 3259 (1998).

$HBCCH_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	BH stretch	2757.7	Ar	IR	1
	3	CC stretch	1859.8	Ar	IR	1

$DBCCD_2$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	BD stretch	2168.2	Ar	IR	1
	3	CC stretch	1774.6	Ar	IR	1

Reference

[1] L. Andrews, D. V. Lanzisera, P. Hassanzadeh, and Y. Hannachi, J. Phys. Chem. A **102**, 3259 (1998).

cyc-$C_3H_3^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	4	CH stretch	3130	Ne	IR	1

cyc-$C_3D_3^+$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	4	CD stretch	2344	Ne	IR	1

Reference

[1] M. Wyss, E. Riaplov, and J. P. Maier, J. Chem. Phys. **114**, 10355 (2001).

CH_2CCH^+

$\tilde{A}\,^1A'$ C_{2v}
$T_0 = 37330(30)$ Ne AB^3 $\tilde{A}$–$\tilde{X}$ 246–268 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	4		1629(50)	Ne	AB	3
	11		667(50)	Ne	AB	3

$\tilde{a}\,^3A_2$ C_{2v}
$T_0 \cong 13900$ gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	3319	gas	TPE	2
	2	CH_2 s-stretch	3130	gas	TPE	2
	3	C≡C stretch	2093[a]	gas	TPE	2
			2080	Ne	IR	3
	4	CH_2 scissors	1465	gas	TPE	2
	5		1106T	gas	TPE	2
b_1	6	CH_2 OPLA	1183	gas	TPE	2
	7	CCH deform.	910T	gas	TPE	2

CD_2CCD^+

$\tilde{A}\,^1A'$ C_{2v}
$T_0 = 37430(30)$ Ne AB^3 $\tilde{A}$–$\tilde{X}$ 246–267 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	4		1501(50)	Ne	AB	3
	11		641(50)	Ne	AB	3

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C≡C stretch	1955	Ne	IR	3

[a] Reassigned by Ref. 3.

References

[1] D. W. Minsek and P. Chen, J. Phys. Chem. **94**, 8399 (1990).
[2] T. Gilbert, R. Pfab, I. Fischer, and P. Chen, J. Chem. Phys. **112**, 2575 (2000).
[3] M. Wyss, E. Riaplov, and J. P. Maier, J. Chem. Phys. **114**, 10355 (2001).

CH_2BNH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BN stretch	1881.0	Ar	IR	1

Reference

[1] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **101**, 824 (1997).

CH_3NB

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NB stretch	1981.1	Ar	IR	1

Reference

[1] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **101**, 824 (1997).

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.

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

$T_0 = 30109$U gas AB[1]CR[12] $\tilde{A},\tilde{B}-\tilde{X}$ 290–353 nm
29146(17) Ne AB[13] $\tilde{B}-\tilde{X}$ 294–343 nm
Ar AB[2] $\tilde{A},\tilde{B}-\tilde{X}$ 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.
a'	5	C–C stretch	961(10)	gas	AB	1
			966(25)	Ne	AB	13
			965(10)	Ar	AB	2
	6	CCH bend	661(25)	Ne	AB	13
	8	C_3 deform.	301(25)	Ne	AB	13

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

$T_0 = 28409(16)$ Ne AB[13] $\tilde{A}-\tilde{X}$ 345–352 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	8	C_3 deform.	285(25)	Ne	AB	13

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3322.29	gas	CC	5,11
			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]MW[10]

CD_2CCD

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

$T_0 = 29189(17)$ Ne AB[13] $\tilde{B}-\tilde{X}$ 310–343 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	6	CCD bend	547(25)	Ne	AB	13
	8	C_3 deform.	301(25)	Ne	AB	13

$\tilde{X}\,^2B_1$ 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

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SiH_2CCH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CC stretch	2055.6	Ar	IR	1
	4	SiH_2 scissors	926.8	Ar	IR	1

SiD_2CCD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CC stretch	1927.2	Ar	IR	1
	4	SiD_2 scissors	701.9	Ar	IR	1

Reference

[1] D. S. Han, C. M. L. Rittby, and W. R. M. Graham, J. Chem. Phys. **109**, 8355 (1998).

$CaOCH_3$

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

$T_0 = 21750$T gas LF[3] $\tilde{C}-\tilde{X}$ 446–462 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CaO stretch	440(5)	gas	LF	3
		Skel. deform.	150(5)	gas	LF	3

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

$T_0 = 17682.431$ gas $CL^1LF^{1,2,4,5}$ $\tilde{B}-\tilde{X}$ 525–590 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CO stretch	1150(5)	gas	LF	1
	4	CaO stretch	491(5)	gas	LF	1,2
e	8	CaOC bend	168(5)	gas	LF	1,2

$B_0 = 0.118$ LF[5]

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

$T_0 = 15930(10)$ gas $CL^1LF^{1,2}$ $\tilde{A}-\tilde{X}$ 605–635 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CO stretch	1140(5)	gas	LF	1, 2
	4	CaO stretch	500(10)	gas	LF	1,2
e	8	CaOC bend	145(5)	gas	LF	1

$A = 68(5)$ gas $LF^{1,2}$

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CO stretch	1156(5)	gas	LF	2
	4	CaO stretch	488(5)	gas	LF	1,2
e	8	CaOC bend	144(5)	gas	LF	1,2

$A_0 = 5.448$T; $B_0 = 0.116$ DR^4LF^5

$CaOCD_3$

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

$T_0 = 17674(5)$ gas LF[1] $\tilde{B}-\tilde{X}$ 528–600 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CO stretch	1156(5)	gas	LF	1
	4	CaO stretch	476(5)	gas	LF	1
e	8	CaOC bend	166(5)	gas	LF	1

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

$T_0 = 15935(10)$ gas LF[1] $\tilde{A}-\tilde{X}$ 584–630 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CO stretch	1156(5)	gas	LF	1
	4	CaO stretch	480(5)	gas	LF	1
e	8	CaOC bend	140(5)	gas	LF	1

$A = 72(5)$ gas LF[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4	CaO stretch	467(5)	gas	LF	1
e	8	CaOC bend	142(5)	gas	LF	1

References

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CH_3BO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CBO a-stretch	1972.4	Ar	IR	1
		CH_3 umbrella	1305.0	Ar	IR	1
e		Deformation	896.8	Ar	IR	1
			895.6			

CD_3BO

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CBO a-stretch	1972.0	Ar	IR	1
e		Deformation	750.0	Ar	IR	1

Reference

[1] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **101**, 1482 (1997).

CH_2BOH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1748.3	Ar	IR	1

CD_2BOD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1724.9	Ar	IR	1

Reference

[1] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **101**, 1482 (1997).

CH_2CCH^-

Threshold for electron detachment from ground-state CH_2CCH^- = 7410(65) gas PE[1,2]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C_3 a-stretch	1857.9	Ne	IR	3
			687.0	Ne	IR	3

CD_2CCD^-

Threshold for electron detachment from ground-state CD_2CCD^- = 7380(65) gas PE[2]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C_3 a-stretch	1802.6	Ne	IR	3

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[1] J. M. Oakes and G. B. Ellison, J. Am. Chem. Soc. **105**, 2969 (1983).
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CH_3BCl

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		B–C stretch	1172.7	Ar	IR	1

CD_3BCl

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		B–C stretch	1161.0	Ar	IR	1

Reference

[1] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **104**, 9295 (2000).

CH_3BBr

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		B–C stretch	1142.4	Ar	IR	1

CD_3BBr

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		B–C stretch	1161.0	Ar	IR	1

Reference

[1] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **104**, 9295 (2000).

CH_2CHO

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

$T_0 = 28784.09(1)$ gas $AB^{1}LF^{2,4,6,12,16}FD^{10}PF^{13}$ $\tilde{B}-\tilde{X}$ 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_2CHO to produce $CH_3 + CO$ was observed between 280 and 300 nm.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	4	CO stretch	1621	gas	FD,PF	10,12,13
					LF,DR	14
	5	CH_2 scissors	1405.23	gas	FD,PF	10,12,13
					LF,DR	14,16
	6	OCH bend	1274	gas	PF,LF,DR	13,14
	7	CH_2 rock	1121.65	gas	LF,FD	2,6,10,12
					PF,DR	13,14,16
	8	CC stretch	917.10	gas	LF,FD	2,6,10,12
					PF,DR	13,14,16
	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

$\tau_0 = 190(2)$ 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

$T_0 = 8190(120)$ gas $AB^{3}PE^{15}$ $\tilde{A}-\tilde{X}$ 1000–1250 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	4	CC stretch	1580(120)	gas	PE	15
	5	CH_2 scissors	1350(120)	gas	PE	15
	9	CCO bend	460(120)	gas	PE	15

$\tilde{X}\,^2A''$ 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	CC stretch	1143	gas	LF,PD	2,6,7,14
	8	CH_2 rock	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

$A_0 = 2.224$; $B_0 = 0.382$; $C_0 = 0.326$ $LF^{6}MW^{8,17}$

CD_2CDO

$\tilde{B}\,^2A''$ 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_3MgF

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 s-stretch	2907.2	Ar	IR	1
	2	CH_3 s-deform.	1127.2	Ar	IR	1
	3	CMgF a-stretch	755.8	Ar	IR	1
e	5	CH_3 a-stretch	2958.5	Ar	IR	1
	7	CH_3 rock	560.2	Ar	IR	1

CD_3MgF

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_3 s-stretch	2211.0	Ar	IR	1
	2	CD_3 s-deform.	880.8	Ar	IR	1
	3	CMgF a-stretch	744.5	Ar	IR	1
e	5	CD_3 a-stretch	2232.6	Ar	IR	1
	7	CD_3 rock	432.3	Ar	IR	1
			431.3			

Reference

[1]W. D. Bare and L. Andrews, J. Am. Chem. Soc. **120**, 7293 (1998).

$HMgCH_2F$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		MgH stretch	1547T	Ar	IR	1

Reference

[1]W. D. Bare and L. Andrews, J. Am. Chem. Soc. **120**, 7293 (1998).

CH_3MgCl

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 s-stretch	2910.4	Ar	IR	1
	2	CH_3 s-deform.	1127.5	Ar	IR	1
	3	CMgCl a-stretch	627.1	Ar	IR	1
e	5	CH_3 a-stretch	2951.3	Ar	IR	1
	7	CH_3 rock	556.6	Ar	IR	1

Reference

[1]W. D. Bare and L. Andrews, J. Am. Chem. Soc. **120**, 7293 (1998).

$HMgCH_2Cl$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		MgH stretch	1555.4T	Ar	IR	1

Reference

[1]W. D. Bare and L. Andrews, J. Am. Chem. Soc. **120**, 7293 (1998).

CH_3MgBr

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 s-stretch	2910.6	Ar	IR	1
	2	CH_3 s-deform.	1125.4	Ar	IR	1
	3	CMgBr a-stretch	599T	Ar	IR	1
e	5	CH_3 a-stretch	2950.9	Ar	IR	1
	7	CH_3 rock	555.3	Ar	IR	1

CD_3MgBr

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD_3 s-stretch	2123.5	Ar	IR	1
	2	CD_3 s-deform.	881.2	Ar	IR	1
	3	CMgBr a-stretch	575T	Ar	IR	1
e	5	CD_3 a-stretch	2138.5	Ar	IR	1
	7	CD_3 rock	429.0	Ar	IR	1

Reference

[1]W. D. Bare and L. Andrews, J. Am. Chem. Soc. **120**, 7293 (1998).

CH_3MgI

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 s-stretch	2910.3	Ar	IR	1
	2	CH_3 s-deform.	1125br	Ar	IR	1
	3	CMgI a-stretch	588T	Ar	IR	1
e	5	CH_3 a-stretch	2950br	Ar	IR	1
	7	CH_3 rock	558.2	Ar	IR	1

Reference

[1]W. D. Bare and L. Andrews, J. Am. Chem. Soc. **120**, 7293 (1998).

$HSc(OH)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ScH stretch	1418.3wT	Ar	IR	2
		ScO_2 a-stretch	729.6T	Ar	IR	1,2

$DSc(OD)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ScO_2 a-stretch	713.3T	Ar	IR	1,2

References

[1] J. W. Kauffman, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **89**, 3547 (1985).
[2] L. Zhang, J. Dong, and M. Zhou, J. Phys. Chem. A **104**, 8882 (2000).

$HY(OH)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		YH stretch	1368.6	Ar	IR	1
		YO_2 a-stretch	616.9	Ar	IR	1

$DY(OD)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		YD stretch	981.6	Ar	IR	1
		YO_2 a-stretch	593.4	Ar	IR	1

Reference

[1] L. Zhang, L. Shao, and M. Zhou, Chem. Phys. **272**, 27 (2001).

$HLa(OH)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		LaH stretch	1229.0	Ar	IR	1
		LaO_2 a-stretch	554.3	Ar	IR	1

$DLa(OD)_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		LaD stretch	880.3	Ar	IR	1
		LaO_2 a-stretch	534.5	Ar	IR	1

Reference

[1] L. Zhang, L. Shao, and M. Zhou, Chem. Phys. **272**, 27 (2001).

CH_2CHO^-

Dipole-Bound State C_s
$T_0 = 14712.747(5)$ gas PD[1,3,4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		C–C stretch	1143	gas	PD	3
		CCO bend	499	gas	PD	3
a''		Torsion	102H	gas	PD	3

$A_0 = 2.221(2)$; $B_0 = 0.376$; $C_0 = 0.320$ PD[3,4]

Threshold for electron detachment from ground-state CH_2CHO^- = 14480(120) gas PE[2,6]

$\tilde{X}$ C_s Structure: PD[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CCO bend	525.82	gas	PD	3,4
a''		Torsion	375T	gas	PD	3

$A_0 = 2.494$; $B_0 = 0.362$; $C_0 = 0.316$ PD[3,4]

CD_2CDO^-

Dipole-Bound State C_s
$T_0 = 14665.97(5)$ gas PD[1,3,5]

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[3,5]

Threshold for electron detachment from ground-state CD_2CDO^- = 14660(240) gas PE[2]

$\tilde{X}$ C_s
$A_0 = 1.554(1)$; $B_0 = 0.319$; $C_0 = 0.264$ PD[3]

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$CH_3S_2^+$

$\tilde{c}\,^3A'$ C_s
$T^a = 25740(230)$ gas PE[1]

$\tilde{B}\,^1A''$ C_s
$T_0 = 16860(230)$ gas PE[1]

$\tilde{b}\,^3A''$ C_s
$T_0 = 13390(230)$ gas PE[1]

$\tilde{A}\,^1A''$ C_s
$T_0 = 10570(230)$ gas PE[1]

$\tilde{a}\,^3A''$ C_s
$T_0 = 5890(230)$ gas PE[1]

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		SS stretch	600(60)	gas	PE	1

[a]From vertical ionization potential.

Reference

[1] M. Ge, J. Wang, Z. Sun, X. Zhu, and D. Wang, J. Chem. Phys. **114**, 3051 (2001).

CH_3O_2

An unstructured gas-phase absorption between 200 and 300 nm, with a maximum at 235 nm, has been assigned[1,3,4,6,7,9] to CH_3O_2. In the gas phase, CH_3O_2 photolyzes on exposure to 248-nm radiation,[8] and, in an argon matrix, on exposure to 254-nm radiation.[5]

$\tilde{A}\,^2A'$ C_s
$T_0 = 7382.8(5)$ gas $AB^2CR^{10}PE^{11}$ $\tilde{A}-\tilde{X}$ 7375–9149 cm^{-1}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		Mixed	1005(10)	gas	PE	11
		Mixed	896(9)	gas	AB,PE	2,11

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH_3 stretch	3032	Ar	IR	12
	2	CH_3 stretch	2954	Ar	IR	12
	3	CH_3 deform.	1448s	Ar	IR	5,12
	4	CH_3 deform.	1410w	Ar	IR	5,12
	5	Mixed	1180m	Ar	IR	5,12
	6	Mixed	1124(5)	gas	PE	11
			1109wm	Ar	IR	5,12
	7	CO stretch	902s	Ar	IR	5,12
	8	COO bend	482(9)	gas	PE	11
			492wm	Ar	IR	5,12
a''	9	CH_3 stretch	3024	Ar	IR	12
	10	CH_3 deform.	1434vs	Ar	IR	5,12

CD_3O_2

$\tilde{A}\,^2A'$ C_s
$T_0 = 7372.6(5)$ gas $CR^{10}PE^{11}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		Mixed	975(10)	gas	PE	11
		Mixed	840(10)	gas	PE	11

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CD_3 stretch	2280wm	Ar	IR	12
	2	CD_3 stretch	2172m	Ar	IR	5,12
	3	CD_3 deform.	1123(7)	gas	PE	11
			1144ms	Ar	IR	5,12
	4	CD_3 deform.	1076s	Ar	IR	5,12
	5	Mixed	1050wm	Ar	IR	12
	6	Mixed	941wm	Ar	IR	12
	7	CO stretch	822vs	Ar	IR	5,12
	8	COO bend	440(7)	gas	PE	11
			446wm	Ar	IR	5,12
a''	9	CD_3 stretch	2273s	Ar	IR	12
	10	CD_3 deform.	1046ms	Ar	IR	5,12
	11	CD_3 rock	860wm	Ar	IR	5,12

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[1] D. A. Parkes, D. M. Paul, C. P. Quinn, and R. C. Robson, Chem. Phys. Lett. **23**, 425 (1973).
[2] H. E. Hunziker and H. R. Wendt, J. Chem. Phys. **64**, 3488 (1976).
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[10] M. B. Pushkarsky, S. J. Zalyubovsky, and T. A. Miller, J. Chem. Phys. **112**, 10695 (2000).
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[12] S. Nandi, S. J. Blanksby, X. Zhang, M. R. Nimlos, D. C. Dayton, and G. B. Ellison, J. Phys. Chem. A **106**, 7547 (2002).

CH_3SCl^+

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			631(60)	gas	PI	1

Reference

[1] B.-M. Cheng, E. P. Chew, C.-P. Liu, J.-S. K. Yu, and C.-H. Yu, J. Chem. Phys. **110**, 4757 (1999).

$CH_3O_2^-$

Threshold for electron detachment from ground-state $CH_3O_2^- = 9370(40)$ gas PE[1]

Reference

[1] S. J. Blanksby, T. M. Ramond, G. E. Davico, M. R. Nimlos, S. Kato, V. M. Bierbaum, W. C. Lineberger, G. B. Ellison, and M. Okumura, J. Am. Chem. Soc. **123**, 9585 (2001).

$ClCH_2OH$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3646	gas	IR	3
			3591	Ar	IR	1
		CH_2 a-stretch	2981	Ar	IR	1
			2971			
		CH_2 s-stretch	2913	Ar	IR	1
		COH bend	1374	gas	IR	2,3
			1393	Ar	IR	1
		CH_2 wag	1318	gas	IR	2,3
			1323	Ar	IR	1
			1319			
			1231	Ar	IR	1
			1176	gas	IR	3
		CH_2 twist	1114	Ar	IR	1
		CO stretch	1083	gas	IR	2,3
			1096	Ar	IR	1
		CH_2 rock	960	gas	IR	2,3
			959	Ar	IR	1
		CCl stretch	697	gas	IR	3
			669	Ar	IR	1
		ClCO deform.	469	Ar	IR	1
			463			
		OH torsion	372	Ar	IR	1
			368			

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[1] H. Kunttu, M. Dahlqvist, J. Murto, and M. Räsänen, J. Phys. Chem. **92**, 1495 (1988).
[2] G. S. Tyndall, T. J. Wallington, M. D. Hurley, and W. F. Schneider, J. Phys. Chem. **97**, 1576 (1993).
[3] T. J. Wallington, W. F. Schneider, I. Barnes, K. H. Becker, J. Sehested, and O. J. Nielsen, Chem. Phys. Lett. **322**, 97 (2000).

CH_3SCl

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			513(60)	gas	PI	1
			244(60)	gas	PI	1

Reference

[1] B.-M. Cheng, E. P. Chew, C.-P. Liu, J.-S. K. Yu, and C.-H. Yu, J. Chem. Phys. **110**, 4757 (1999).

$HCCCNH^+$

$\tilde{X}$ $C_{\infty v}$

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[3,4]

References

[1] S. K. Lee and T. Amano, Astrophys. J. **323**, L145 (1987).
[2] K. Kawaguchi, M. Kajita, K. Tanaka, and E. Hirota, J. Mol. Spectrosc. **144**, 451 (1990).
[3] K. Kawaguchi, Y. Kasai, S. Ishikawa, M. Ohishi, N. Kaifu, and T. Amano, Astrophys. J. **420**, L95 (1994).
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HOCH=C=C:

In an argon matrix, the threshold for rearrangement to propynal (HC≡CCHO) lies between 380 and 360 nm.[1]

On broad-band irradiation, short-lived absorptions, attributed to the *cisoid*-rotamer, appear[2] at 1999.6 and 1254.3.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C_3 a-stretch	1992.5vs	Ar	IR	1,2
		COH bend	1460.8wm	Ar	IR	1,2
		Mixed	1280.5w	Ar	IR	2
		Deformation	1223.1wm	Ar	IR	1,2
		Skel. stretch	1016.3wm	Ar	IR	1,2

References

[1] B. J. Ortman, R. H. Hauge, J. L. Margrave, and Z. H. Kafafi, J. Phys. Chem. **94**, 7973 (1990).
[2] J. Szczepanski, S. Ekern, and M. Vala, J. Phys. Chem. **99**, 8002 (1995).

CH_2CFO

$\tilde{B}\,^2A''$ C_s
$T_0 = 29867.4$ gas LF[1–4] $\tilde{B}-\tilde{X}$ 307–335 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CO stretch	1790	gas	LF	1,4
	4	CH_2 scissors	1409	gas	LF	4
	5	CF stretch	1253	gas	LF	1,4
	6	CH_2 rock	911	gas	LF	1,4
	7	CC stretch	874	gas	LF	1,4
	8	FCO bend	537	gas	LF	1,4
	9	CCO bend	421	gas	LF	1,4

$\tau_0 = 81.0(5)$ ns gas LF[1]
$1/2(A_0 + B_0) = 0.345(4)$; $C_0 = 0.181(4)$ LF[2]

$\tilde{X}\,^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CO stretch	1724	gas	LF	1
	4	CH_2 scissors	1475	gas	LF	4
	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

$1/2(A_0+B_0)=0.360(6)$; $C_0=0.185(6)$ LF[2]

CD_2CFO

$\tilde{B}\,^2A''$ C_s

$T_0=29867$ gas LF[4] $\tilde{B}-\tilde{X}$ 316–335 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CO stretch	1772	gas	LF	4
	4	CF stretch	1241	gas	LF	4
	5	CD_2 scissors	1073	gas	LF	4
	6	CC stretch	827	gas	LF	4
	7	CD_2 rock	783	gas	LF	4
	8	CCF bend	530	gas	LF	4
	9	CCO bend	370	gas	LF	4

$\tau_0=78(11)$ ns gas LF[4]

$\tilde{X}\,^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CO stretch	1735	gas	LF	4
	4	CF stretch	1248	gas	LF	4
	5	CD_2 scissors	1043	gas	LF	4
	6	CC stretch	863	gas	LF	4
	7	CD_2 rock	774T	gas	LF	4
	8	CCF bend	597	gas	LF	4
	9	CCO bend	370	gas	LF	4

References

[1] M. Furubayashi, I. Bridier, S. Inomata, N. Washida, and K. Yamashita, J. Chem. Phys. **106**, 6302 (1997).
[2] S. A. Wright and P. J. Dagdigian, J. Chem. Phys. **107**, 9755 (1997).
[3] M. Yamaguchi, M. Furubayashi, S. Inomata, and N. Washida, Chem. Phys. Lett. **298**, 93 (1998).
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t-CHClCHO

In the gas phase, a fluorescence spectrum with origin at 29040 has been attributed[1] to *t*-CHClCHO.

Reference

[1] N. Washida, M. Furubayashi, T. Imamura, I. Bridier, and A. Miyoshi, J. Chem. Phys. **107**, 6998 (1997).

$CH_2=SiCl_2$

In an Ar matrix, absorption maximum at 246 nm.[1]

$\tilde{X}$[a] C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		Si=C stretch	1008m	Ar	IR	1
b_2		CH_2 rock	732s	Ar	IR	1
		$SiCl_2$ a-stretch	593m	Ar	IR	1

[a]Assigned using density functional theory calculations of Ref. 2.

References

[1] G. Maier, G. Mihm, and H. P. Reisenauer, Angew. Chem. **93**, 615 (1981); Angew. Chem. Int. Ed. Engl. **20**, 597 (1981).
[2] V. N. Khabashesku, K. N. Kudin, and J. L. Margrave, J. Mol. Struct. **443**, 175 (1998).

$HCCl_2OH$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3611	gas	IR	2
		COH bend	1388	gas	IR	1,2
		CH a-rock	1221	gas	IR	1,2
		CO stretch	1105	gas	IR	1,2
			1003	gas	IR	1
		CCl_2 a-stretch	740	gas	IR	2

References

[1] G. S. Tyndall, T. J. Wallington, M. D. Hurley, and W. F. Schneider, J. Phys. Chem. **97**, 1576 (1993).
[2] T. J. Wallington, W. F. Schneider, I. Barnes, K. H. Becker, J. Sehested, and O. J. Nielsen, Chem. Phys. Lett. **322**, 97 (2000).

C_5H

$\tilde{X}\,^2\Pi$ $C_{\infty v}$

$A_{eff}=24.20$ MW[3]

$B_0=0.080$ MW[1,3]

C_5D

$\tilde{X}\,^2\Pi$ $C_{\infty v}$

$A_{eff}=24.2$ MW[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).
[3] M. C. McCarthy, W. Chen, A. J. Apponi, C. A. Gottlieb, and P. Thaddeus, Astrophys. J. **520**, 158 (1999).

SiCCCCH

$\tilde{X}\ ^2\Pi$ $C_{\infty v}$
$B = 0.047$ MW[1]

Reference

[1] M. C. McCarthy, A. J. Apponi, C. A. Gottlieb, and P. Thaddeus, J. Chem. Phys. **115**, 870 (2001).

CCCHCN

$\tilde{X}$ C_s
$A_0 = 1.067$; $B_0 = 0.098$; $C_0 = 0.089$ MW[1]

Reference

[1] M. C. McCarthy, A. J. Apponi, V. D. Gordon, C. A. Gottlieb, P. Thaddeus, T. D. Crawford, and J. F. Stanton, J. Chem. Phys. **111**, 6750 (1999).

HCCCCN

$\tilde{X}$ $C_{\infty v}$
$B_0 = 0.077$ MW[1]

Reference

[1] J. Tang, Y. Sumiyoshi, and Y. Endo, Chem. Phys. Lett. **315**, 69 (1999).

(*cyc*-HC_3)CN

$\tilde{X}$ C_s
$A_0 = 1.144$; $B_0 = 0.117$; $C_0 = 0.106$ MW[1]

Reference

[1] M. C. McCarthy, J.-U. Grabow, M. J. Travers, W. Chen, C. A. Gottlieb, and P. Thaddeus, Astrophys. J. **513**, 305 (1999).

NCCH=C=O

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	CH stretch	3076.7w	Ar	IR	2
	2	CN stretch	2240.2w	Ar	IR	1,2
	3	CCO a-stretch	2162.8vs	Ar	IR	1,2
	4	CH bend	1364.4w	Ar	IR	2
a″	10	CH bend	552.8wm	Ar	IR	2

NCCD=C=O

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	CD stretch	2273.7	Ar	IR	2
	2	CN stretch	2235.3	Ar	IR	2
	3	CCO a-stretch	2155.8	Ar	IR	2
	4		1325.5	Ar	IR	2
a″	10	CD bend	539.3	Ar	IR	2

References

[1] D. W. J. Moloney, M. W. Wong, R. Flammang, and C. Wentrup, J. Org. Chem. **62**, 4240 (1997).
[2] G. Maier, H. P. Reisenauer, and K. Rademacher, Chem. Eur. J. **4**, 1957 (1998).

c-CHFCFO

In the gas phase, a fluorescence spectrum with origin at 31644 has been attributed[1] to *c*-CHFCFO.

References

[1] N. Washida, M. Furubayashi, T. Imamura, I. Bridier, and A. Miyoshi, J. Chem. Phys. **107**, 6998 (1997).

t-CHFCFO

In the gas phase, a fluorescence spectrum with origin at 31270 has been attributed[1] to *t*-CHFCFO.

References

[1] N. Washida, M. Furubayashi, T. Imamura, I. Bridier, and A. Miyoshi, J. Chem. Phys. **107**, 6998 (1997).

CHClCFO

In the gas phase, a fluorescence spectrum with origin at 30715 has been tentatively attributed[1] to CHClCFO.

References

[1] N. Washida, M. Furubayashi, T. Imamura, I. Bridier, and A. Miyoshi, J. Chem. Phys. **107**, 6998 (1997).

$HOONO_2$

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
			1726.2vs	Ar	IR	14
	3	OH bend	1396.9wm	gas	IR	1,3,4,7,12,15
	4	NO_2 s-stretch	1304.2s	gas	IR	1-4,7,12
			1292.7m	Ar	IR	14
	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).
[2] S. Z. Levine, W. M. Uselman, W. H. Chan, J. G. Calvert, and J. H. Shaw, Chem. Phys. Lett. **48**, 528 (1977).
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[11] R. D. May and D. B. Peterson, J. Mol. Spectrosc. **150**, 647 (1991).
[12] R. D. May and R. R. Friedl, J. Quant. Spectrosc. Radiat. Transfer **50**, 257 (1993).
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[14] T. G. Koch and J. R. Sodeau, J. Phys. Chem. **99**, 10824 (1995).
[15] S. Höjer, R. D. May, and C. E. Miller, J. Quant. Spectrosc. Radiat. Transfer **55**, 273 (1996).

HSO_4

$\tilde{A}$

$T_0 = 5240(1130)$ gas PE[1]

References

[1] X.-B. Wang, J. B. Nicholas, and L.-S. Wang, J. Phys. Chem. A **104**, 504 (2000).

CCl_3OH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3604	gas	IR	1
		COH bend	1311	gas	IR	1
		CO stretch	1113	gas	IR	1
		CCl_3 stretch	784	gas	IR	1

References

[1] T. J. Wallington, W. F. Schneider, I. Barnes, K. H. Becker, J. Sehested, and O. J. Nielsen, Chem. Phys. Lett. **322**, 97 (2000).

HSO_4^-

Threshold for electron detachment from ground-state HSO_4=38320(800) gas PE[1]

References

[1] X.-B. Wang, J. B. Nicholas, and L.-S. Wang, J. Phys. Chem. A **104**, 504 (2000).

$HOOClO_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	OH stretch	3526.7	Ar	IR	1
	2	HOO bend	1282.6	Ar	IR	1
	3	ClO_2 a-stretch	1207.4	Ar	IR	1
	4	ClO_2 s-stretch	1046.4	Ar	IR	1
	5	OO stretch	893.2	Ar	IR	1

$DOOClO_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	OD stretch	2604.7	Ar	IR	1
	2	ClO_2 a-stretch	1207.4	Ar	IR	1
	3	ClO_2 s-stretch	1048.3	Ar	IR	1
	4	DOO bend	956.7	Ar	IR	1
	5	OO stretch	889.7	Ar	IR	1

References

[1] T. Svensson, B. Nelander, A. Bernhardsson, and G. Karlström, J. Phys. Chem. A **103**, 4432 (1999).

Al_5C

$\tilde{C}$ C_{2v}
T_0= 11540(650) gas PE[1]

$\tilde{B}$ C_{2v}
T_0= 3630(580) gas PE[1]

$\tilde{A}$ C_{2v}
T_0= 1690(520) gas PE[1]

References

[1] A. I. Boldyrev, J. Simons, X. Li, and L.-S. Wang, J. Chem. Phys. **111**, 4993 (1999).

Al_5C^-

Threshold for electron detachment from ground-state Al_5C=21060(320) gas PE[1]

References

[1] A. I. Boldyrev, J. Simons, X. Li, and L.-S. Wang, J. Chem. Phys. **111**, 4993 (1999).

TiC_5

$\tilde{A}$
T_0=7640(560) gas PE[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			240(60)	gas	PE	1

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TiC_5^-

Threshold for electron detachment from ground-state TiC_5^-=14100(400) gas PE[1]

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[1] X.-B. Wang, C.-F. Ding, and L.-S. Wang, J. Phys. Chem. A **101**, 7699 (1997).

C_6

(2) $^3\Sigma_u^-$ $D_{\infty h}$
T_0=42108(35) Ne AB[15]

(5) $^3\Pi_u$ $D_{\infty h}$
T_0= 40090(32)T Ne AB[15] $^3\Pi_u - \tilde{X}$ 241-249 nm
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]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	3	Stretch	644(45)	Ne	AB	15

$^3\Sigma_u^-$ $D_{\infty h}$
T_0=19558(5) Ne AB[10,15] $^3\Sigma_u^- - \tilde{X}$ 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

$^3\Pi_u$ $D_{\infty h}$
T_0=8880(160) gas PE[14]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	3	Stretch	640(50)	gas	PE	14

$^3\Sigma_u^+$ $D_{\infty h}$
T_0=6850(120) gas PE[14]

$^1\Delta_g$ $D_{\infty h}$
T_0=1340(120) gas PE_{14}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	2016(50)	gas	PE	14
	2	Sym. stretch	1686(50)	gas	PE	14

$\tilde{X}\ ^3\Sigma_g^-$ $D_{\infty h}$ 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,PE	6,14
			2050T	Ar	IR	11
	2	Sym. stretch	1694(50)	gas	PE	14
	3	Stretch	637(50)	gas	PE	14
Σ_u^+	4	Asym. stretch	1959.86	gas	DL	8
			1958.7	Ne	IR	9,10,13
			1952.0	Ar	IR	3,4,7
			1951.2	Kr	IR	11
			1956.8	H_2	IR	13
	5	Asym. stretch	1199.4	Ne	IR	9
			1197.3	Ar	IR	1,3,7
			1197.0	Kr	IR	11
Π_g	7	Bend	246(50)H	gas	PE	5,14
Π_u	9	Bend	90(50)H	gas	PE	14

B_0=0.048 DL[8]

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cyc-C_6

$\tilde{X}$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	4		1694.9	Ar	IR	1,2

References

[1] S. L. Wang, C. M. L. Rittby, and W. R. M. Graham, J. Chem. Phys. **107**, 6032 (1997).
[2] J. D. Presilla-Márquez, J. A. Sheehy, J. D. Mills, P. G. Carrick, and C. W. Larson, Chem. Phys. Lett. **274**, 439 (1997).

SiC_4Si

$\tilde{a}$ $D_{\infty h}$
$T_0 = 888(32)$ gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		1790(20)	gas	PE	2
	2		990(20)	gas	PE	2

$\tilde{X}\,^3\Sigma^-$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		1870(20)	gas	PE	2
	2		1200(20)	gas	PE	2
Σ_u^+	4	C=C stretch	1807.4	Ar	IR	1
	5	Si–C stretch	719.1	Ar	IR	1

References

[1] J. D. Presilla-Márquez, C. M. L. Rittby, and W. R. M. Graham, J. Chem. Phys. **106**, 8367 (1997).
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Si_6

$\tilde{A}$
$T_0 = 6450T$ gas PE[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			323(20)	gas	PE	3

$\tilde{X}\,^1A_{1g}$ 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

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C_6^-

Threshold for electron detachment from ground-state $C_6^- = 33725(10)$ gas PE[1,2,9]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]MPD[11]PE[12] $\tilde{C}-\tilde{X}$ 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	605	gas	PD,MPD	5,11
			607(5)	Ne	AB	4
			605T	Ar	AB	6
Π_g	8		245H	gas	PD	5
Π_u	9		110H	gas	PD	5

Internal conversion to vibrationally excited levels of the $\tilde{B}$ and $\tilde{A}$ states occurs in 730(50) fs gas PE[12]

$\tilde{A}\,^2\Sigma_g^+$ $D_{\infty h}$
$T_0 = 9352(2)$ 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^+	1	Sym. stretch	2083	Ar	Ra	10
	2	Sym. stretch	1775	Ar	Ra	10
	3	C–C stretch	564	gas	PD	5
			634	Ar	Ra	10
Σ_u^+	4	Asym. stretch	1938.5	Ne	IR	7
			1936.7	Ar	IR	6,10
Π_g	7		220T	gas	PE	3
	8		201H	gas	PD	5
			234H	Ar	Ra	10
Π_u	9		111T	gas	PE	3

$A = -29(2)$ gas PE[3]

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[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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SiC_4Si^-

Threshold for electron detachment from ground-state $SiC_4Si^- = 20520(50)$ gas PE[1]

Reference

[1] G. E. Davico, R. L. Schwartz, and W. C. Lineberger, J. Chem. Phys. **115**, 1789 (2001).

C_5N

$^2\Pi$ $C_{\infty v}$
$T_0 = 21259(9)$ Ne AB[2] $^2\Pi-\tilde{X}$ 427–471 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		CC,CN stretch	2122(13)	Ne	AB	2
		C–C stretch	1515(13)	Ne	AB	2
		C–C stretch	652(13)	Ne	AB	2
Π		Deformation	135(7)H	Ne	AB	2

$\tilde{X}\,^2\Sigma$ $C_{\infty v}$
$B_0 = 0.0468$ MW[1]

References

[1] Y. Kasai, Y. Sumiyoshi, Y. Endo, and K. Kawaguchi, Astrophys. J. **477**, L65 (1997).
[2] M. Grutter, M. Wyss, and J. P. Maier, J. Chem. Phys. **110**, 1492 (1999).

$NCC{\equiv}CCN^+$

$\tilde{D}\,^2\Pi_u$ $D_{\infty h}$
$T_0 = 25500(160)$ gas PE[1,3]

$\tilde{C}\,^2\Sigma_u^+$ $D_{\infty h}$
$T_0 = 18720(160)$ gas PE[1,3]

$\tilde{B}\,^2\Sigma_g^+$ $D_{\infty h}$
$T_0 = 17430(160)$ gas PE[1,3]

$\tilde{A}\,^2\Pi_g$ $D_{\infty h}$

$T_0 = 16780.31$ gas $EF^2LF^3AB^6$ $\tilde{A}-\tilde{X}$ 528–720 nm
16679 Ne LF^4 $\tilde{A}-\tilde{X}$ 530–816 nm
16709 Ne LF^4AB^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

$\tau = 13(2)$ ns gas EF^2PEFCO^3
$A_0 = -45(10)$ gas AB^6
$B_0 = 0.044$ AB^6

$\tilde{X}\,^2\Pi_u$ $D_{\infty h}$

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		2015	Ne	LF,IR	4,7
	5		1208[a]	Ne	LF	4

$A_0 = -45(10)$ gas AB^6
$B_0 = 0.045$ AB^6

[a]From overtones and combination bands.

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[1] G. Bieri, E. Heilbronner, V. Hornung, E. Kloster-Jensen, J. P. Maier, F. Thommen, and W. Von Niessen, Chem. Phys. **36**, 1 (1979).
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C_5N^-

$\tilde{X}\,^1\Sigma$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+			2116	Ne	IR	1

Reference

[1] M. Grutter, M. Wyss, and J. P. Maier, J. Chem. Phys. **110**, 1492 (1999).

C_5O

$\tilde{X}\,^1\Sigma^+$ $C_{\infty v}$ Structure: MW[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2251.7T	Ar	IR	2

$B_0 = 0.046$ MW[1]

References

[1] T. Ogata, Y. Ohshima, and Y. Endo, J. Am. Chem. Soc. **117**, 3593 (1995).
[2] M. Dibben, J. Szczepanski, C. Wehlburg, and M. Vala, J. Phys. Chem. A **104**, 3584 (2000).

C_5S

$\tilde{X}\,^1\Sigma^+$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2124.5	Ar	IR	2

$B_0 = 0.031$ MW[1]

References

[1] Y. Kasai, K. Obi, Y. Ohshima, Y. Hirahara, Y. Endo, K. Kawaguchi, and A. Murakami, Astrophys. J. **410**, L45 (1993).
[2] J. Szczepanski, R. Hoduss, J. Fuller, and M. Vala, J. Phys. Chem. A **103**, 2975 (1999).

NCCCNC

$\tilde{X}$ $C_{\infty v}$ Structure: MW[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡C stretch	2295.72	gas	IR	3
			2287.1s	Ar	IR	1,2
	2	–C≡N stretch	2209.62	gas	IR	3
			2203.6s	Ar	IR	1,2
	3	–N≡C stretch	2052.98	gas	IR	3
			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

$B_0 = 0.047$ MW[3,4]

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[1] A. M. Smith, G. Schallmoser, A. Thoma, and V. E. Bondybey, J. Chem. Phys. **98**, 1776 (1993).
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Al_3O_3

$\tilde{B}$

$T_0 = 18560(800)$ gas PE[1]

$\tilde{A}$

$T_0 = 6450(440)$ gas PE[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			610(60)[a]	gas	PE	1

[a]Ref. 1 presents evidence for the existence of an isomer, for which the vibrational spacing in the first photoelectron band is 720(60). A more detailed assignment has been proposed by Ref. 2.

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[1] H. Wu, X. Li, X.-B. Wang, C.-F. Ding, and L.-S. Wang, J. Chem. Phys. **109**, 449 (1998).
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Cr_2O_4

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			716.2	Ar	IR	1
			643.1	Ar	IR	1

Reference

[1] G. V. Chertihin, W. D. Bare, and L. Andrews, J. Chem. Phys. **107**, 2798 (1997).

$Al_3O_3^-$

Threshold for electron detachment from ground-state $Al_3O_3^- = 22590(160)$ gas PE[1]

Evidence for the participation of a second electronic state of $Al_3O_3^-$ in its photoelectron spectrum is presented by Ref. 2.

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$(SiNN)_2$

$\tilde{X}$ C_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_u		NN a-stretch	2080	N_2	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, and J. Glatthaar, Organomet. **19**, 4775 (2000).

OCNNCO

In an argon matrix, an absorption maximum at 45450 (220 nm) has been assigned[1] to OCNNCO.

$\tilde{X}$ C_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	NCO stretch	2235T	Ar	IR	1
	2	NCO stretch	1460T	Ar	IR	1
	3	NN stretch	840T	Ar	IR	1
a_u	6	OPLA bend	533.5w	Ar	IR	1
b_u	9	NCO stretch	2208	gas	IR	1
			2200.6vs	Ar	IR	1
	11	Bend	661.0w	Ar	IR	1

Reference

[1] G. Maier, M. Naumann, H. P. Reisenauer, and J. Eckwert, Angew. Chem. **108**, 1800 (1996); Angew. Chem. Int. Ed. Engl. **35**, 1696 (1996).

$(GeO)_3$

$\tilde{X}$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1		475.0	Ar	Ra	3
	2		305.0	Ar	Ra	3
e'	5	GeO stretch	828.6s	Ar	IR,Ra	1–3
			824	N_2	IR	1
	6	GeO stretch	438.2w	Ar	IR,Ra	1,3
			440	N_2	IR	1
	7		193.0	Ar	Ra	3

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[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] A. Zumbusch and H. Schnöckel, J. Chem. Phys. **108**, 8092 (1998).

$O_2CCO_2^+$

Photodestruction of gas-phase $O_2CCO_2^+$ occurs in the near infrared and visible spectral regions, with onset[3] below 9400 and maximum[1,2] near 15400 (650 nm).

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO_2 a-stretch	2130.8	Ne	IR	4,5
			1274.4	Ne	IR	4,5
			1274.0	Ar	IR	4

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$S_2CCS_2^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CS_2 a-stretch	1385.2	Ne	IR	1
			1379.7	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Chem. Phys. **112**, 6576 (2000).

$(NO)_3^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO stretch	1790T	gas	PF	1

Reference

[1] A. Mouhandes and A. J. Stace, J. Chem. Phys. **111**, 9517 (1999).

$O_2CCO_2^-$

Maximum in the photoelectron spectrum of $(CO_2)_2^-$ near 20170 (2.5 eV) gas PE[1–3]

$\tilde{X}$ D_{2d}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	5	CO_2 s-stretch	1189.2	Ne	IR	4,6,7
			1184.7	Ar	IR	5
	6	Deformation	679.2T	Ne	IR	6,7
e	7	CO_2 a-stretch	1852.4	Ne	IR	4,6,7
			1856.7	Ar	IR	5

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$FAl(O_2)_2$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		892.4	Ar	IR	1
b_2	11		705.3	Ar	IR	1

Reference

[1] J. Bahlo, H.-J. Himmel, and H. Schnöckel, Angew. Chem. Int. Ed. **40**, 4696 (2001).

$c\text{-}(NO)_3^-$

Maximum in the photoelectron spectrum of c-$(NO)_3^-$ at 29850(160), or 3.70(2) eV gas PE[1]

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1369.9	Ne	IR	2,3
			1001.9	Ne	IR	2
			693.8	Ne	IR	2

References

[1] T. Tsukuda, M. Saeki, L. Zhu, and T. Nagata, Chem. Phys. Lett. **295**, 416 (1998).
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[3] L. Andrews and M. Zhou, J. Chem. Phys. **111**, 6036 (1999).

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	6,10,13–15
			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	2,6,11,13–15
			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	6,13,15
			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 $\nu_6+\nu_{10}$.

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O_2PPO_2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		PO_2 a-stretch	1473.1	Ar	IR	1–3
		PO_2 s-stretch	1158.1	Ar	IR	1–3
		PO_2 deform.	479.4	Ar	IR	1,3

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$C_2F_4^+$

$\tilde{H},\tilde{I}\,^2B_{3g}$, $^2B_{3u}$ D_{2h}
$T_0=73020(320)$ gas PE[1,4]TPE[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2	CF stretch	806(40)	gas	PE,TPE	1,5

$\tilde{G}\,^2B_{2g}$ D_{2h}
$T^a=65190(320)$ gas PE[2–4]

$\tilde{F}\,^2B_{1u}$ D_{2h}
$T_0=59460(400)$ gas PE[1–4]TPE[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2	CF s-stretch	766(40)	gas	PE,TPE	1,5
	3	CF_2 scissors	330(80)	gas	PE	1

$\tilde{B},\tilde{C},\tilde{D},\tilde{E}\,^2A_g$, $^2B_{2u}$, ^2A_u, $^2B_{1g}$ D_{2h}
$T^a\cong52000$ gas PE[1–4]

$\tilde{A}\,^2B_{3g}$ D_{2h}
$T^a=46880(320)$ gas PE[1–4]

$\tilde{X}\,^2B_{3u}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	C=C stretch	1686(40)	gas	PE,TPE	1–3,5
	2	CF s-stretch	766(40)	gas	PE,TPE	1–3,5
	3	CF_2 scissors	371(40)	gas	PE,TPE	2,3,5

[a]From vertical ionization potential.

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UOF_4

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		UO stretch	834.7	Ar	IR	1

Reference

[1] P. F. Souter and L. Andrews, J. Mol. Struct. **412**, 161 (1997).

CF_3O_2

In the gas phase, an absorption maximum near 47620 (210 nm) has been assigned[5,6] to CF_3O_2. In a neon matrix, the corresponding absorption maximum has been observed[7] at 48430 (206.5 nm).

$\tilde{A}\,^2A'$ C_s
$T_0=6656(3)$ gas CR[8]

Vib. sym.	No.	Approximate typeofmode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CO stretch	1192(5)T	gas	CR	8
	3	OO stretch	980(5)	gas	CR	8

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CF_3 a-stretch	1309.0vs	Ne	IR	7
			1303.9vs	Ar	IR	2–4,7
	2	CF_3 s-stretch	1178.3ms	Ne	IR	7
			1172.5s	Ar	IR	1–4,7
	3	O–O stretch	1099.6m	Ne	IR	7
			1093.0m	Ar	IR	1–4,7
	4	CO stretch	872.7w	Ne	IR	7
			869.2w	Ar	IR	2,7
	5	CF_3 s-deform.	694.8w	Ne	IR	7
			693.2m	Ar	IR	2–4,7
	6	CF_3 a-deform.	495.0w	Ne	IR	7
			491.2	Ar	IR	7
	7	COO deform.	449.6vw	Ne	IR	7
			447.6vw	Ar	IR	2,7
	8	CF_3 rock	289.6vw	Ne	IR	7
			286.8vw	Ar	IR	2,7
a''	9	CF_3 a-stretch	1266.1s	Ne	IR	7
			1261.8vs	Ar	IR	2–4,7
	10	CF_3 a-deform.	596.9w	Ne	IR	7
			595.2w	Ar	IR	2,4,7
	11	CF_3 rock	402.7vw	Ne	IR	7
			401.2	Ar	IR	7

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[1] R. R. Smardzewski, R. A. DeMarco, and W. B. Fox, J. Chem. Phys. **63**, 1083 (1975).
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$(SO_2)_2^-$ [a]

Threshold for electron detachment from ground-state $(SO_2)_2^-$ = 15300(1600) gas PE[2,4]; vertical detachment energy=22270(160) gas PE[6]

Gas-phase absorption maxima[1,3,5] at 25000 (400 nm) and 16700 (600 nm) result from the photodissociation of $(SO_2)_2^-$ into $SO_2+SO_2^-$.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SO stretch	1267.4	Ne	IR	7
			1265.9			
		SO stretch	1256.6	Ne	IR	7
			1256.1			
			1015.7	Ne	IR	7
			622.7	Ne	IR	7

[a] Two or more nearly isoenergetic structures may contribute to the observed spectrum.

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SF_5^+

$\tilde{X}$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	3	SF stretch	1008.2vs	Ne	IR	1
	4	Deformation	633.2m	Ne	IR	1
e'	5	SF stretch	1074.8vs	Ne	IR	1
	6	Deformation	579.6m	Ne	IR	1

Reference

[1] C. L. Lugez, M. E. Jacox, R. A. King, and H. F. Schaefer III, J. Chem. Phys. **108**, 9639 (1998).

PF_5^-

$\tilde{X}$ C_{4v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PF stretch	815.6ms	Ne	IR	1
	3		455.9mT	Ne	IR	1
e	7	PF stretch	735.0vs	Ne	IR	1

Reference

[1] C. L. Lugez, K. K. Irikura, and M. E. Jacox, J. Chem. Phys. **108**, 8381 (1998).

SF_5

$\tilde{X}$ C_{4v} Structure: ESR[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Eq. s-stretch	884.5	Ar	IR	5
	3	SF stretch	553.8	Ne	IR	6
			552m	Ar	IR	3,4
e	7	SF a-stretch	817.0	Ne	IR	6
			813.1vs	Ar	IR	3–5

References

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SF_5^-

$\tilde{X}$ C_{4v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SF stretch	795.8	Ne	IR	4
			795.5m	Ar	IR	2,3
e	7	SF stretch	602.9	Ne	IR	4
			596s[a]	Ar	IR	1,2
	8	Deformation	470.5	Ne	IR	4
			470w	Ar	IR	2

[a]This absorption was attributed to SF_6^- by Ref. 1. Reassignment to SF_5^- is dictated by the close correspondence, discussed in Ref. 2, of these three absorptions to peaks observed for solid $CsSF_5$.

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[4] C. L. Lugez, M. E. Jacox, R. A. King, and H. F. Schaefer III, J. Chem. Phys. **108**, 9639 (1998).

8.13. Seven-Atomic Molecules

$Pd(H_2)_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		HH stretch	2909	Ar	IR	1
		PdH stretch	745.7	Ne	IR	1
			730.1	Ar	IR	1
		Deformation	319.5	Ar	IR	1

$Pd(D_2)_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		DD stretch	2070	Ar	IR	1
		PdD stretch	560.6	Ne	IR	1
			549.4	Ar	IR	1
		Deformation	236.6	Ar	IR	1

Reference

[1] L. Andrews, X. Wang, M. E. Alikhani, and L. Manceron, J. Phys. Chem. A **105**, 3052 (2001).

CH_3GaH_2

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	GaH_2 s-stretch	1898.0	Ar	IR	1
a''	11	GaH_2 a-stretch	1892.0	Ar	IR	1

Reference

[1] J. Müller, H. Sternkicker, U. Bergmann, and B. Atakan, J. Phys. Chem. A **104**, 3627 (2000).

C_2H_5

3p Rydberg state

In the gas phase, an absorption with maximum at 205 nm has been assigned[6,7] to the $3p-\tilde{X}$ transition of C_2H_5. The detection of this band in MPI studies[9] is consistent with the assignment to a Rydberg state.

3s Rydberg state

In the gas phase, a broad, unstructured absorption with maximum at 246 nm has been assigned[1,3,6,7] to the $3s-\tilde{X}$ transition of C_2H_5.

$\tilde{X}$ C_s Structure: MO[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CH_2 s-stretch	3037.02	gas	LD	13
			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	528.12	gas	DL	10,12
			540vs	Ar	IR	2,4,5,8
a''		CH_2 a-stretch	3128.69	gas	LD	13
			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

$A_0=9.629$; $(B_0+C_0)/2=0.730$; $(B_0-C_0)/4=0.014$ DL[12]

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	2199mT	Ar	IR	4,5
		CD_3 s-stretch	2094m	Ar	IR	4,5
			2092.2	H_2	IR	14
		2-CD stretch	2048m	Ar	IR	4,5
			2050.0	H_2	IR	14
		CD_3 deform.	1070mT	Ar	IR	4,5
		CD_3 deform.	1035mT	Ar	IR	4,5
		CCD_2 umbrella	398vs	Ar	IR	4,5
a''		CD_2 a-stretch	2249mT	Ar	IR	4,5
		CD_3 a-stretch	2170sT	Ar	IR	4,5
		CD_3 deform.	1041mT	Ar	IR	4,5
			2350T	H_2	IR	14
			2343T	H_2	IR	14
			2060.7T	H_2	IR	14
			1188.7	H_2	IR	14

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cyc-$BHCHCH_2$

$\tilde{X}$ C_1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2621.6	Ar	IR	1
			864.3	Ar	IR	1
			637.6	Ar	IR	1

cyc-$BDCDCD_2$

$\tilde{X}$ C_1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1962.2	Ar	IR	1
			650.9T	Ar	IR	1
			530.4	Ar	IR	1

Reference

[1] L. Andrews, D. V. Lanzisera, P. Hassanzadeh, and Y. Hannachi, J. Phys. Chem. A **102**, 3259 (1998).

H_2BCCH_2

$\tilde{X}$ C_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BH_2 a-stretch	2568.7	Ar	IR	1
		C=C stretch	1770.6	Ar	IR	1
			1347.1	Ar	IR	1
			847.7w	Ar	IR	1
			826.5	Ar	IR	1

D_2BCCD_2

$\tilde{X}$ C_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BD_2 a-stretch	1933.5	Ar	IR	1
		C=C stretch	1732.1	Ar	IR	1
			650.9T	Ar	IR	1

Reference

[1] L. Andrews, D. V. Lanzisera, P. Hassanzadeh, and Y. Hannachi, J. Phys. Chem. A **102**, 3259 (1998).

CH_3CCH^+

$\tilde{C}$
$T^a = 55100(800)$ gas PE[1]

$\tilde{B}$
$T^a = 39000(800)$ gas PE[1]

$\tilde{A}$ C_{3v}
$T_0 = 26790(100)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4	CH_3 deform.	1290(40)	gas	PE	1

$\tilde{X}\,^2E$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	3226.7T	Ne	IR	3
	2	CH stretch	2767T	gas	PI	2
	3	CC stretch	1996(38)	gas	PE,PI	2
	5	CC stretch	940(40)	gas	PE	1
e	9	CCH deform.	586(74)	gas	PI	2
	10	Deformation	289(65)	gas	PI	2

[a]From vertical ionization potential.

References

[1] C. Baker and D. W. Turner, Proc. R. Soc. A **308**, 19 (1968).
[2] G. H. Ho, M. S. Lin, Y. L. Wang, and T. W. Chang, J. Chem. Phys. **109**, 5868 (1998).
[3] D. Forney, M. E. Jacox, C. L. Lugez, and W. E. Thompson, J. Chem. Phys. **115**, 8418 (2001).

$H_2CCCH_2^+$

$\tilde{B}$
$T^a = 61400(800)$ 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.
			1320(6)	gas	PE	3,4
			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.
		CH_2 stretch	3047.3wm	Ne	IR	5
		CH_2 stretch	2956.0m	Ne	IR	5
		CH_2 deform.	1314.4s	Ne	IR	5
			880.4m	Ne	IR	5
b_1	4	Torsion	745(5)	gas	PE	3,4
			738.4wm	Ne	IR	5

$D_2CCCD_2^+$

$\tilde{X}\,^2E$ D_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD_2 stretch	2295.5wm	Ne	IR	5
		CD_2 stretch	2177.2wm	Ne	IR	5
			2169.6wm			
		CD_2 deform.	962.4m	Ne	IR	5
			724.6wm	Ne	IR	5
b_1	4	Torsion	565(50)	gas	PE	1
			583.6wm	Ne	IR	5

[a]From vertical ionization potential.

References

[1] R. K. Thomas and H. Thompson, Proc. R. Soc. London, Ser. A **339**, 29 (1974).
[2] L. S. Cederbaum, W. Domcke, and H. Köppel, Chem. Phys. **33**, 319 (1978).
[3] Z. Z. Yang, L. S. Wang, Y. T. Lee, D. A. Shirley, S. Y. Huang, and W. A. Lester, Jr., Chem. Phys. Lett. **171**, 9 (1990).
[4] P. Baltzer, B. Wannberg, M. Lundqvist, L. Karlsson, D. M. P. Holland, M. A. MacDonald, and W. von Niessen, Chem. Phys. **196**, 551 (1995).
[5] D. Forney, M. E. Jacox, C. L. Lugez, and W. E. Thompson, J. Chem. Phys. **115**, 8418 (2001).

cyc-CH_2CH_2Si

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_2 deform.	1417.1w	Ar	IR	1
	3	CC stretch	1011.9wm	Ar	IR	1
	4	CH_2 deform.	869.6w	Ar	IR	1
	5	Ring deform.	601.4wm	Ar	IR	1
b_1	9	CH stretch	3032.0wm	Ar	IR	1
	10	CH_2 deform.	719.4w	Ar	IR	1
b_2	12	CH stretch	2966.3wm	Ar	IR	1
	13	CH_2 deform.	1376.7w	Ar	IR	1
	14	CH_2 deform.	919.4wm	Ar	IR	1
	15	Ring deform.	592.1vs	Ar	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, and H. Egenolf, Eur. J. Org. Chem. **1998**, 1313.

H_2CCHCH:

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_2 wag	786.6T	Xe	IR	1

Reference

[1] G. Maier, C. Lautz, and S. Senger, Chem. Eur. J. **6**, 1467 (2000).

$H_2CCHSiH$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH_2 stretch	3056.1w	Ar	IR	1
	2	CH stretch	2997.0w	Ar	IR	1
	3	CH stretch	2976.5w	Ar	IR	1
	4	SiH stretch	1979.4vs	Ar	IR	1
	5	Mixed	1566.9w	Ar	IR	1
	6	CH_2 deform.	1388.2wm	Ar	IR	1
	8	CH_2 deform.	1004.8w	Ar	IR	1
	9	Deform.	812.7wm	Ar	IR	1
	10	Deform.	665.2wm	Ar	IR	1
a''	12	CH deform.	1009.3w	Ar	IR	1
	13	CH_2 deform.	985.2wm	Ar	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, and H. Egenolf, Eur. J. Org. Chem. **1998**, 1313.

H_2CCSiH_2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	3008.2	Ar	IR	1
	2	SiH stretch	2205.9	Ar	IR	1
	4	CH_2 deform.	1371.0w	Ar	IR	1
	5	SiH_2 deform.	930.3vs	Ar	IR	1
b_1	8	CH stretch	3069.1	Ar	IR	1
b_2	12	SiH stretch	2221.6	Ar	IR	1
	13	CH_2 deform.	917.6vs	Ar	IR	1
	14	$CSiH_2$ deform.	656.2vs	Ar	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, and H. Egenolf, Eur. J. Org. Chem. **1998**, 1313.

CH_3BNH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NH stretch	3690.5	Ar	IR	1
		BN stretch	1940.2	Ar	IR	1

Reference

[1] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **101**, 824 (1997).

CH_3NBH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NB stretch	1949.2	Ar	IR	1

Reference

[1] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **101**, 824 (1997).

CH_2BNH_2

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BN stretch	1743.5	Ar	IR	1

Reference

[1] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **101**, 824 (1997).

CH_3CNH^+

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NH stretch	3527.29	gas	LD	1,2

$B_0 = 0.287$ $LD^{1,2}MW^3$

References

[1] T. Amano, Astrophys. J. **330**, L137 (1988).
[2] T. Amano, J. Mol. Spectrosc. **153**, 654 (1992).
[3] C. A. Gottlieb, A. J. Apponi, M. C. McCarthy, P. Thaddeus, and H. Linnartz, J. Chem. Phys. **113**, 1910 (2000).

CH_3CHO^+

$\tilde{E}$ C_s
$T_0 = 47930(400)$ gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CO stretch	1200(40)	gas	PE	2

$\tilde{C},\tilde{D}$ C_s
$T_0 = 37840(400)$ gas PE[1,2]

$\tilde{B}$ C_s
$T_0 = 28160(400)$ gas PE[1,2]

$\tilde{A}$ C_s

$T_0 = 18560(240)$ gas PE[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CO stretch	1210(40)	gas	PE	1,2
		CCO deform.	440(40)	gas	PE	1,2

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CH stretch	2815(10)	gas	PE	3
		CH stretch	2570(40)	gas	PE	2
			1428(10)	gas	PE	3
		CH_3 deform.	1315(10)	gas	PE	1–3
		CH deform.	1100(40)	gas	PE	1,2
			1032(10)	gas	PE	3
			823(10)	gas	PE	3
	10	CH_3 rock	363(10)	gas	PE	3
a''	14	CH_3 rock	742(10)	gas	PE	1–3
	15	Torsion	145(10)	gas	PE	3

CD_3CDO^+

$\tilde{A}$ C_s

$T_0 = 18560T$ gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CO stretch	1210(40)	gas	PE	2
		CCO bend	440(40)	gas	PE	2

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CH stretch	1890(40)	gas	PE	2
		CO stretch	1550(40)	gas	PE	2
			960(40)	gas	PE	2
			830(40)	gas	PE	2
		CCO deform.	320(40)	gas	PE	2

References

[1] D. Chadwick and R. Katrib, J. Electron Spectrosc. Relat. Phenom. **3**, 39 (1974).
[2] T. Cvitaš, H. Güsten, and L. Klasinc, J. Chem. Phys. **64**, 2549 (1976).
[3] H.-T. Kim and S. L. Anderson, J. Chem. Phys. **114**, 3018 (2001).

syn-CH_2=CHOH

$\tilde{X}$ C_s Structure: MW[1,3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3633.5m	gas	IR	5,6
			3620s	Ar	IR	2,4
	2	CH stretch	3121.7(2)	gas	IR	5
	5	C=C stretch[a]	1663m	gas	IR	5,6
			1626m			
			1662vs	Ar	IR	2,4
			1622s			
	6		1411.8vw	gas	IR	5,6
			1409.4	Ar	IR	4
	7		1300.0vw	gas	IR	5,6
			1326w	Ar	IR	4
	8		1259.7m	gas	IR	5,6
			1300.2m	Ar	IR	4
	9	CO stretch+	1118vs	gas	IR	5,6
		OH deform.[b]	1078vs			
			1121s	Ar	IR	2,4
			1079vs			
	10		947.6w	gas	IR	5
			943.4w	Ar	IR	4
	11		486.1w	Ar	IR	4
a''	12		960m	gas	IR	6
			971.4m	Ar	IR	4
	13	H_2C=C OPLA	816.66s	gas	IR	5,6
			813.7s	Ar	IR	2,4
	14		698.9w	gas	IR	5
			698vw	Ar	IR	4
	15	Torsion	388H	gas	IR	6
			413s	Ar	IR	2,4

$A_0 = 1.990$; $B_0 = 0.352$; $C_0 = 0.299$ MW[1,3]IR[6]

syn-CD_2=CDOD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		OD stretch	2677	Ar	IR	2
		C=C stretch	1590	Ar	IR	2
			1584			
		CO stretch+	926	Ar	IR	2
		OD deform.	922			
a''		D_2C=C OPLA	651	Ar	IR	2
		Torsion	310	Ar	IR	2

$A_0 = 1.342$; $B_0 = 0.312$; $C_0 = 0.253$ MW[3]

[a] Fermi resonance between ν_5 and $2\nu_{13}$.
[b] Fermi resonance between ν_9 and $(\nu_{14} + \nu_{15})$.

References

[1] S. Saito, Chem. Phys. Lett. **42**, 399 (1976).
[2] M. Hawkins and L. Andrews, J. Am. Chem. Soc. **105**, 2523 (1983).
[3] M. Rodler and A. Bauder, J. Am. Chem. Soc. **106**, 4025 (1984).
[4] M. Rodler, C. E. Blom, and A. Bauder, J. Am. Chem. Soc. **106**, 4029 (1984).
[5] Y. Koga, T. Nakanaga, K. Sugawara, A. Watanabe, M. Sugie, H. Takeo, S. Kondo, and C. Matsumura, J. Mol. Spectrosc. **145**, 315 (1991).
[6] D.-L. Joo, A. J. Merer, and D. J. Clouthier, J. Mol. Spectrosc. **197**, 68 (1999).

anti-CH_2=CHOH

Relative intensities of microwave lines for the two isomers of CH_2=OH indicate that the *anti*-isomer lies 380(50), or 4.5(6) kJ/mol, above the *syn*-isomer.[1]

$\tilde{X}$ C_s
A_0=2.097; B_0=0.349; C_0=0.299 MW[1]

Reference

[1] M. Rodler, J. Mol. Spectrosc. **114**, 23 (1985).

t-CH_3OSiH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	SiH stretch	1929.1vs	Ar	IR	1
			1964.7vs			
	4	CH_2 deform.	1473.6vw	Ar	IR	1
	5	CH_3 deform.	1443.9w	Ar	IR	1
	6	CH_3 deform.	1186.2wm	Ar	IR	1
	7	Mixed	1084.8s	Ar	IR	1
	8	SiH deform.	859.4ms	Ar	IR	1
	9	SiO stretch	749.3wm	Ar	IR	1
a''	12	CH_2 deform.	1457.6w	Ar	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, and H. Egenolf, Monatsh. Chem. **130**, 227 (1999).

c-CH_3OSiH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	SiH stretch	1849.6vs	Ar	IR	1
			1910.7vs			
	4	CH_2 deform.	1461.3w	Ar	IR	1
	5	CH_3 deform.	1438.7w	Ar	IR	1
	6	CH_3 deform.	1174.7w	Ar	IR	1
	7	Mixed	1096.2s	Ar	IR	1
	8	SiH deform.	881.4w	Ar	IR	1
	9	SiO stretch	741.8m	Ar	IR	1
a''	12	CH_2 deform.	1452.6w	Ar	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, and H. Egenolf, Monatsh. Chem. **130**, 227 (1999).

CH_3CNO

$\tilde{X}$ C_{3v} Structure: MW[1,2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_3 s-stretch	2943w	gas	IR	5
	2	CNO a-stretch	2311vs	gas	IR	5
			2309	Ar	IR	4
	3	CH_3 s-deform.	1394	gas	IR	5
			1381	Ar	IR	4
	4	CNO s-stretch	1348	gas	IR	5
			1332	Ar	IR	4
	5	CC stretch	785	gas	IR	5
			780	Ar	IR	4
e	6	CH_3 a-stretch	3022vwT	gas	IR	5
	7	CH_3 a-deform.	1453vw	gas	IR	5
	8	CH_3 rock	1034vwT	gas	IR	5
	9	CNO bend	477vw	gas	IR	5

B_0=0.131 MW[1–3]

CD_3CNO

$\tilde{X}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CNO a-stretch	2297	Ar	IR	4
		CNO s-stretch	1341	Ar	IR	4

References

[1] H. K. Bodenseh and K. Morgenstern, Z. Naturforsch. **25A**, 150 (1970).
[2] P. B. Blackburn, R. D. Brown, F. R. Burden, J. G. Crofts, and I. R. Gillard, Chem. Phys. Lett. **7**, 102 (1970).
[3] M. Winnewisser, E. F. Pearson, J. Galica, and B. P. Winnewisser, J. Mol. Spectrosc. **91**, 255 (1982).
[4] Z. Mielke, M. Hawkins, and L. Andrews, J. Phys. Chem. **93**, 558 (1989).
[5] T. Pasinszki and N. P. C. Westwood, J. Phys. Chem. A **105**, 1244 (2001).

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

Reference

[1] J. Fulara, P. Freivogel, D. Forney, and J. P. Maier, J. Chem. Phys. **103**, 8805 (1995).

(*cyc*-HC=CHC)=C=C:

$\tilde{X}$ C_{2v}
A_0=1.067; B_0=0.118; C_0=0.106 MW[1]

(*cyc*-DC=CDC)=C=C:

$\tilde{X}$ C_{2v}
$A_0 = 0.808$; $B_0 = 0.112$; $C_0 = 0.098$ MW[1]

Reference

[1] C. A. Gottlieb, M. C. McCarthy, V. D. Gordon, J. M. Chakan, A. J. Apponi, and P. Thaddeus, Astrophys. J. **509**, L141 (1998).

HCCCH=C=C:

$\tilde{X}$ C_s
$A_0 = 1.061$; $B_0 = 0.096$; $C_0 = 0.088$ MW[1]

DCCCD=C=C:

$\tilde{X}$ C_s
$A_0 = 0.844$; $B_0 = 0.090$; $C_0 = 0.081$ MW[1]

Reference

[1] C. A. Gottlieb, M. C. McCarthy, V. D. Gordon, J. M. Chakan, A. J. Apponi, and P. Thaddeus, Astrophys. J. **509**, L141 (1998).

H_2C_5:

$\tilde{X}$ C_{2v}
$A_0 = 9.26$; $B_0 = 0.077$; $C_0 = 0.076$ 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*-HC_3)CCH

$\tilde{X}$ C_s
$A_0 = 1.155$; $B_0 = 0.114$; $C_0 = 0.104$ MW[1]

(*cyc*-DC_3)CCD

$\tilde{X}$ C_s
$A_0 = 0.994$; $B_0 = 0.104$; $C_0 = 0.094$ MW[1]

Reference

[1] M. J. Travers, M. C. McCarthy, C. A. Gottlieb, and P. Thaddeus, Astrophys. J. **483**, L135 (1997).

HSiCCCCH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CH stretch	3328.0w	Ar	IR	1
		CC stretch	2155.7m	Ar	IR	1
		SiH stretch	2029.1vs	Ar	IR	1
		CC stretch	2016.4s	Ar	IR	1
		CC stretch	999.6w	Ar	IR	1
		SiH deform.	806Tvs	Ar	IR	1
		SiC stretch	466.0w	Ar	IR	1
a''		CCC deform.	593.7w	Ar	IR	1

DSiCCCCD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CD stretch	2591.4m	Ar	IR	1
		CC stretch	2118.2vs	Ar	IR	1
		CC stretch	1936.3vw	Ar	IR	1
		SiD stretch	1474.2s	Ar	IR	1
		CC stretch	985.1w	Ar	IR	1
		SiH deform.	628Ts	Ar	IR	1
		SiC stretch	456.5vw	Ar	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, and A. Meudt, Eur. J. Org. Chem. **1998**, 1285.

$Si(CCH)_2$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CH stretch	3312.9s 3296.7	Ar	IR	1
		CC stretch	2012.5w 2004.3	Ar	IR	1
		SiC stretch	605.9w 602.4	Ar	IR	1
b_1		CH deform.	630.0vs 618.9	Ar	IR	1
b_2		CH stretch	3312.9s 3296.7	Ar	IR	1
		CC stretch	2007.3s 1999.5	Ar	IR	1
		CH deform.	621.6m 618.9	Ar	IR	1

$Si(CCD)_2$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CD stretch	2578.4w	Ar	IR	1
			2567.2			
		CC stretch	1894.2w	Ar	IR	1
			1885.8			
		SiC stretch	597.9s	Ar	IR	1
b_2		CD stretch	2578.4w	Ar	IR	1
			2567.2			
		CC stretch	1888.9vs	Ar	IR	1
			1861.1			
			612.6vs	Ar	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, and A. Meudt, Eur. J. Org. Chem. **1998**, 1285.

H_2CCCCN

$\tilde{X}$ C_{2v}
B_{eff}=0.073 MW[1]

Reference

[1] W. Chen, M. C. McCarthy, M. J. Travers, E. W. Gottlieb, M. R. Munrow, S. E. Novick, C. A. Gottlieb, and P. Thaddeus, Astrophys. J. **492**, 849 (1998).

cyc-(HC=CHN=C=N)

In an argon matrix,[1] irradiation of *cyc*-(CH=CHN=C=N) at wavelengths longer than 570 nm leads to the formation of (*cyc*-HC=CHN)CN.

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4	CH deform.	1077.8w	Ar	IR	1
	5	NCN s-stretch	979.2s	Ar	IR	1
			967.7s			
	6	NCN deform.	718.1m	Ar	IR	1
b_1	9	OPLA	672.9s	Ar	IR	1
			670.0s			
b_2	12	NCN a-stretch	1707.3vs	Ar	IR	1
			1684.7vs			
	13	CH a-deform.	1207.3m	Ar	IR	1
			1196.7m			

Reference

[1] G. Maier and J. Endres, Chem. Eur. J. **5**, 1590 (1999).

(*cyc*-HC=CHN)CN

In an argon matrix,[1] a prominent absorption at 41000 (244 nm) has been assigned to (*cyc*-HC=CHN)CN. Exposure of the deposit to 254-nm radiation leads to the formation of $H_2C=C=NCN$.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH s-stretch	3235.1w	Ar	IR	1
			3233.6w	N_2	IR	1
	2	CN stretch	2207.4s	Ar	IR	1
			2217.6vs	N_2	IR	1
			2207.4vs			
	3	C=C stretch	1712.6w	Ar	IR	1
			1714.1w	N_2	IR	1
	4	N–C stretch	1051.8m	Ar	IR	1
			1049.0s	N_2	IR	1
	5	CH deform.	960.0w	Ar	IR	1
			961.8w	N_2	IR	1
	6	Mixed	803.2w	Ar	IR	1
			803.2w	N_2	IR	1
	7	Mixed	613.6m	Ar	IR	1
			618.8w	N_2	IR	1
	8	Mixed	562.8m	Ar	IR	1
			580.7m	N_2	IR	1
			571.3m			
a''	10	CH a-stretch	3185.7s	Ar	IR	1
			3183.1s			
			3183.7s	N_2	IR	1
			3181.6s			
	11	CH deform.	958.0w	Ar	IR	1
	13	NCN deform.	636.7vw	Ar	IR	1
			635.0w	N_2	IR	1

Reference

[1] G. Maier and J. Endres, Chem. Eur. J. **5**, 1590 (1999).

$H_2C=C=NCN$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH s-stretch	3044.7w	Ar	IR	1
			3035.4w	N_2	IR	1
	2	CN stretch	2267.0m	Ar	IR	1
			2249.7m			
			2232.8m			
			2253.8m	N_2	IR	1
			2235.9m			
	3	CCN a-stretch	2048.9vs	Ar	IR	1
			2041.8vs	N_2	IR	1
	5	Mixed	1222.0vw	Ar	IR	1
			1221.6w	N_2	IR	1
	6	Mixed	857.9vw	Ar	IR	1
			862.5vw	N_2	IR	1
	7	CH_2 wag	733.5m	Ar	IR	1
			749.9m	N_2	IR	1
			747.3m			
	8	Skel. deform.	596.3vw	Ar	IR	1
			601.4vw	N_2	IR	1
a''	11	CH a-stretch	3136.4vw	Ar	IR	1
			3123.3vw	N_2	IR	1

Reference

[1] G. Maier and J. Endres, Chem. Eur. J. **5**, 1590 (1999).

cyc-(C=NCHNCH)

$\tilde{X}\,^3A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	Mixed	1452.0s	Ar	IR	1
	4	Mixed	1358.9s	Ar	IR	1
	5	CH a-deform.	1250.6w	Ar	IR	1
	6	CH s-deform.	1210.3m	Ar	IR	1
	7	NCN deform.	1114.0s	Ar	IR	1
	8	Mixed	988.6s	Ar	IR	1
			981.1s			
	9	C–C: stretch	971.9m	Ar	IR	1
	10	NCN deform.	864.1w	Ar	IR	1
a''	13	CH deform.	810.0m	Ar	IR	1
	14	Ring deform.	516.1m	Ar	IR	1

Reference

[1] G. Maier and J. Endres, Eur. J. Org. Chem. 2535 (2000).

HC−N=CHCN

In an argon matrix, an absorption maximum at 36100 (277 nm) can be assigned to HC–N=CHCN.[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	3	CN stretch	2216.1w	Ar	IR	1
			2216.3	N_2	IR	1
	4	NC stretch	1980.9s	Ar	IR	1
			1973.2s			
			1985.0s	N_2	IR	1
			1975.4s			
	8	CH deform.	848.0w	Ar	IR	1
			847.3w	N_2	IR	1
	9	:CH deform.	730.7vs	Ar	IR	1
			713.2vs			
			735.7vs	N_2	IR	1
			713.9vs			
	10	:CH deform.	575.5w	Ar	IR	1
			576.3w	N_2	IR	1
	12	Skel. deform.	442.8m	Ar	IR	1
			449.3m	N_2	IR	1

Reference

[1] G. Maier and J. Endres, Eur. J. Org. Chem. 2535 (2000).

cyc-(HC=NCH)CN

In an argon matrix, an absorption maximum at 38900 (257 nm) can be assigned to *cyc*-(HC=NCH)CN.[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	4	C=N stretch	1676.2m	Ar	IR	1
			1671.5m	N_2	IR	1
	6	Mixed	1214.2m	Ar	IR	1
			1209.4m	N_2	IR	1
	7	=CH deform.	1025.1w	Ar	IR	1
			1028.1w	N_2	IR	1
	8	CH deform.	977.1m	Ar	IR	1
			980.7m	N_2	IR	1
	9	CH deform.	917.7s	Ar	IR	1
			919.4s	N_2	IR	1
	10	=CH deform.	768.0m	Ar	IR	1
			750.7m	N_2	IR	1
	11	Ring deform.	708.4w	Ar	IR	1
	12	Mixed	561.3vw	Ar	IR	1
			562.8vw	N_2	IR	1
	13	CCN deform.	533.9vw	Ar	IR	1
			535.1vw	N_2	IR	1

Reference

[1] G. Maier and J. Endres, Eur. J. Org. Chem. 2535 (2000).

HNC=C=CHCN

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NH stretch	3331.6w	Ar	IR	1
	3	CN stretch	2238.9w	Ar	IR	1
	4	CCN stretch	2070.4vs	Ar	IR	1
	7	Mixed	950.5vw	Ar	IR	1
	8	NH deform.	890.7s	Ar	IR	1
	9	Mixed	830.9vw	Ar	IR	1
	11	Mixed	598.0vw	Ar	IR	1

Reference

[1] G. Maier and J. Endres, Eur. J. Org. Chem. 2535 (2000).

C_6H

$\tilde{B}\,^2\Pi$ $C_{\infty v}$

$T_0 = 18990.1(3)$ gas CR[8,10] $\tilde{B}-\tilde{X}$ 484–528 nm

18854(5) Ne AB[7] $\tilde{B}-\tilde{X}$ 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

$A_{eff} = -23.69$ gas CR[10,11]

$B_0 = 0.046$ CR[8,10,11]

$\tilde{A}\,^2\Sigma^+$ $C_{\infty v}$
$T_0 = 1460(50)$ gas PE[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	C≡C stretch	2202(70)	gas	PE	9

$\tilde{X}\,^2\Pi$ $C_{\infty v}$

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

$A_{eff} - 15.11$ gas $MW^{3-5,11,12}$
$B_0 = 0.046$ $MW^{1-5,11,12}$

C_6D

$\tilde{B}\,^2\Pi$ $C_{\infty v}$
$T_0 = 19041.26$ gas $CR^{8,10,11}$ $\tilde{B}-\tilde{X}$ 524–526 nm
18900(10) Ne AB^8
$A_{eff} = -24.08$ gas CR^{11}
$B_0 = 0.044$ CR^{11}

$\tilde{A}\,^2\Sigma^+$ $C_{\infty v}$
$T_0 = 1452(50)$ gas PE[9]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	C≡C stretch	2202(70)	gas	PE	9

$\tilde{X}\,^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		C≡C stretch	1862.4	Ar	IR	6

$A_{eff} = -15.13$ MW^{11}
$B_0 = 0.044$ MW^{11}

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SiC_5H

$\tilde{X}\,^2\Pi$ $C_{\infty v}$
$B = 0.029$ MW^1

Reference

[1] M. C. McCarthy, A. J. Apponi, C. A. Gottlieb, and P. Thaddeus, J. Chem. Phys. **115**, 870 (2001).

$H(C{\equiv}C)_2CN^+$

$\tilde{C}\,^2\Pi$ $C_{\infty v}$
$T_0 = 27350(160)$ gas PE[1]

$\tilde{B}\,^2\Sigma^+$ $C_{\infty v}$
$T_0 = 21860(160)$ gas PE[1]

$\tilde{A}\,^2\Pi$ $C_{\infty v}$
$T_0 = 17178.04$ gas EF^1AB^4 $\tilde{A}-\tilde{X}$ 580–670 nm
17098(20) Ne AB^2LF^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

$\tau_0 = 15(2)$ ns gas EF^1
$A_0 = -32.58(41)$ gas AB^4
$B_0 = 0.044$ AB^4

$\tilde{X}\,^2\Pi$ $C_{\infty v}$

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

$A_0 = -35.71(41)$ gas AB^4
$B_0 = 0.045$ AB^4

$D(C{\equiv}C)_2CN^+$

$\tilde{A}\,^2\Pi$ $C_{\infty v}$
$T_0 = 17188.50$ gas AB^4
$A_0 = -33.38(57)$ gas AB^4
$B_0 = 0.042$ AB^4

$\tilde{X}\,^2\Pi$ $C_{\infty v}$
$A_0 = -36.47(57)$ AB^4
$B_0 = 0.043$ AB^4

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C_6H^-

Threshold for electron detachment from ground-state $C_6H^- = 30730(120)$ gas PE[1]

C_6D^-

Threshold for electron detachment from ground-state $C_6D^- = 30700(120)$ gas PE[1]

Reference

[1] T. R. Taylor, C. Xu, and D. M. Neumark, J. Chem. Phys. **108**, 10018 (1998).

$H(C{\equiv}C)_2NC$

$\tilde{X}$ $C_{\infty v}$
$B_0 = 0.0467$ MW[1]

Reference

[1] P. Botschwina, Ä. Heyl, W. Chen, M. C. McCarthy, J.-U. Grabow, M. J. Travers, and P. Thaddeus, J. Chem. Phys. **109**, 3108 (1998).

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

$\tilde{a}$ $D_{\infty h}$
$T^a = 13800(80)$ gas PE[11]

$\tilde{X}\ ^1\Sigma_g^+$ $D_{\infty h}$ Structure: DL[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_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	6,7,10
			2127.8	Ar	IR	8
			2120.4	Kr	IR	9
	5	Asym. stretch	1898.376	gas	DL	3
			1897.5	Ne	IR	6,7,10
			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]

[a] From vertical ionization potentials.

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C_6Si

$\tilde{X}$ $C_{\infty v}$ Structure: MW[2]
$B_0 = 0.020$ MW[1,2]

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Si_7

$\tilde{A}$
$T_0 = 9200(400)$ gas PE[4]

$\tilde{X}$ D_{5h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1		435	N_2	Ra	1
	2		385(20)	gas	PE	3,4
			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

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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

$\tilde{B}\ ^2\Pi_u$ $D_{\infty h}$
$T_0 = 20298$ gas MPD[5,7,9] $\tilde{B}-\tilde{X}$ 447–493 nm
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	2038	gas	MPD	5,7,9
			2058(10)	Ne	AB	6
	2		1569(9)	Ne	AB	6
	3		532	gas	MPD	7,9
			575(8)	Ne	AB	6

$\tilde{A}\ ^2\Pi_u$ $D_{\infty h}$
$T_0 = 15930$ gas MPD[5,7,9,10] $\tilde{A}-\tilde{X}$ 496–627 nm
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	1870	gas	MPD	5,7,9,10
			1877(6)	Ne	AB	6
	2		1452	gas	MPD	7,9,10
			1457(5)	Ne	AB	6
	3		543	gas	MPD	5,7,9,10
			562(5)	Ne	AB	6

$A = 0.6(4)$ MPD[10]

$\tilde{X}\ ^2\Pi_g$ $D_{\infty h}$

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	3,8

$A = 27.4(2)$ MPD[10]

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Si_7^-

Threshold for electron detachment from ground-state $Si_7^- = 14930(160)$ gas PE[1]

Reference

[1] C. Xu, T. R. Taylor, G. R. Burton, and D. M. Neumark, J. Chem. Phys. **108**, 1395 (1998).

C_5N_2

$\tilde{A}\ ^3\Sigma_u^-$ $D_{\infty h}$
$T_0 = 22832.7$ gas CR[2] $\tilde{A}-\tilde{X}$ 403–438 nm
22762.9(2)T Ne AB^1LF^1
22737.3(2)T Ar AB^1LF^1 $\tilde{A}-\tilde{X}$ 375–610 nm
22731.8(2)T N_2 AB^1LF^1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1		1958	gas	CR	2
			1961.3(2)T	Ne	AB	1
			1960.5(2)	Ar	AB	1
	8		601.2(2)T	Ar	AB	1
	9		508.5(2)T	Ar	AB	1

$B_0 = 0.028$ CR[2]

$\tilde{X}\,^3\Sigma_g^-$ $D_{\infty h}$

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

$B_0 = 0.028$ CR^2

[a]Center of split transition.

References

[1] A. M. Smith, C. Engel, A. Thoma, G. Schallmoser, B. E. Wurfel, and V. E. Bondybey, Chem. Phys. **184**, 233 (1994).
[2] H. Linnartz, O. Vaizert, P. Cias, L. Grüter, and J. P. Maier, Chem. Phys. Lett. **345**, 89 (2001).

Al_3O_4

$\tilde{A}$

$T_0 = 12260(970)$ gas PE[1]

Reference

[1] H. Wu, X. Li, X.-B. Wang, C.-F. Ding, and L.-S. Wang, J. Chem. Phys. **109**, 449 (1998).

Fe_2O_5

$\tilde{A}$

$T_0 = 1450(400)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			790(60)	gas	PE	1

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			750(50)	gas	PE	1

Reference

[1] H. Wu, S. R. Desai, and L.-S. Wang, J. Am. Chem. Soc. **118**, 5296 (1996); J. Am. Chem. Soc. **118**, 7434 (1996).

$Al_3O_4^-$

Threshold for electron detachment from ground-state $Al_3O_4^- = 28880(650)$ gas PE[1]

Reference

[1] H. Wu, X. Li, X.-B. Wang, C.-F. Ding, and L.-S. Wang, J. Chem. Phys. **109**, 449 (1998).

$Fe_2O_5^-$

Threshold for electron detachment from ground-state $Fe_2O_5^- = 31300(320)$ gas PE[1]

Reference

[1] H. Wu, S. R. Desai, and L.-S Wang, J. Am. Chem. Soc. **118**, 5296 (1996); J. Am. Chem. Soc. **118**, 7434 (1996).

$V(NO)_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO a-stretch	1724.0	Ne	IR	2
			1715.1	Ar	IR	1

References

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **103**, 478 (1999).
[2] L. Andrews and X. Wang, J. Phys. Chem. A **106**, 1196 (2002).

$Nb(NO)_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO stretch	1673.2	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 10025 (1998).

$Ta(NO)_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO stretch	1676.9	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **102**, 10025 (1998).

$Mn(NO)_3$

$\tilde{X}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NO stretch	1824.1	Ar	IR	1
e		NO stretch	1721.8	Ne	IR	2
			1713.2	Ar	IR	1
		MnNO deform.	594.1	Ar	IR	1
			591.0			
		MnN stretch	534.3	Ar	IR	1

References

[1] L. Andrews, M. Zhou, and D. W. Ball, J. Phys. Chem. A **102**, 10041 (1998).
[2] L. Andrews and X. Wang, J. Phys. Chem. A **106**, 1196 (2002).

$Fe(NO)_3$

$\tilde{X}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NO stretch	1794.6	Ar	IR	1
e		NO stretch	1757.8	Ne	IR	1
			1742.6	Ar	IR	1
		FeN stretch	513.4	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 3915 (2000).

$Ru(NO)_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO stretch	1741.1	Ne	IR	1
			1738.9	Ar	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 8689 (2000).

$Os(NO)_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO stretch	1745.5	Ar	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 8689 (2000).

$Co(NO)_3$

$\tilde{X}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NO stretch	1825.6	Ne	IR	1
			1814.6	Ar	IR	1
		CoN stretch	579.3	Ar	IR	1
e		NO stretch	1782.1	Ne	IR	1
			1770.1	Ar	IR	1
		CoN stretch	493.8	Ar	IR	1

Reference

[1] M. Zhou and L. Andrews, J. Phys. Chem. A **104**, 3915 (2000).

$Rh(NO)_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO stretch	1757.7	Ne	IR	1
			1749.0	Ar	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 11897 (2000).

$Ir(NO)_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO stretch	1753.7	Ne	IR	1
			1745.5	Ar	IR	1

Reference

[1] A. Citra and L. Andrews, J. Phys. Chem. A **104**, 11897 (2000).

$Al_2O_5^-$

Threshold for electron detachment from ground-state $Al_2O_5^- = 30260(240)$ gas PE[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Sym. stretch	1170(60)	gas	PE	1

Reference

[1] S. R. Desai, H. Wu, C. M. Rohlfing, and L.-S. Wang, J. Chem. Phys. **106**, 1309 (1997).

$O_2N\text{-}O\text{-}NO_2$

In the gas phase, continuous absorption begins near 420 nm, and has its maximum beyond 200 nm.[11,15]

$\tilde{X}$ C_2[a] Structure: ED[6]MW[13]DL[14]

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,DL	1,2,5,8,11,14
			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 and diode laser spectral observations of Refs. 13 and 14 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.

References

[1] W. G. Fateley, H. A. Bent, and B. Crawford, Jr., J. Chem. Phys. **31**, 204 (1959).
[2] I. C. Hisatsune, J. P. Devlin, and Y. Wada, Spectrochim. Acta **18**, 1641 (1962).
[3] E. L. Varetti and G. C. Pimentel, J. Chem. Phys. **55**, 3813 (1971).
[4] G. R. Smith and W. A. Guillory, J. Mol. Spectrosc. **68**, 223 (1977).
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[14] J. L. Domenech, G. T. Fraser, A. R. Hight Walker, W. J. Lafferty, and R. D. Suenram, J. Mol. Spectrosc. **184**, 172 (1997).
[15] M. H. Harwood, J. B. Burkholder, and A. R. Ravishankara, J. Phys. Chem. A **102**, 1309 (1998).

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[1–3,6,8]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[1–3,6,8]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.

References

[1] D. C. Frost, C. A. McDowell, J. S. Sandhu, and D. A. Vroom, J. Chem. Phys. **46**, 2008 (1967).
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[7] A. J. Yencha, D. B. Thompson, A. J. Cormack, D. R. Cooper, M. Zubek, P. Bolognesi, and G. C. King, Chem. Phys. **216**, 227 (1997).
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SF_6^-

$\tilde{X}$ O_h

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
t_{1u}	3		619.8T	Ne	IR	1

Reference

[1] C. L. Lugez, M. E. Jacox, R. A. King, and H. F. Schaefer III, J. Chem. Phys. **108**, 9639 (1998).

8.14. Eight-Atomic Molecules

$GaBH_6$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	BH_2 s-stretch	2482m	gas	IR	1
			2482m	N_2	IR	1
			2465m			
	2	GaH_2 s-stretch	1982w	gas	IR	1
			1965m	N_2	IR	1
	3	Mixed	1937m	gas	IR	1
			1925m	N_2	IR	1
	4	Mixed	1435s	gas	IR	1
			1432s	N_2	IR	1
			1422s			
	5	BH_2 scissors	1130m	gas	IR	1
			1125m	N_2	IR	1
			1120m			
			1105s			
	6	GaH_2 scissors	729m	gas	IR	1
			730s	N_2	IR	1
	7	Mixed	468m	gas	IR	1
			460s	N_2	IR	1
			452m			
b_1	10	Mixed	2007m	gas	IR	1
			2018s	N_2	IR	1
	11	Mixed	1315w	gas	IR	1
			1330w	N_2	IR	1
			1290m			
	12	BH_2 wag	782vw	gas	IR	1
			770w	N_2	IR	1
	13	GaH_2 wag	544m	gas	IR	1
			570m	N_2	IR	1
			560m			
b_2	14	BH_2 a-stretch	2558m	gas	IR	1
			2558m	N_2	IR	1
			2536m			
	15	GaH_2 a-stretch	2005m	gas	IR	1
			1992s,br	N_2	IR	1
	16	BH_2 rock	930vw	gas	IR	1
	17	GaH_2 rock	620w	gas	IR	1
			630w	N_2	IR	1
			612w			

$GaBD_6$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	BD_2 s-stretch	1823m	gas	IR	1
	2	GaD_2 s-stretch	1428w	gas	IR	1
	3	Mixed	1383m	gas	IR	1
	4	Mixed	1060s	gas	IR	1
	5	BD_2 scissors	850w	gas	IR	1
	6	GaD_2 scissors	527m	gas	IR	1
	7	Mixed	412s	gas	IR	1
b_1	10	Mixed	1450m	gas	IR	1
	11	Mixed	980w	gas	IR	1
	13	GaD_2 wag	421s	gas	IR	1
b_2	14	BD_2 a-stretch	1933.5m	gas	IR	1
	15	GaD_2 a-stretch	1447m	gas	IR	1
	16	BD_2 rock	670w	gas	IR	1
	17	GaD_2 rock	442m	gas	IR	1

Reference

[1] A. J. Downs, T. M. Greene, E. Johnsen, P. T. Brain, C. A. Morrison, S. Parsons, C. R. Pulham, D. W. H. Rankin, K. Aarset, I. M. Mills, E. M. Page, and D. A. Rice, Inorg. Chem. **40**, 3482 (2001).

$ZnC_2H_5^+$

$\tilde{X}\,^1A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	6	CH_3 bend	1380(3)	gas	TPE	1
	7	Wag	1107(3)	gas	TPE	1
	8	CC stretch	1015(3)	gas	TPE	1
	9	Wag	933(3)	gas	TPE	1
	10	ZnC stretch	424(3)	gas	TPE	1
	11	ZnCC bend	217(3)	gas	TPE	1
a''	17	CH_2 rock	683(3)	gas	TPE	1
	18	CH_3 torsion	238(3)	gas	TPE	1

Reference

[1] M. B. Pushkarsky, V. L. Stakhursky, and T. A. Miller, J. Phys. Chem. A **104**, 9184 (2000).

ZnC_2H_5

$\tilde{A}\,^2A'$ C_s

$T_0 = 22515(5)$ gas LF[1]MPI[2] $\tilde{A}-\tilde{X}$ 425–475 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	7	Wag	1087(3)	gas	MPI	2
	8	CC stretch	1011(5)	gas	LF,MPI	1,2
	10	ZnC stretch	424(5)	gas	LF,MPI	1,2
	11	ZnCC bend	245(5)	gas	LF,MPI	1,2
a''	18	CH_3 torsion	218HT	gas	MPI	2

$\tilde{X}\,^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	7	Wag	1109(5)T	gas	LF	1
	8	CC stretch	987(5)T	gas	LF	1
	9	Wag	915(5)T	gas	LF	1
	10	ZnC stretch	387(5)	gas	LF	1
	11	ZnCC bend	180(5)	gas	LF	1

References

[1] S. J. Pooley and A. M. Ellis, J. Mol. Spectrosc. **185**, 48 (1997).
[2] M. B. Pushkarsky, V. L. Stakhursky, and T. A. Miller, J. Phys. Chem. A **104**, 9184 (2000).

CdC_2H_5

$\tilde{A}$ C_s

The absence of structure in the excitation spectrum of this transition suggests[1] that predissociation occurs in the $\tilde{A}$ state of CdC_2H_5.

$T_0 = 21374(5)$ gas LF[1] $\tilde{A}-\tilde{X}$ 467–488 nm

$\tilde{X}\,^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			880(5)	gas	LF	1
	10	CdC stretch	278(5)	gas	LF	1
	11	CdCC bend	157(5)	gas	LF	1

Reference

[1] A. J. Bezant and A. M. Ellis, J. Mol. Spectrosc. **185**, 54 (1997).

$H_2BC_2H_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BH_2 a-stretch	2570.2	Ar	IR	1
			1536.8	Ar	IR	1
			1414.1w	Ar	IR	1
			1213.9	Ar	IR	1
			1031.3w	Ar	IR	1

$D_2BC_2D_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1472.5	Ar	IR	1

Reference

[1] L. Andrews, D. V. Lanzisera, P. Hassanzadeh, and Y. Hannachi, J. Phys. Chem. A **102**, 3259 (1998).

$CH_3B{=}CH_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		B=C stretch	1631.2	Ar	IR	1

Reference

[1] L. Andrews, D. V. Lanzisera, P. Hassanzadeh, and Y. Hannachi, J. Phys. Chem. A **102**, 3259 (1998).

$GaNH_2CH_3^+$

$\tilde{X}\,^1A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		NH_3 rock	515T	gas	TPE	1
		GaN stretch	299 (ω)	gas	TPE	1
		Bend	124 (ω)	gas	TPE	1

Reference

[1] S. Li, G. K. Rothschopf, D. Pillai, B. R. Sohnlein, B. M. Wilson, and D.-S. Yang, J. Chem. Phys. **115**, 7968 (2001).

$CH_2CHCH_2^+$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	5	CH_2 s-rock	1239(7)	gas	TPE	2
	6	C_3 s-stretch	1027(7)	gas	TPE	2
	7	C_3 bend	431(7)	gas	PE,TPE	1,2
a_2	9	CH_2 a-twist	612(7)	gas	TPE	2
b_1	10	CH OPLA	1078(7)	gas	TPE	2
	12	CH_2 s-twist	274(7)	gas	TPE	2
b_2	17	C_3 a-stretch	1236(7)	gas	TPE	2

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$GaNH_2CH_3$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		GaNC bend	93	gas	TPE	1

Reference

[1] S. Li, G. K. Rothschopf, D. Pillai, B. R. Sohnlein, B. M. Wilson, and D.-S. Yang, J. Chem. Phys. **115**, 7968 (2001).

CH_2CHCH_2

8*s* C_{2v}
$T_0 = 63398(5)$ gas MPI[25]

7*s* C_{2v}
$T_0 = 62620(5)$ gas MPI[25]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	7	C_3 bend	429(5)	gas	MPI	25

6*s* C_{2v}
$T_0 = 61337(5)$ gas MPI[25]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	7	C_3 bend	439(5)	gas	MPI	25

4*s* C_{2v}
$T_0 = 53708(5)$ gas MPI[25]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	6	C_3 stretch	1034(5)	gas	MPI	25
	7	C_3 bend	429(5)	gas	MPI	25

3*d* C_{2v}
$T_0 = 52114(5)$ gas MPI[25]

$\tilde{D}\,^2B_2$ 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

$\tau_0 = 12$ ps gas MPI[20]

$\tilde{C}\,^2B_1$ C_{2v} Structure: MPI[18]
$T_0 = 40305.5(5)$ gas AB^2MPI[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

$\tau_0 = 15$ ps gas MPI[20]
$A_0 \cong 1.619$; $B_0 \cong 0.351$; $C_0 \cong 0.288$ MPI[11]

$\tilde{B}\,^2A_1$ (3*s*) 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

$\tau_0 = 20$ ps gas MPI[20]

$\tilde{A}\,^2B_1$ C_2
$T_0 = 24485$ gas AB^1CR[24] $\tilde{A}-\tilde{X}$ 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			1241	gas	AB,CR	1,24
			1005	gas	AB,CR	1,24
			908	gas	AB,CR	1,24
			359	gas	AB,CR	1,24

$\tilde{X}\,^2A_2$ C_{2v} Structure: DL[12]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH_2 s-stretch	3113.98	gas	LD,CC	21,22
			3109wm	Ar	IR	4–6,26
	2	CH stretch	3052w	Ar	IR	4–6,26
	3	CH stretch	3027vw	Ar	IR	26
	4	CH_2 scissors	1488(4)	gas	Ra	10,15
			1478w	Ar	IR	4–6,26
	5	Mixed	1245(3)	gas	Ra	10,15
			1242vw	Ar	IR	4–6,26
	6	Mixed	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
			983.6wm	Ar	IR	4–6,9,26
	11	CH_2 s-wag	801.72	gas	DL,PE	12,19
			801.1vs	Ar	IR	3–6,9,26
	12	CH_2 s-twist	518(4)	gas	MPI,Ra	7,8,10,15
						16,18
			510.1wm	Ar	IR	4–6,9,26
b_2	13	CH_2 a-stretch	3110.60	gas	LD,CC	21–23
			3107w	Ar	IR	26
	14	CH stretch	3020w	Ar	IR	4–6,26
	15	CH_2 scissors	1464wm	Ar	IR	4–6,26
	16	Mixed	1390vw	Ar	IR	4–6,26
	17	C_3 stretch	1182	Ar	IR	6,26

$A_0=1.802$; $B_0=0.346$; $C_0=0.290$ DL[12]LD[21,23]

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	2285w	Ar	IR	6,26
	3	CD stretch	2215w	Ar	IR	6
	4	CD_2 scissors	1272(8)	gas	Ra	17
			1263	Ar	IR	6,26
	5	Mixed	1020(8)	gas	Ra	17
			1018w	Ar	IR	6,26
	6	Mixed	835(20)	gas	MPI,PE	7,19
			844vw	Ar	IR	26
	7	C_3 deform.	350(8)	gas	MPI,Ra	7,17–19
					PE	
a_2	9	CD_2 torsion	372H	gas	Ra	17
b_1	10	OPLA	762H	gas	Ra	17
			767w	Ar	IR	26
	11	Deform.	678(10)H	gas	PR	19
			646.5vs	Ar	IR	6,9,26
	12	Deform.	403(8)	gas	Ra,MPI	17,18
b_2	14	CD_2 stretch	2209	Ar	IR	6,26
	15	CD_2 scissors	1387wm	Ar	IR	26
	16	Mixed	1062w	Ar	IR	6,26
	17	Mixed	900w	Ar	IR	26

[a]Evidence presented in Refs. 14 and 18 suggests that this state may be slightly nonplanar.

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$C_2H_3NH_2$

$\tilde{X}$ C_1[a] Structure: MW[3–5]IR[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	5	CH stretch	2987	gas	IR	2
			2976			
	6	C=C stretch	1672	gas	IR	2
			1668			
	7	NH_2 scissors	1625T	gas	IR	2
	8	CH_2 scissors	1454	gas	IR	2
	10	C–N stretch	1260	gas	IR	2
			1248			
	11	NH_2 rock	1084	gas	IR	2
			1078			
	12		1046	gas	IR	2
			1039			
	14		812s	gas	IR	2
			805s			
	15		674.44	gas	IR	2,4,5,7
	17		469.91	gas	IR	4,5,7
	18	NH_2 wag	614.76[b]	gas	IR	2,4,5,7
			569.58[c]	gas	IR	2,4,5,7
			331.92[d]	gas	IR	4,5,7
			286.71[e]	gas	IR	4,5,7

$A_0 = 1.879$; $B_0 = 0.335$; $C_0 = 0.286$ 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 45.5 cm^{-1}.
[b]$1^- - 0^+$.
[c]$1^- - 0^-$.
[d]$1^+ - 0^+$.
[e]$1^+ - 0^-$.

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$CH_3CH_2O^+$

$T^a = 22190(120)$ gas PE[1]

$\tilde{b}\,^1A''$ C_s
$T^a = 9280(120)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1170(60)	gas	PE	1

$\tilde{a}\,^1A'$ C_s
$T^a = 5320(120)$ gas PE[1]

$\tilde{X}\,^3A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1260(60)	gas	PE	1

[a]From vertical ionization potentials.

Reference

[1] J. Wang, Z. Sun, X. Zhu, M. Ge, and D. Wang, Chem. Phys. Lett. **340**, 98 (2001).

CH_3CHOH^+

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1600(30)	gas	PE	1

CD_3CDOD^+

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1590(30)	gas	PE	1

Reference

[1] J. M. Dyke, A. P. Groves, E. P. F. Lee, and M. H. Zamanpour Niavaran, J. Phys. Chem. A **101**, 373 (1997).

$C_2H_5S^+$

$\tilde{B}\,^3A'$ C_s
$T^a = 34940(240)$ gas PE[2]

$\tilde{A}\,^3A''$ C_s
$T^a = 26380(240)$ gas PE[2]

$\tilde{b}\,^1A''$ C_s
$T^a = 11460(240)$ gas PE[2]

$\tilde{a}\,^1A'$ C_s
$T^a = 9920(240)$ gas PE[2]

$\tilde{X}\,^3A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CS stretch	670(30)	gas	PE	1,2

[a]From vertical ionization potentials.

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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

$\tau_0 = 1.7(2)\ \mu s$ gas LF^3EM^4
$A_0 = 1.117(2)$; $B_0 = 0.311(2)$; $C_0 = 0.268(2)$ LF^6

$\tilde{A}\,^2A'$ C_s
$T_0 = 355(10)$ gas PE[7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			685T	gas	PE	7

$\tilde{X}\,^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CH_2 wag	1370	gas	LF	3
		CH_2 scissors	1295(10)	gas	PE	7
		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

C_2D_5O

$\tilde{A}\,^2A'$ C_s
$T_0 = 275(10)$ gas PE[7]

[a] Assignment to overtone of CCO bend cannot be excluded.

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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

$\tau = 75$ ns gas LF^1

$\tilde{A}\,^2A'$ C_s
$T_0 = 240(30)$ gas PE^3

$\tilde{X}\,^2A''$ 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

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$C_2H_5O^-$

Threshold for electron detachment from ground-state $C_2H_5O^-$ = 13810(30) gas PE^{1-3}

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1250(400)	gas	PE	1

$C_2D_5O^-$

Threshold for electron detachment from ground-state $C_2D_5O^-$ = 13710(30) gas PE[1–3]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1200(400)	gas	PE	1

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$HFeCH{=}C{=}CH_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C_3 a-stretch	1832.0	Ar	IR	1,2
		FeH stretch	1737.8	Ar	IR	1,2
		CH_2 scissors	1413.8	Ar	IR	1
		CH_2 wag	820.2	Ar	IR	1,2
		FeC stretch	431.4	Ar	IR	1,2
			428.7			

$DFeCH{=}C{=}CD_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C_3 a-stretch	1799.0	Ar	IR	1,2
		FeD stretch	1250.0	Ar	IR	1,2
		CD_2 wag	585.5	Ar	IR	1,2

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$HCCCH_2FeH$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3314.4	Ar	IR	1,2
		FeH stretch	1697.5	Ar	IR	1,2

$DCCCD_2FeD$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		FeD stretch	1204.3	Ar	IR	1,2

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$HFeCCCH_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_3 s-stretch	2881.8	Ar	IR	1,2
		CC stretch	2117.1	Ar	IR	1,2
			2114.7			
			2110.5			
		FeH stretch	1721.9	Ar	IR	1,2
		CH_3 deform.	1373.8	Ar	IR	2
		CH_3 rock	984.9	Ar	IR	1,2
		C–C stretch	911.0	Ar	IR	1,2

$DFeCCCD_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CC stretch	2113.5	Ar	IR	1,2
			2109.5			
		CD_3 s-stretch	2036.9	Ar	IR	2
		FeD stretch	1239.0	Ar	IR	1,2
			1236.2			
			1234.9			
		CD_3 deform.	1113.2	Ar	IR	1,2
			1112.2			
		C–C stretch	897.0	Ar	IR	1,2
			895.1			

References

[1] D. W. Ball, R. G. S. Pong, and Z. H. Kafafi, J. Am. Chem. Soc. **115**, 2864 (1993).
[2] D. W. Ball, R. G. S. Pong, and Z. H. Kafafi, J. Phys. Chem. **98**, 10720 (1994).

CH_3FeCCH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3328.1	Ar	IR	1
		CH_3 stretch	2963.8	Ar	IR	1
		CC stretch	1977.4	Ar	IR	1,2
			1975.5			
			1965.5			
		CH_3 deform.	1455.6	Ar	IR	1
			1439.4			
		CH_3 s-deform.	1163.7	Ar	IR	1,2
			1161.9			
		CH bend	669.7	Ar	IR	1,2
		FeC stretch	566.0	Ar	IR	1,2
			564.7			
		CH_3 rock	551.0	Ar	IR	1,2
			540.8			

CD_3FeCCD

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CC stretch	1864.3	Ar	IR	1,2
			1861.4			
			1851.5			
			1850.8			
		CD_3 s-deform.	912.5	Ar	IR	2
		FeC stretch	520.4	Ar	IR	1,2
			519.2			
		CD_3 rock	421.8	Ar	IR	2
			416.4			

References

[1] D. W. Ball, R. G. S. Pong, and Z. H. Kafafi, J. Am. Chem. Soc. **115**, 2864 (1993).
[2] D. W. Ball, R. G. S. Pong, and Z. H. Kafafi, J. Phys. Chem. **98**, 10720 (1994).

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
			1237.7	Xe	IR	9
		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
			573.3	Xe	IR	9

cyc-C_4D_4

$\tilde{X}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{1u}		C=C stretch	1456w	Ar	IR	4
b_{2u}		CD deform.	1043wm	Ar	IR	4
		Ring deform.	609wm	Ar	IR	4
b_{3u}		CD OPLA	421vs	Ar	IR	4

References

[1] O. L. Chapman, C. L. McIntosh, and J. Pacansky, J. Am. Chem. Soc. **95**, 614 (1973).
[2] C. Y. Lin and A. Krantz, J. Chem. Soc., Chem. Commun. 1111 (1972).
[3] G. Maier, H.-G. Hartan, and T. Sayrac, Angew. Chem. **88**, 252 (1976); Angew. Chem., Int. Ed. Engl. **15**, 226 (1976).
[4] S. Masamune, F. A. Souto-Bachiller, T. Machiguchi, and J. E. Bertie, J. Am. Chem. Soc. **100**, 4889 (1978).
[5] G. Maier, Angew. Chem. **100**, 317 (1988); Angew. Chem. Int. Ed. Engl. **27**, 309 (1988).
[6] A. M. Orendt, B. R. Arnold, J. G. Radziszewski, J. C. Facelli, K. D. Malsch, H. Strub, D. M. Grant, and J. Michl, J. Am. Chem. Soc. **110**, 2648 (1988).
[7] B. R. Arnold, J. G. Radziszewski, A. Campion, S. S. Perry, and J. Michl, J. Am. Chem. Soc. **113**, 692 (1991).
[8] B. R. Arnold and J. Michl, J. Phys. Chem. **97**, 13348 (1993).
[9] G. Maier and C. Lautz, Eur. J. Org. Chem. **1998**, 769.

$H_2C=C=CHCH$:

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C_3 a-stretch[a]	1942	Ar	IR	1
		C_3 a-stretch[a]	1881	Ar	IR	1
			877	Ar	IR	1

[a] It is likely that more than one stereoisomer contributes to the observed absorptions.

Reference

[1] R. Wrobel, W. Sander, D. Cremer, and E. Kraka, J. Phys. Chem. A **104**, 3819 (2000).

$H_3C(cyc\text{-}CSiCH)$

In an argon matrix, irradiation at 313 nm results in isomerization to $H_3CCCSiH$.[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3014.9wm	Ar	IR	1
		CH_3 stretch	2973.4m	Ar	IR	1
			2963.6			
		CH_3 stretch	2929.5m	Ar	IR	1
			2915.3			
		CH_3 stretch	2850.0wm	Ar	IR	1
		C=C stretch	1562.8wm	Ar	IR	1
		CH_3 deform.	1440.5wm	Ar	IR	1
		CH_3 deform.	1433.9wm	Ar	IR	1
		CH_3 deform.	1360.9w	Ar	IR	1
		CH_3 rock	1140.4wm	Ar	IR	1
		CH_3 rock	1016.9w	Ar	IR	1
		CH bend	964.1wm	Ar	IR	1
		CC stretch	953.3s	Ar	IR	1
		CH bend	823.4m	Ar	IR	1
		Si–(CH) stretch	744.0vs	Ar	IR	1
		Si–(CCH_3) stretch	576.5m	Ar	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, J. Jung, H. Pacl, and H. Egenolf, Eur. J. Org. Chem. **1998**, 1297.

$cyc\text{-}CH_2CHCHSi$

In an argon matrix, irradiation at 405 or 366 nm results in isomerization to $H_2CCHCHSi$, whereas irradiation at 313 nm results in isomerization to $H_2CCCHSiH$.[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3062.6w	Ar	IR	1
		CH_2 stretch	3017.3w	Ar	IR	1
		CH_2 stretch	2972.0m	Ar	IR	1
		CH stretch	2931.5w	Ar	IR	1
		CH_2 scissors	1422.1w	Ar	IR	1
		CH deform.	1405.0w	Ar	IR	1
		CH deform.	1247.7vw	Ar	IR	1
		CH_2 twist	1129.2wm	Ar	IR	1
		CH deform.	1028.6wm	Ar	IR	1
		CC stretch	993.0w	Ar	IR	1
		CH_2 wag	970.2wm	Ar	IR	1
		CH deform.	879.2m	Ar	IR	1
		CH deform.	823.2s	Ar	IR	1
		SiC stretch	765.0vs	Ar	IR	1
		SiCC deform.	719.8wm	Ar	IR	1
		CCC deform.	549.3w	Ar	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, J. Jung, H. Pacl, and H. Egenolf, Eur. J. Org. Chem. **1998**, 1297.

$H_3CCHCSi$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SiCC stretch	1681.4	Ar	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, J. Jung, H. Pacl, and H. Egenolf, Eur. J. Org. Chem. **1998**, 1297.

$H_2CCHCHSi$

In an argon matrix, irradiation at 313 nm results in isomerization to $H_2CCCHSiH$.[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_2 stretch	3103.4m	Ar	IR	1
		CH_2 stretch	3052.5w	Ar	IR	1
		CH stretch	3040.3vw	Ar	IR	1
		CH stretch	3010.6w	Ar	IR	1
		C=C stretch	1594.6m	Ar	IR	1
		CC stretch	1167.5m	Ar	IR	1
		CH bend	979.7m	Ar	IR	1
		CH_2 wag	881.0vs	Ar	IR	1
			877.3			
		CH_2 twist	541.2w	Ar	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, J. Jung, H. Pacl, and H. Egenolf, Eur. J. Org. Chem. **1998**, 1297.

$H_3CCCSiH$

In an argon matrix, irradiation at 313 or 254 nm results in isomerization to $H_3CCHCSi$ and $H_3CSiCCH$.[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_3 stretch	2982.0w	Ar	IR	1
		CH_3 stretch	2933.0w	Ar	IR	1
		CH_3 stretch	2860w	Ar	IR	1
		C≡C stretch	2151.1s	Ar	IR	1
			2142.7			
		SiH stretch	1970.8vs	Ar	IR	1
			1964.1			
		CH_3 deform.	1442.5w	Ar	IR	1
		CH_3 deform.	1437.6vw	Ar	IR	1
		SiH bend	826.7m	Ar	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, J. Jung, H. Pacl, and H. Egenolf, Eur. J. Org. Chem. **1998**, 1297.

$H_3CSiCCH$

In an argon matrix, irradiation at wavelengths longer than 385 nm results in isomerization to $H_2CSiHCCH$.[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3308.6vs	Ar	IR	1
		C≡C stretch	2001.2ms	Ar	IR	1
		CH_3 deform.	1430.0w	Ar	IR	1
		CH_3 deform.	1218.8m	Ar	IR	1
		Si–CH_3 stretch	620.2s	Ar	IR	1
		Si–CCH stretch	588.4vs	Ar	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, J. Jung, H. Pacl, and H. Egenolf, Eur. J. Org. Chem. **1998**, 1297.

$H_2CCCHSiH$

In an argon matrix, irradiation at 313 or 254 nm results in isomerization to $H_3CCHCSi$ and $H_3CSiCCH$.[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_2 stretch	3023.9vw	Ar	IR	1
		CH stretch	2980.2vw	Ar	IR	1
		SiH stretch	1993.8vs	Ar	IR	1
			1988.3			
		CCC stretch	1915.5vs	Ar	IR	1
			1908.0			
		SiCC stretch	1184.4wm	Ar	IR	1
			1179.4			
		SiH bend	860.4wm	Ar	IR	1
		CH_2 wag	798.4m	Ar	IR	1
		HSiCH deform.	682.3wm	Ar	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, J. Jung, H. Pacl, and H. Egenolf, Eur. J. Org. Chem. **1998**, 1297.

$H_2CSiHCCH$

In an argon matrix, irradiation at 313 nm results in isomerization to $H_3CSiCCH$.[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		≡CH stretch	3314.5vs	Ar	IR	1
		SiH stretch	2224.0s	Ar	IR	1
		C≡C stretch	2047.5s	Ar	IR	1
		CH_2 scissors	1331.6m	Ar	IR	1
		SiH bend	858.2vs	Ar	IR	1
		CH_2 wag	716.2m	Ar	IR	1
		CH_2 rock	689.5s	Ar	IR	1
		≡CH bend	669.2ms	Ar	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, J. Jung, H. Pacl, and H. Egenolf, Eur. J. Org. Chem. **1998**, 1297.

$H_3Si(cyc\text{-}CSiCH)$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3017.2w	Ar	IR	1
		SiH stretch	2190T	Ar	IR	1
		CC stretch	1498.8wm	Ar	IR	1
			1484.0			
		CH deform.	1029.3	Ar	IR	1
			1026.6			
		SiH deform.	953.1wm	Ar	IR	1
		SiH deform.	921.8T	Ar	IR	1
		SiH deform.	919.3vs	Ar	IR	1
		SiC stretch	840.8wm	Ar	IR	1
		SiC stretch	749.7wm	Ar	IR	1
		SiCC deform.	665.7wm	Ar	IR	1
		Mixed	650.6wm	Ar	IR	1
			655.5			

$D_3Si(cyc\text{-}CSiCD)$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SiD stretch	1600T	Ar	IR	1
		CC stretch	1472.5w	Ar	IR	1
		CD deform.	911.2w	Ar	IR	1
		SiC stretch	803.2ms	Ar	IR	1
		SiD deform.	695.4	Ar	IR	1
		SiD deform.	694.4vs	Ar	IR	1
		SiD deform.	677.9w	Ar	IR	1
		SiC stretch	652.0w	Ar	IR	1
		SiCC deform.	522.0w	Ar	IR	1
		CD deform.	508.3	Ar	IR	1
			505.8			

Reference

[1] G. Maier, H. P. Reisenauer, and A. Meudt, Eur. J. Org. Chem. **1998**, 1291.

$HSiCCSiH_3$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SiH stretch	2200Tw	Ar	IR	1
		SiH stretch	2030.2vw	Ar	IR	1
			2006.6			
		SiH deform.	938.3vw	Ar	IR	1
		SiH deform.	922.5vs	Ar	IR	1
		SiH deform.	808.0vw	Ar	IR	1
		SiC stretch	784.0s	Ar	IR	1
			780.0			
		Mixed	680.2vw	Ar	IR	1

$DSiCCSiD_3$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SiD stretch	1600Tw	Ar	IR	1
		SiD stretch	1477.0vw	Ar	IR	1
			1458.7			
		SiC stretch	782.8vs	Ar	IR	1
		SiD deform.	686.1s	Ar	IR	1
		SiD deform.	622.0vw	Ar	IR	1
		Mixed	531.0vw	Ar	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, and A. Meudt, Eur. J. Org. Chem. **1998**, 1291.

$HCCSiSiH_3$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3294.1wm	Ar	IR	1
			3291.1			
		SiH_3 stretch	2168T	Ar	IR	1
		SiH_3 deform.	856.0vs	Ar	IR	1
			854.5			
		HCC deform.	690.1wm	Ar	IR	1
		SiC stretch	586.0m	Ar	IR	1

Reference

[1] G. Maier, H. P. Reisenauer, and A. Meudt, Eur. J. Org. Chem. **1998**, 1291.

H_2C_5H

$\tilde{X}$ C_{2v}

$1/2(B_0+C_0)=0.072$ MW[1]

Reference

[1] W. Chen, S. E. Novick, M. C. McCarthy, and P. Thaddeus, J. Chem. Phys. **109**, 10190 (1998).

$C_6H_2^+$

$\tilde{B}\,^2\Pi_u$ $D_{\infty h}$

$T_0=27350(160)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			650(80)	gas	PE	1

$\tilde{A}\,^2\Pi_g$ $D_{\infty h}$

$T_0=16654.69$ gas $EF^{2,3}LF^3AB^{6,7}$ $\tilde{A}-\tilde{X}$ 485–725 nm

16570 Ne LF^4AB^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	617.8	gas	LF,EF AB	2,3,7
			620	Ne	LF,AB	4,5
Π_g	10	Skel. bend	244T	gas	LF	3
			248H	Ne	LF	4

$\tau_0=17(2)$ ns gas EF^2

$A_0=-28.41(28)$ AB^6

$B_0=0.044$ AB^6

$\tilde{X}\,^2\Pi_u$ $D_{\infty h}$

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

$A_0=-31.40(28)$ AB^6

$B_0=0.045$ AB^6

$C_6D_2^+$

$\tilde{A}\,^2\Pi_g$ $D_{\infty h}$
$T_0 = 16686.51$ gas AB^6
$A_0 = -28.40(49)$ AB^6
$B_0 = 0.040$ AB^6

$\tilde{X}\,^2\Pi_u$ $D_{\infty h}$
$A_0 = -31.31(49)$ AB^6
$B_0 = 0.041$ AB^6

References

[1] F. Brogli, E. Heilbronner, V. Hornung, and E. Kloster-Jensen, Helv. Chim. Acta **56**, 2171 (1973).
[2] M. Allan, E. Kloster-Jensen, and J. P. Maier, Chem. Phys. **17**, 11 (1976).
[3] D. Klapstein, R. Kuhn, J. P. Maier, M. Ochsner, and W. Zambach, J. Phys. Chem. **88**, 5176 (1984).
[4] A. M. Smith, J. Agreiter, M. Härtle, C. Engel, and V. E. Bondybey, Chem. Phys. **189**, 315 (1994).
[5] P. Freivogel, J. Fulara, D. Lessen, D. Forney, and J. P. Maier, Chem. Phys. **189**, 335 (1994).
[6] W. E. Sinclair, D. Pfluger, H. Linnartz, and J. P. Maier, J. Chem. Phys. **110**, 296 (1999).
[7] D. Pfluger, W. E. Sinclair, H. Linnartz, and J. P. Maier, Chem. Phys. Lett. **313**, 171 (1999).

H_2C_6:

$\tilde{X}$ C_{2v}
$A_0 = 8.95$; $B_0 = 0.0450$; $C_0 = 0.0447$ 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).

$F_2C{=}(cyc\text{-}C_3H_2)$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		C=C stretch	1906.9wm	Ar	IR	1
		Ring stretch	1563.2wm	Ar	IR	1
		Deformation	1198.1vs	Ar	IR	1
		Breathing	705w	Ar	IR	1
b_1		H_2 deform.	623.6wm	Ar	IR	1
b_2		CF_2 a-stretch	1215s	Ar	IR	1
		HCCH rock	1038.3w	Ar	IR	1

Reference

[1] C. Kötting, W. Sander, and M. Senzlober, Chem. Eur. J. **4**, 2360 (1998).

$F_2C{=}CHCCH$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1731.1vs	Ar	IR	1
			1348.1ms	Ar	IR	1
			1223.3m	Ar	IR	1
			914.2wm	Ar	IR	1
			659.0w	Ar	IR	1

Reference

[1] C. Kötting, W. Sander, and M. Senzlober, Chem. Eur. J. **4**, 2360 (1998).

$F_2C{=}C{=}C{=}CH_2$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2114.3s	Ar	IR	1
			1703.5vs	Ar	IR	1
			1404.8m	Ar	IR	1
			1239.4s	Ar	IR	1
			1167.1m	Ar	IR	1

Reference

[1] C. Kötting, W. Sander, and M. Senzlober, Chem. Eur. J. **4**, 2360 (1998).

C_7H

$\tilde{X}\,^2\Pi_{1/2}$ $C_{\infty v}$
$A_{\text{eff}} = 26.17$; $B_0 = 0.029$ $MW^{1,2}$

C_7D

$\tilde{X}\,^2\Pi_{1/2}$ $C_{\infty v}$
$A_{\text{eff}} = 26.15$; $B_0 = 0.028$ $MW^{1,2}$

References

[1] M. J. Travers, M. C. McCarthy, C. A. Gottlieb, and P. Thaddeus, Astrophys. J. **465**, L77 (1996).
[2] M. C. McCarthy, M. J. Travers, A. Kovács, C. A. Gottlieb, and P. Thaddeus, Astrophys. J. Suppl. **113**, 105 (1997).

SiC_6H

$\tilde{X}\,^2\Pi$ $C_{\infty v}$
$B = 0.019$ MW^1

Reference

[1] M. C. McCarthy, A. J. Apponi, C. A. Gottlieb, and P. Thaddeus, J. Chem. Phys. **115**, 870 (2001).

HC_6N

$\tilde{A}\,^3\Sigma^-$ $C_{\infty v}$
$T_0 = 21208.60(5)$ gas CR[2] $\tilde{A}-\tilde{X}$ 432–472 nm
21181(10) Ne AB[2] $\tilde{A}-\tilde{X}$ 432–472 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		CC stretch	1942.5(5)	gas	CR	2
			1950(15)	Ne	AB	2
Π		Bend	234HT	Ne	AB	2

$\tilde{X}\,^3\Sigma^-$ $C_{\infty v}$
$B_0 = 0.028$ MW[1]

DC_6N

$\tilde{A}\,^3\Sigma^-$ $C_{\infty v}$
$T_0 = 21282.10(5)$ gas CR[2] $\tilde{A}-\tilde{X}$ 431–471 nm
21239(10) Ne AB[2] $\tilde{A}-\tilde{X}$ 431–471 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		CC stretch	1926.0	gas	CR	2
			1935(15)	Ne	AB	2
Π		Bend	172HT	Ne	AB	2

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[1] V. D. Gordon, M. C. McCarthy, A. J. Apponi, and P. Thaddeus, Astrophys. J. **540**, 2886 (2000).
[2] O. Vaizert, T. Motylewski, M. Wyss, E. Riaplov, H. Linnartz, and J. P. Maier, J. Chem. Phys. **114**, 7918 (2001).

(*cyc*-HC_3)CCCN

$\tilde{X}$ C_s
$A_0 = 1.150$; $B_0 = 0.035$; $C_0 = 0.034$ MW[1]

Reference

[1] M. C. McCarthy, J.-U. Grabow, M. J. Travers, W. Chen, C. A. Gottlieb, and P. Thaddeus, Astrophys. J. **513**, 305 (1999).

Nb_8

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			180(15)	gas	PE	1

Reference

[1] T. P. Marcy and D. G. Leopold, Int. J. Mass Spectrom. **195/196**, 653 (2000).

Nb_8^-

Threshold for electron detachment from ground-state $Nb_8^- = 12210(65)$ gas PE[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			165(20)	gas	PE	1

Reference

[1] T. P. Marcy and D. G. Leopold, Int. J. Mass Spectrom. **195/196**, 653 (2000).

Ag_8

The resonant two-photon ionization of helium clusters containing Ag_8 shows a narrow peak at 31950 (3.96 eV) and a broader peak at 32190 (3.99 eV).[3]

In solid neon, the corresponding absorption maximum for Ag_8 has been observed[2] at 31550 (3.91 eV). In solid argon, this maximum appears[1] at 31390 (3.89 eV), and a fluorescence maximum has been detected[4] at 31220 (3.87 eV).

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[1] W. Harbich, S. Fedrigo, and J. Buttet, Z. Phys. D **26**, 138 (1993).
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[4] C. Félix, C. Sieber, W. Harbich, J. Buttet, I. Rabin, W. Schulze, and G. Ertl, Phys. Rev. Lett. **86**, 2992 (2001).

C_8

(2) $^3\Sigma_u^-$ $D_{\infty h}$
$T_0 = 36071(26)$ Ne AB[9]

$T_0 = 32934(22)$ Ne AB[9] $D_{\infty h}$ 285–304 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	3		1639(34)	Ne	AB	9
	4		473(32)	Ne	AB	9

$^3\Sigma_u^-$ $D_{\infty h}$
$T_0 = 15630(5)$ Ne AB[3,9] $^3\Sigma_u^- - \tilde{X}$ 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

$^3\Pi_g$ $D_{\infty h}$
$T_0 = 8310(160)$ gas PE[8]

$^3\Sigma_u^+$ $D_{\infty h}$
$T_0 = 6290(160)$ gas PE[8]

$^1\Sigma_g^+$ $D_{\infty h}$
$T_0 = 930(120)$ gas PE[8]

$^1\Delta_g$ $D_{\infty h}$
$T_0 = 570(120)$ gas PE[8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1903(50)	gas	PE	8
	3	Sym. stretch	1355(50)T	gas	PE	8

$\tilde{X}\,^3\Sigma_g^-$ $D_{\infty h}$ Structure: ESR[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1928(50)	gas	PE	8
	3	Sym. stretch	1361(50)	gas	PE	8
Σ_u^-	5		2067.8	Ne	IR	3,6,7
			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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[1] R. J. Van Zee, R. F. Ferrante, K. J. Zeringue, and W. Weltner, Jr., J. Chem. Phys. **88**, 3465 (1988).
[2] D. W. Arnold, S. E. Bradforth, T. N. Kitsopoulos, and D. M. Neumark, J. Chem. Phys. **95**, 8753 (1991).
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cyc-C_8

$\tilde{X}$ D_{4h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e_u	12	Stretch	1844.2	Ar	IR	1,2

References

[1] S. L. Wang, C. M. L. Rittby, and W. R. M. Graham, J. Chem. Phys. **107**, 7025 (1997).
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C_8^-

Threshold for electron detachment from ground-state $C_8^- = 35330(50)$ gas PE[1,2,6]

(2) $^2\Pi_u$ $D_{\infty h}$
$T_0 = 16305$ gas PD[4]MPD[8] 446–614 nm
16295(5) Ne AB[7] 438–614 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		2104	gas	MPD	8
			2125(10)	Ne	AB	7
	2		1821(10)	Ne	AB	7
	4		469(8)	Ne	AB	7
Π_g	8		487(5)H	Ne	AB	7

$\tilde{C}\,^2\Pi_u$ $D_{\infty h}$
$T_0 = 13014$ gas PD[4]MPD[8] $\tilde{C}-\tilde{X}$ 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		2039	gas	MPD	8
			2055(5)	Ne	AB	3
	3		959(5)	Ne	AB	3
	4		450	gas	PD, MPD	4,8
			475(5)	Ne	AB	3

$^2\Sigma_u^+$ $D_{\infty h}$
$T_0 = 9545(2)$ Ne AB[7] 817–1048 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		2010(4)	Ne	AB	7
	2		1956(4)	Ne	AB	7

$\tilde{X}\,^2\Pi_g$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	6		1796.0	Ne	IR	5

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SiC_7

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1		2100.8	Ar	IR	1

Reference

[1] X. D. Ding, S. L. Wang, C. M. L. Rittby, and W. R. M. Graham, J. Phys. Chem. A **104**, 3712 (2000).

C_7N

$^2\Pi$ $C_{\infty v}$

$T_0 = 17185(6)$ Ne AB[1] $^2\Pi - \tilde{X}$ 482–582 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		CC,CN stretch	2086(8)	Ne	AB	1
		C–C stretch	1630(8)	Ne	AB	1
		C–C stretch	739(8)	Ne	AB	1
		C–C stretch	523(8)T	Ne	AB	1
Π		Deformation	134(5)H	Ne	AB	1

Reference

[1] M. Grutter, M. Wyss, and J. P. Maier, J. Chem. Phys. **110**, 1492 (1999).

$NC(C{\equiv}C)_2CN^+$

$\tilde{E}\,^2\Pi_u$ $D_{\infty h}$

$T_0 = 30420(160)$ 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]

$\tilde{A}\,^2\Pi_u$ $D_{\infty h}$

$T_0 = 15245.74$ gas $EF^1AB^4CR^4$ $\tilde{A}-\tilde{X}$ 630–770 nm

15130[a] Ne AB^2LF^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

$B_0 = 0.019$ AB^4CR^4

$\tilde{X}\,^2\Pi_g$ $D_{\infty h}$

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

$B_0 = 0.019$ AB^4CR^4

[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_7N^-

$^1\Sigma^+$ $C_{\infty v}$

$T_0 = 36496(27)$ Ne AB[1] $^1\Sigma^+ - \tilde{X}$ 249–274 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		CC,CN stretch	2054(38)	Ne	AB	1
		C–C stretch	1599(38)	Ne	AB	1
		C–C stretch	1069(38)	Ne	AB	1
		C–C stretch	472(38)	Ne	AB	1

$\tilde{X}\,^1\Sigma^+$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+			2124	Ne	IR	1
			2074	Ne	IR	1

Reference

[1] M. Grutter, M. Wyss, and J. P. Maier, J. Chem. Phys. **110**, 1492 (1999).

C_7O

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2244.2vsT	Ar	IR	2
			2198.3sT	Ar	IR	2

$B_0 = 0.019$ MW[1]

References

[1] T. Ogata, Y. Ohshima, and Y. Endo, J. Am. Chem. Soc. **117**, 3593 (1995).
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$F_2C=C=CFCF$:

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C_3 a-stretch (cis)	2006.8	Ar	IR	1
		C_3 a-stretch (trans)	1995.6ms	Ar	IR	1
		C_3 s-stretch	1444.4wm	Ar	IR	1
		CF_2 a-stretch	1268.0m	Ar	IR	1
		:CF stretch (cis)	1194.5	Ar	IR	1
		:CF stretch (trans)	1186.5s	Ar	IR	1
		=CF stretch	1174.2vs	Ar	IR	1

Reference

[1] C. Kötting, W. Sander, and M. Senzlober, Chem. Eur. J. **4**, 2360 (1998).

$F_2C=(cyc\text{-}C_3F_2)$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		Skel. breathing	2000.1wm	Ar	IR	1
			1241.9m	Ar	IR	1
			874.5ms	Ar	IR	1
b_2		FCCF a-stretch	1317.8vs	Ar	IR	1
		CF_2 a-stretch	1252.8ms	Ar	IR	1

Reference

[1] C. Kötting, W. Sander, and M. Senzlober, Chem. Eur. J. **4**, 2360 (1998).

8.15. Hydrocarbons With More Than Eight Atoms

$t\text{-}H_2C=CH-CH=CH_2^+$

$\tilde{E}$
$T_0=49210(80)$ gas PE[1,5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1130(80)	gas	PE	5

$\tilde{D}$
$T^a=39000(800)$ gas PE[5]

$\tilde{C}$
$T_0=33000(80)$ gas PE[1,5]

An absorption maximum which appears at 33890 (295 nm) in an argon matrix has been attributed[2] to *t*-butadiene cation.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1290(80)	gas	PE	5

$\tilde{B}$
$T^a=25250(800)$ gas PE[1,5]

$\tilde{A}$
$T_0=18720(80)$ gas PE[1,5]

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_g	4	C=C stretch	1620(2)	gas	PE,TPI	5–7
	5		1479(2)	gas	TPI	6
	6		1281(2)	gas	TPI	6
	7		1259(2)	gas	PE,TPI	5–7
	8		923(2)	gas	TPI	6
	9		511(2)	gas	PE,TPI	5–7
a_u	11		1000.9	Ar	IR	3,4
b_g	14		1000(2)	gas	TPI	6
	15		901(2)	gas	TPI	6
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.

References

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[7] J. Liu and S. L. Anderson, J. Chem. Phys. **114**, 6618 (2001).

$H_2CCHC(CH_3)$:

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1454.6m	Xe	IR	1
			1421.5m	Xe	IR	1
			1402.8w	Xe	IR	1
			1354.4vw	Xe	IR	1
			874.6m	Xe	IR	1
			767.1s	Xe	IR	1

Reference

[1] G. Maier, C. Lautz, and S. Senger, Chem. Eur. J. **6**, 1467 (2000).

cyc-C_5H_5

$\tilde{A}\,^2A_2''$ D_{5h} Structure: LF[9]
$T_0 = 29572.166(2)$ gas $AB^{1,3,4}LF^{6,8,11,12}$ $\tilde{A}-\tilde{X}$ 306–395 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	2		1055	gas	LF	11,12
e_1''	8	CH deform.	166H	gas	AB,LF	1,3,4,9,11,12
e_2'	11		1019	gas	LF	11,12
	12		797	gas	AB,LF	4,9,11,12

$\tau_0 = 64.9(5)$ ns gas $LF^{7,11}$
$B_0 = 0.286$; $C_0 = 0.144$ $LF^{8,9}$

$\tilde{X}\,^2E_1''$ D_{5h} Structure: $ESR^2AB^4LF^9$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	2		1071	gas	LF	12
a_2'	3		1244	gas	LF	12
a_2''	4		681	gas	LF	12
			661vs	Ar	IR	10
e_1'	5	CH stretch	3079wm	Ar	IR	10
	6		1383m	Ar	IR	10
	7		1001	gas	LF	12
e_1''	8		766H	gas	LF	12
e_2'	10		1320	gas	LF	12
	11		1041	gas	LF	12
	12		872	gas	PD,LF	5,6,9,12
e_2''	13		861H	gas	LF	12
	14		576H	gas	LF	12

$B_0 = 0.296$; $C_0 = 0.148$ $LF^{8,9}$

cyc-C_5D_5

$\tilde{A}\,^2A_2''$ D_{5h}
$T_0 = 29819.434(2)$ gas $AB^4LF^{9,12}$ $\tilde{A}-\tilde{X}$ 319–365 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	2		994	gas	LF	12
e_1''	8	CD deform.	116H	gas	AB,LF	4,12
e_2'	11		798T	gas	LF	12
e_2''	14		296H	gas	LF	12

$B_0 = 0.233$; $C_0 = 0.117$ LF^9

$\tilde{X}\,^2E_1''$ D_{5h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	2		1045	gas	LF	12
a_2''	4		562H	gas	LF	12
e_1''	8		616H	gas	LF	12
e_2'	10		1353	gas	LF	12
	11		861	gas	LF	12
e_2''	13		743H	gas	LF	12
	14		414H	gas	LF	12

$B_0 = 0.240$; $C_0 = 0.120$ LF^9

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o-C_6H_4

(**o-Benzyne**)
Absorption maxima at 40650 and 50250 (246 and 199 nm) have been reported[6,7] for o-benzyne isolated in an argon matrix.

An absorption maximum at 26320 (380 nm) has been assigned[6,7] to o-benzyne isolated in an argon matrix. In a neon matrix, this absorption maximum appears at 28730 (348 nm).[8]

$\tilde{a}\,^3B_2$ C_{2v}
$T_0 = 13140(50)$ gas $PE^{4,9}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1520(40)	gas	PE	9
			1395(30)	gas	PE	4,9
			1275(30)	gas	PE	9
			560(20)	gas	PE	4,9

$\tilde{X}\,^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	3094wm	Ne	IR	8
			3088	N_2	IR	2
	2	CH stretch	3071w	Ne	IR	8
	3	C≡C stretch	1860(15)	gas	PE	4,9
			1846w	Ne	IR	8
	4	Mixed	1415vw	Ne	IR	8
	5	Mixed	1271w	Ne	IR	8
	6	CH deform.	1055wm	Ne	IR	8
			1053m	Ar	IR	1
			1056	N_2	IR	2,5
	7	Ring stretch	1010(40)	gas	PE	4,9
			1039m	Ne	IR	8
			1038m	Ar	IR	1
			1039	N_2	IR	2,5
	8	Ring stretch	982wm	Ne	IR	8
	9	Ring deform.	600(15)	gas	PE	4,9
			589vw	Ne	IR	8
b_1	14	CH wag	838vw	Ne	IR	8
	15	CH wag	737s	Ne	IR	8
			736vs	Ar	IR	1
			743	N_2	IR	2,5
	16	Ring torsion	388wm	Ne	IR	8
b_2	17	CH stretch	3086m	Ne	IR	8
	18	CH stretch	3049vw	Ne	IR	8
	19	Ring stretch	1451m	Ne	IR	8
			1451m	Ar	IR	1
			1448	N_2	IR	2,5
	20	Mixed	1394wm	Ne	IR	8
			1395	N_2	IR	5
			1355	N_2	IR	5
	21	Mixed	1307vw	Ne	IR	8
	22	Mixed	1094w	Ne	IR	8
	23	Ring deform.	849ms	Ne	IR	8
			849s	Ar	IR	1
			847	N_2	IR	2,5
	24	Ring deform.	472vs	Ne	IR	8
			469vs	Ar	IR	1
			472	N_2	IR	2,5

$A_0 = 0.233$; $B_0 = 0.190$; $C_0 = 0.105$ MW[3]

o-C_6D_4

$\tilde{a}\,^3B_2$ C_{2v}
$T_0 = 13180(100)$ gas PE[4,9]

Vib.	No.	Approximate	cm^{-1}	Med.	Type	Refs.
a_1			1515(30)	gas	PE	9
			1265(30)	gas	PE	4,9
			550(30)	gas	PE	4

$\tilde{X}\,^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD stretch	2311wm	Ne	IR	8
			2293	N_2	IR	2
	2	CD stretch	2295vw	Ne	IR	8
	3	C≡C stretch	1860(15)	gas	PE	4,9
			1844vw	Ne	IR	8
	4	Mixed	1364w	Ne	IR	8
	5	Mixed	1198w	Ne	IR	8
	6	Ring stretch	980(20)	gas	PE	4
			995wm	Ne	IR	8
	7	CD deform.	853w	Ne	IR	8
	8	Ring stretch	792wm	Ne	IR	8
	9	Ring deform.	580(20)	gas	PE	4,9
			579vw	Ne	IR	8
b_1	14	CD wag	679vw	Ne	IR	8
	15	CD wag	571m	Ne	IR	8
	16	Ring torsion	336w	Ne	IR	8
b_2	17	CD stretch	2314wm	Ne	IR	8
	18	CD stretch	2285vw	Ne	IR	8
	19	Ring stretch	1411w	Ne	IR	8
	20	Mixed	1293w	Ne	IR	8
			1293	N_2	IR	2
	21	Mixed	1112vw	Ne	IR	8
			1108	N_2	IR	2
	22	Mixed	875vw	Ne	IR	8
	23	Ring deform.	790m	Ne	IR	8
			792	N_2	IR	2
	24	Ring deform.	469vs	Ne	IR	8
			471	N_2	IR	2

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m-C_6H_4

(***m*-Benzyne**)

$\tilde{a}$ C_{2v}
$T_0 = 7350(110)$ gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			970(15)	gas	PE	2

$\tilde{X}$ 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
			300T	gas	PE	2
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

m-C_6D_4

$\tilde{a}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			955(20)	gas	PE	2

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			300T	gas	PE	2

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p-C_6H_4

(***p*-Benzyne**)

$\tilde{a}$ D_{2h}
$T_0 = 1330(130)$ gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	4		995(20)	gas	PE	2
	5		610(15)	gas	PE	2

$\tilde{X}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	4		990(20)	gas	PE	2
	5		635(20)	gas	PE	2
b_{1u}	10		1403w	Ne	IR	1
	11		976w	Ne	IR	1
			980s	Ar	IR	1
	12	Ring deform.	918w	Ne	IR	1
b_{2u}	16		1331w	Ne	IR	1
	17		1207w	Ne	IR	1
b_{3u}	23	CH wag	721s	Ne	IR	1
			725s	Ar	IR	1
	24	Ring torsion	435w	Ne	IR	1

p-C_6D_4

$\tilde{a}$ D_{2h}
$T_0 = 1350(130)$ gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	4		945(40)	gas	PE	2
	5		590(20)	gas	PE	2

$\tilde{X}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	5		615(20)	gas	PE	2
b_{1u}	12	Ring deform.	767	Ar	IR	1

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o-$C_6H_4^-$

Threshold for electron detachment from ground-state *o*-$C_6H_4^-$ = 4550(55) 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			600(30)	gas	PE	1,2

o-$C_6D_4^-$

Threshold for electron detachment from ground-state *o*-$C_6D_4^-$ = 4490(65) gas PE[1,2]

$\tilde{X}\,^2B_2$ C_{2v}

Vib.	No.	Approximate	cm^{-1}	Med.	Type meas.	Refs.
a_1			580(30)	gas	PE	1

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m-$C_6H_4^-$

Threshold for electron detachment from ground-state m-$C_6H_4^-$ 6870(90) in the gas phase, estimated from collision-induced dissociation branching ratios.[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			885(20)	gas	PE	1

m-$C_6D_4^-$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			910(40)	gas	PE	1

Reference

[1] P. G. Wenthold, R. R. Squires, and W. C. Lineberger, J. Am. Chem. Soc. **120**, 5279 (1998).

p-$C_6H_4^-$

Threshold for electron detachment from ground-state p-$C_6H_4^-$ = 10210(65) gas PE[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			615(30)	gas	PE	1

p-$C_6D_4^-$

Threshold for electron detachment from ground-state p-$C_6D_4^-$ = 10170(65) gas PE[1]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			605(30)	gas	PE	1

Reference

[1] P. G. Wenthold, R. R. Squires, and W. C. Lineberger, J. Am. Chem. Soc. **120**, 5279 (1998).

$C_6H_5^+$

$\tilde{a}\,^3B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CH stretch	2790(100)	gas	PE	1

$\tilde{X}\,^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_1		CH deform.	713	Ar	IR	2
b_2		CH stretch	3110	Ar	IR	2

$C_6D_5^+$

$\tilde{a}\,^3B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CH stretch	2370(110)	gas	PE	1

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C_6H_5

$\tilde{C}\,^2B_2$ C_{2v}
T_0 = 47281 Ar AB[11]

$\tilde{B}\,^2A_1$ C_{2v}
A broad gas-phase absorption with maximum near 40820 (245 nm) has been attributed[7] to C_6H_5. It may correspond with a broad, unstructured absorption maximum observed[11] at 42535 (235 nm) in an argon matrix.

$\tilde{A}\,^2B_1$ C_{2v}
T_0 = 18908 gas AB[1] $\tilde{A}$–$\tilde{X}$ 440–530 nm
19589 Ar AB[11]
This weak absorption is overlapped by more prominent absorption of C_6H_5O.

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[9] 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	3086w	Ar	IR,Ra	6,8,10,12,13,14
	2	CH s-stretch	3072vw	Ar	IR,Ra	10,12,13,14
	3	CH s-stretch	3037vw	Ar	IR,Ra	13,14
	4	Ring stretch	1497vw	Ar	IR,Ra	13,14
	5	Ring stretch	1441wm	Ar	IR,Ra	8,10,12,13,14
	6	CH deform.	1154vw	Ar	IR,Ra	13,14
	7	Ring deform.	1027wm	Ar	IR,Ra	6,8,10,12,13,14
	8	Ring breathing	997vw	Ar	IR,Ra	13,14
	9	Ring deform.	968(15)	gas	PE	9
			976w	Ar	IR,Ra	8,10,13,14
	10	Ring deform.	600(10)	gas	PE	9
			605w	Ar	IR,Ra	8,10,13,14
a_2	11	OPLA CH deform.	945T	Ar	Ra	14
	12	OPLA CH deform.	816T	Ar	Ra	14
b_1	14	CH deform.	990vw	Ar	IR,Ra	10,13,14
	15	CH deform.	874w	Ar	IR,Ra	10,13,14
	16	CH deform.	706vs	Ar	IR,Ra	2–6,8,10,12–14
	17	CH deform.	657w	Ar	IR,Ra	8,12–14
	18	Deformation	416w	Ar	IR,Ra	10,13,14
b_2	19	CH a-stretch	3071wm	Ar	IR,Ra	8,10,12–14
	20	CH a-stretch	3060vw	Ar	IR,Ra	8,10,13,14
	21	Ring stretch	1593w	Ar	IR,Ra	13,14
	22	Ring stretch	1432wm	Ar	IR,Ra	6,8,10,12–14
	23	CH deform.	1310vw	Ar	IR,Ra	13,14
	24	Ring deform.	1283vw	Ar	IR,Ra	13,14
	25	CH deform.	1159vw	Ar	IR,Ra	13,14
	26	Ring deform.	1063w	Ar	IR,Ra	8,10,13,14
	27	Ring stretch	587vw	Ar	IR,Ra	8,10,13,14

C_6D_5

$\tilde{X}\,^2A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD stretch	2292	Ar	IR	13
	2	CD stretch	2290	Ar	IR	13
	3	CD stretch	2282	Ar	IR	13
	4		1494	Ar	IR	13
	5		1314	Ar	IR	13
	6		960(20)	gas	PE	9
			851	Ar	IR	13
	7		803	Ar	IR	13
	10		588(10)	gas	PE	9
			590	Ar	IR	13
b_1	17	CD deform.	517s	Ar	IR	2,5,13
	18		382	Ar	IR	13
b_2	19	CD stretch	2271	Ar	IR	13
	20	CD stretch	2264	Ar	IR	13
	21		1561	Ar	IR	13
	22		1312	Ar	IR	13
	23		1297	Ar	IR	13
	26		806	Ar	IR	13
	27		547	Ar	IR	13

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$C_6H_6^+$

$\tilde{F}\,^2A_{1g}$ D_{6h}
$T^a = 61320(10)$ gas PE[1,5,16]

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	960(10)	gas	PE	1,16

$\tilde{E}\,^2B_{1u}$ D_{6h}
$T^a = 50265(10)$ gas PE[1,5,16]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1[b](2)	CH stretch	1694(8)	gas	PE	16

$\tilde{D}\,^2B_{2u}$ D_{6h}
$T^a = 44700(100)$ gas PE[5,16]

$\tilde{C}\,^2E_{1u}$ D_{6h}
$T^a = 38220(100)$ gas PE[5,16]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e_{2g}	18 (6)	Ring deform.	508T	gas	PE	16

$\tilde{B}\,^2A_{2u}$ D_{6h}
$T^a = 25310(100)$ gas PE[5,16]

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 $\tilde{B}$–$\tilde{X}$ transition of $C_6H_6^+$ produced by vacuum-ultraviolet photolysis of benzene isolated in a neon matrix.[2]

$T_0 \cong 19840$ Ar LF[3]AB[4] 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

$\tilde{A}\,^2E_{2g}$ D_{6h}

$T_0 = 18117$ gas PF[9]PRI[13,15]PE[16] $\tilde{A}-\tilde{X}$ 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 $\tilde{A}$ state.

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1[b] (2)	CH stretch	2856(10)	gas	PE	1,16
	2 (1)	Ring stretch	976(8)[c]	gas	PF,PE	9,16
a_{2u}	4 (11)	CH bend (E_{2u})	506	gas	PRI	15
e_{1u}	14 (18)	CH bend (B_{1u})	551	gas	PRI	15
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.	617[d]	gas	PE,PRI	1,15,16
e_{2u}	19 (17)	CH bend (E_{2u})	635	gas	PF,PRI	9,15
		(A_{2u})	579			
	20 (16)	Ring deform. (E_{2u})	300	gas	PF,PRI	9,15
		(A_{2u})	228			

$\tilde{X}\,^2E_{1g}$ 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	966	gas	PE,MPI	1,6,8,16
b_{2g}	8 (4)	Ring deform.	422[e]	gas	PE,MPI	6,15
e_{1g}	11 (10)	CH bend	835(15)	gas	MPI	8
e_{2g}	16 (8)	Ring stretch	1557(8)[f]	gas	PE	1,6,16
			1480(10)T	Ar	LF	3
	17 (9)	CH bend	1230(15)[f]	gas	PE, MPI	1,6,8
	18 (6)	Ring deform.	676.4[f]	gas	TPE,PE	1,6,8,12,
		(E_{1g})			MPI	15,16
			630(10)T	Ar	LF	3
		(B_{2g})	365.4[g]	gas	TPE,PE	12,15,16
					MPI	
		(B_{1g})	345.4[h]	gas	TPE,MPI	6,12,15
e_{2u}	20 (16)	Ring deform.	300(10)	gas	PE,MPI	6,8,15,16

$B_0 = 0.189$; $C_0 = 0.095$ PE[7]TPE[11]TPI[14]

$C_6D_6^+$

$\tilde{F}\,^2A_{1g}$ D_{6h}

T[a] $\cong 62000$ gas PE[1,17]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1[b] (2)	CD stretch	2240(100)	gas	PE	1,17
	2 (1)	Ring stretch	920(100)	gas	PE	1,17

$\tilde{E}\,^2B_{1u}$ D_{6h}

T[a] $\cong 50000$ gas PE[1,17]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1[b] (2)	CD stretch	1610T	gas	PE	1,17

$\tilde{B}\,^2A_{2u}$ 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

$\tilde{A}\,^2E_{2g}$ D_{6h}

T[a] $= 18362$ gas PE[1,17]PRI[15]

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
a_{2u}	4 (11)	CD bend	486	gas	PRI	15
e_{1u}	14 (18)	CD bend (B_{1u})	451	gas	PRI	15
		(B_{2u})	425			
e_{2g}	16 (8)	Ring stretch	1450(100)	gas	PE	1,17
	17 (9)	CD bend	870(100)	gas	PE	1,17
	18 (6)	Ring deform.	569	gas	PE,PRI	1,15,17
e_{2u}	19 (17)	CD bend (E_{2u})	604	gas	PRI	15
		(A_{2u})	546			
	20 (16)	Ring deform. (E_{2u})	218	gas	PRI	15
		(A_{2u})	151			

$\tilde{X}\,^2E_{1g}$ 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	1,6,17
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. (E_{1g})	634[f]	gas	PE,MPI	1,6,15,17
			590(10)T	Ar	LF	3
		(B_{2g})	356	gas	MPI	15
		(B_{1g})	335[i]	gas	PE,MPI	6,15
e_{2u}	20 (16)	Ring deform. (E_{1u})	262	gas	PE,MPI	6,15

$B = 0.155$; $C = 0.076$ 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] Ref. 16 gives 652(8).

[e] Ref. 16 gives 468(8).

[f] $j = \pm 1/2$.

[g] $j = +3/2$.

[h] $j = -3/2$.

[i] $j = 3/2$.

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HC_7H

$^3\Sigma_u^-$ $D_{\infty h}$

$T_0 = 19818.0$ gas CR[2,3] $^3\Sigma_u^- - \tilde{X}$ 459–505 nm
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	1954.5(2)	gas	CR	3
			1961(5)	Ne	AB	1
	4		647(5)	Ne	AB	1
Π		CH bend	286HT	Ne	AB	1

DC_7D

$^3\Sigma_u^-$ $D_{\infty h}$

$T_0 = 19943.2$ gas CR[2] $^3\Sigma_u^- - \tilde{X}$ 457–502 nm
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	1926.6(2)	gas	CR	3
			1935(5)	Ne	AB	1
	4		551(5)	Ne	AB	1
Π		CD bend	202HT	Ne	AB	1

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(*cyc*-HC_3)(C≡C)$_2$H

$\tilde{X}$ C_s

$A_0 = 1.158$; $B_0 = 0.035$; $C_0 = 0.034$ MW[1]

(*cyc*-DC_3)(C≡C)$_2$D

$\tilde{X}$ C_s

$A_0 = 0.997(2)$; $B_0 = 0.033$; $C_0 = 0.032$ MW[1]

Reference

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3,5-$C_6H_3CH_3$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CH_3 deform.	1533wm	Ar	IR	1
		Ring deform.	1462ms	Ar	IR	1
		CH wag	824m	Ar	IR	1
		CH wag	768m	Ar	IR	1
		Deformation	570wm	Ar	IR	1
a''		CH_3 deform.	1570wm	Ar	IR	1
		Mixed	1000wm	Ar	IR	1
		Ring deform.	543vs	Ar	IR	1

Reference

[1] W. Sander and M. Exner, J. Chem. Soc., Perkin Trans. **2**, 2285 (1999).

C_6H_5CH

In an argon matrix, absorption maxima have been observed[2,3] at 240 and 245 nm. A weaker absorption maximum has also been observed[3] at 300 nm.

In an argon matrix, structured absorption has been observed[1–3] between 372 and 430 nm.

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3		3073ms	Ar	IR	1–3
	5		3060wm	Ar	IR	3
	6		3035wm	Ar	IR	3
	7		1562vw	Ar	IR	3
	8		1538w	Ar	IR	3
			1505(5)m	Ar	IR	1
	9		1458wm	Ar	IR	1,3
	10		1428wm	Ar	IR	1,3
			1390(5)m	Ar	IR	1
	11		1325vw	Ar	IR	3
	12		1290vw	Ar	IR	3
	13		1264w	Ar	IR	3
			1210(5)wm	Ar	IR	1
	14		1160vw	Ar	IR	3
	15		1149vw	Ar	IR	3
	16		1091w	Ar	IR	3
	17		1017w	Ar	IR	1,3
	18		976w	Ar	IR	3
			945(5)wm	Ar	IR	1
	19		840wm	Ar	IR	3
	20		788wm	Ar	IR	3
	21		612vw	Ar	IR	3
			550(5)wm	Ar	IR	1
	22		525vw	Ar	IR	3

	23		343wm	Ar	IR	3
a″	26		884wm	Ar	IR	1,3
	27		835vw	Ar	IR	3
	28		741vs	Ar	IR	1–3
	29		670m	Ar	IR	1–3
	30		497wm	Ar	IR	3
	31		443ms	Ar	IR	1–3
	32		392vw	Ar	IR	3

C_6D_5CD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	2		2289m	Ar	IR	3
	3		2271vs	Ar	IR	3
	5		2257w	Ar	IR	3
	6		2245wm	Ar	IR	3
	7		1518vw	Ar	IR	3
	8		1485vw	Ar	IR	3
	9		1338wm	Ar	IR	3
	10		1329w	Ar	IR	3
	11		1256w	Ar	IR	3
	14		944w	Ar	IR	3
	15		854w	Ar	IR	3
	16		837vw	Ar	IR	3
	17		842w	Ar	IR	3
	18		823wm	Ar	IR	3
	19		762m	Ar	IR	3
	20		658m	Ar	IR	3
	21		585w	Ar	IR	3
	23		295wm	Ar	IR	3
a″	24		815w	Ar	IR	3
	26		740m	Ar	IR	3
	28		630m	Ar	IR	3
	29		525vs	Ar	IR	3
	30		429w	Ar	IR	3
	31		354s	Ar	IR	3
	32		339wm	Ar	IR	3

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cyc-C_7H_6

(1,2,4,6-Cycloheptatetraene)

In an argon matrix, the onset of absorption occurs near 390 nm, with increasing absorption out to the limit of the measurements, near 220 nm.[2,4]

$\tilde{X}$ C_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1		3048wm	Ar	IR	4
	2		3041ms	Ar	IR	4
	3		3021w	Ar	IR	4
	4		1527w	Ar	IR	4
	5		1422w	Ar	IR	1,4
	6		1364wm	Ar	IR	1,4
	7		1211vw	Ar	IR	4
	8		1104w	Ar	IR	4
	9		1012vw	Ar	IR	4
	10		966wm	Ar	IR	1,4
	11		913wm	Ar	IR	1,2,4
	12		826vw	Ar	IR	4
	13		798vw	Ar	IR	4
	14		689m	Ar	IR	1–4
	15		581m	Ar	IR	1,2,4
	16		404m	Ar	IR	1,4
	17		302wm	Ar	IR	4
b	18		3038vs	Ar	IR	1,2,4
	20		3013wm	Ar	IR	1,2,4
	21		1823wm	Ar	IR	1–4
	22		1579w	Ar	IR	4
	23		1380wm	Ar	IR	1–4
	24		1285w	Ar	IR	4
	25		1189w	Ar	IR	1,4
	26		1019w	Ar	IR	4
	27		952w	Ar	IR	4
	28		874wm	Ar	IR	4
	29		772s	Ar	IR	1–4
	30		679vs	Ar	IR	1,2,4
	31		482w	Ar	IR	4
	32		362wm	Ar	IR	4
	33		298w	Ar	IR	4

cyc-C_7D_6

$\tilde{X}$ C_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	2		2263ms	Ar	IR	4
	3		2234vw	Ar	IR	4
	4		1499w	Ar	IR	4
	5		1312m	Ar	IR	4
	6		1221wm	Ar	IR	4
	7		915w	Ar	IR	4
	8		869w	Ar	IR	4
	9		828vw	Ar	IR	4
	11		765wm	Ar	IR	4
	12		724m	Ar	IR	4
	13		654wm	Ar	IR	4
	14		598wm	Ar	IR	4
	15		507m	Ar	IR	4
	16		394m	Ar	IR	4
	17		266wm	Ar	IR	4
b	18		2275vs	Ar	IR	4
	19		2254ms	Ar	IR	4
	20		2221wm	Ar	IR	4
	21		1800wm	Ar	IR	4
	22		1528w	Ar	IR	4
	23		1184wm	Ar	IR	4
	24		1006vw	Ar	IR	4
	25		892vw	Ar	IR	4
	26		843wm	Ar	IR	4
	27		823vw	Ar	IR	4
	29		660vs	Ar	IR	4
	30		543s	Ar	IR	4
	31		435w	Ar	IR	4
	32		314wm	Ar	IR	4
	33		262w	Ar	IR	4

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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}

$T_0=22850$T gas AB[11]EM[11]LF[22,24]MPI[28]
Vibronically coupled to modes of b_2 symmetry in the $\tilde{A}$ state.[11,22,24,27,28]
$A^b=0.179$; $B^b=0.088$; $C^b=0.059$ 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]MPI[28] $\tilde{A},\tilde{B}-\tilde{X}$ 429–471 nm
22003 Ne AB[6] $\tilde{A},\tilde{B}-\tilde{X}$ 429–455 nm
21862 Ar LF[13] $\tilde{A},\tilde{B}-\tilde{X}$ 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	11,17,18
					LF	22
			402	Ne	AB	6
	6b	Ring deform.	328[c]	gas	AB	11,17,18
					LF	22
			344	Ne	AB	6

$\tau_{0(1)}=0.4\ \mu s$; $\tau_{0(2)}=1.85\ \mu s$ 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)	gas	PE	23,29
			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	5,8,10,20
					PE,MPI	23,28,29
			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, MPI	5,8,10,18 20,28
			612	Ar	LF	13
	18b	CH deform.	356	gas	EM,LF	5,8,18,20
					MPI	28
			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

$\tau\cong1340$ 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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$C_6H_5CH_2^-$

Threshold for electron detachment from ground-state $C_6H_5CH_2^-$ = 7360(50) gas PE[2,3]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			945	gas	MPD	1
			514(15)	gas	PE	3

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C_8H

$^2\Pi_{3/2}$ $C_{\infty v}$
T_0 = 15973.5(2) gas CR[5] $^2\Pi-\tilde{X}$ 554–626 nm
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		2077.6(3)	gas	CR	5
			2080(5)	Ne	AB	1
	5		1591.2(3)	gas	CR	5
			1607(5)	Ne	AB	1
	6		783(5)	Ne	AB	1

A = −36.8(2) gas CR[5]

$\tilde{A}\,^2\Sigma^+$ $C_{\infty v}$
T_0 = 2041(50) gas PE[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		C≡C stretch	2016(70)	gas	PE	4

$\tilde{X}\,^2\Pi_{3/2}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		C≡C stretch	1661(50)	gas	PE	4

A_{eff} = −19.33 MW[2,3,6]
B_0 = 0.0196 MW[2,3,6]

C_8D

$^2\Pi_{3/2}$ $D_{\infty h}$
$T_0 = 16004.0(3)$ gas CR[5] $^2\Pi - \tilde{X}$ 568–625 nm
15873(5) Ne AB[5] $^2\Pi - \tilde{X}$ 572–630 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3		2073.8(6)	gas	CR	5
			2064(7)	Ne	AB	5
	5		1592.3(4)	gas	CR	5
			1604(7)	Ne	AB	5

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C_8H^-

Threshold for electron detachment from ground-state $C_8H^- = 32000(80)$ gas PE[1]

$^1\Sigma^+$ $C_{\infty v}$
$T_0 = 35174(25)$ Ne AB[2] $^1\Sigma^+ - \tilde{X}$ 275–285 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		C–C stretch	720(35)	Ne	AB	2
		C–C stretch	464(35)	Ne	AB	2

$\tilde{X}\ ^1\Sigma^+$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		CC stretch	2106	Ne	IR	2
		CC stretch	2021	Ne	IR	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

$\tilde{A}\ ^2\Pi_u$ $D_{\infty h}$
$T_0 = 14143.18$ gas $PE^1EF^2EM^5CR^5$
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

$\tau_0 \leqslant 6$ ns gas EF^2
$B_0 = 0.019$ EM^5CR^5

$\tilde{X}\ ^2\Pi_g$ $D_{\infty h}$

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

$B_0 = 0.019$ EM^5CR^5

$C_8D_2^+$

$\tilde{A}\ ^2\Pi_u$ $D_{\infty h}$
$T_0 = 14169.52$ gas EM^5CR^5
$B_0 = 0.017$ EM^5CR^5

$\tilde{X}\ ^2\Pi_g$ $D_{\infty h}$
$B_0 = 0.018$ EM^5CR^5

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cyc-C_8H_6

$\tilde{a}$
$T_0 = 5710(50)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CC stretch	2060(20)	gas	PE	1
			1490(20)	gas	PE	1

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CC stretch	2185(20)	gas	PE	1
			1500(20)	gas	PE	1
			295(20)	gas	PE	1

Reference

[1] P. G. Wenthold and W. C. Lineberger, J. Am. Chem. Soc. **119**, 7772 (1997).

cyc-$C_8H_6^-$

Threshold for electron detachment from ground-state *cyc*-$C_8H_6^-$ = 5710(50) gas PE[1]

Reference

[1] P. G. Wenthold and W. C. Lineberger, J. Am. Chem. Soc. **119**, 7772 (1997).

p-HC≡C_6H_4≡CH

In a nitrogen matrix,[1] this species has strong bands at 27400 (365 nm), 25710 (389 nm), 23920 (418 nm) and 21740 (460 nm), as well as a long, regularly structured tail out to 700 nm.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3051.0w	N_2	IR	1
			1258.2wm	N_2	IR	1
			1248.2wm	N_2	IR	1
			1239.0wm	N_2	IR	1
			1237.5wm			
			956.6w	N_2	IR	1
			847.4wm	N_2	IR	1
			844.5m			
			826.6wm	N_2	IR	1
			817.4vs	N_2	IR	1
			815.4m			
			814.4m			
			768.9wm	N_2	IR	1
			629.8wm	N_2	IR	1
			618.6s	N_2	IR	1
			615.1s			
			612.5m			
			457.3ms	N_2	IR	1
			455.0wm			

Reference

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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

$\tilde{a}$ $D_{\infty h}$

T^a = 10730(80) gas PE[15]

$\tilde{X}\ ^1\Sigma_g^+$ $D_{\infty h}$

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	12–14
			1998.0[b]	Ar	IR	1,2,5,12
			1994.2	Kr	IR	12
			2007.3	H_2	IR	10,14
	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] From vertical ionization potentials.

[b] 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

$\tilde{C}\,^2\Pi_g$ $D_{\infty h}$
$T_0 = 29334$ gas MPD[7]
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

$\tilde{B}\,^2\Pi_g$ $D_{\infty h}$
$T_0 = 16462$ gas MPD[5,7,9] $\tilde{B}-\tilde{X}$ 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		1991	gas	MPD	7,9
			2001(6)	Ne	AB	6

$\tilde{A}\,^2\Pi_g$ $D_{\infty h}$
$T_0 = 13068$ gas MPD[5,7,9]
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	3,8
	7	Asym. stretch	1583.3	Ar	IR	3,8

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cum-C_9H^- [a]

$^1A'$ C_s
$T_0 = 29014(10)$ gas MPD[1] $^1A'-\tilde{X}$ 326–345 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		C=C stretch	1668(10)	gas	MPD	1

[a] This isomer of C_9H^-, with cumulenic bonding, lies at a somewhat higher energy than the acetylenic isomer.

Reference

[1] M. Tulej, F. Güthe, M. Schnaiter, M. V. Packhov, D. A. Kirkwood, J. P. Maier, and G. Fischer, J. Phys. Chem. A **103**, 9712 (1999).

acet-C_9H^-

$^3\Sigma^-$ $C_{\infty v}$
$T_0 = 27630(10)$ gas MPD[1] $^3\Sigma^- - \tilde{X}$ 337–362 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		C≡C stretch	1978(10)	gas	MPD	1
		C–C stretch	680(10)	gas	MPD	1

Reference

[1] M. Tulej, F. Güthe, M. Schnaiter, M. V. Packhov, D. A. Kirkwood, J. P. Maier, and G. Fischer, J. Phys. Chem. A **103**, 9712 (1999).

HC_9H

$^3\Sigma_u^-$ $D_{\infty h}$
$T_0 = 17184.6$ gas CR[2,3] $^3\Sigma_u^- - \tilde{X}$ 521–582 nm
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	1976.0(2)	gas	CR	2,3
			1969(5)	Ne	AB	1
			770(5)	Ne	AB	1

DC_9D

$^3\Sigma_u^-$ $D_{\infty h}$
$T_0 = 17262.5$ gas CR[2,3] $^3\Sigma_u^- - \tilde{X}$ 519–580 nm
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	1968.4(2)	gas	CR	2,3
			1966(5)	Ne	AB	1

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cyc-$(HC_3)(C{\equiv}C)_3H$

$\tilde{X}$ C_s
$A_0 = 1.157$T; $B_0 = 0.015$; $C_0 = 0.015$ MW[1]

Reference

[1] M. C. McCarthy, M. J. Travers, W. Chen, C. A. Gottlieb, and P. Thaddeus, Astrophys. J. **498**, L89 (1998).

C_{10}

(2) $^3\Sigma_u^-$ $D_{\infty h}$
$T_0 = 29985(18)$ Ne AB[2] 324–334 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	5		401(25)	Ne	AB	2

$D_{\infty h}$
$T_0 = 27925(16)$ Ne AB[2] 349–358 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	5		364(22)	Ne	AB	2

$\tilde{X}\ ^3\Sigma_g^-$ $D_{\infty h}$

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

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[1] P. Freivogel, M. Grutter, D. Forney, and J. P. Maier, Chem. Phys. **216**, 401 (1997).
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cyc-C_{10}

$^1\Sigma_{1u}$ D_{10h}
$T_0 = 31636(20)$ Ne AB[1] 308–316 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g			374(30)	Ne	AB	1

Reference

[1] M. Grutter, M. Wyss, E. Riaplov, J. P. Maier, S. D. Peyerimhoff, and M. Hanrath, J. Chem. Phys. **111**, 7397 (1999).

C_{10}^-

REMPD studies[4] suggest the formation of cyclic species of C_{10}^- when the anion is generated at low laser fluence.

(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

$\tilde{C}\ ^2\Pi_g$ $D_{\infty h}$
$T_0 = 10380(5)$ gas MPD[4]
10338(5) Ne AB[1] $\tilde{C} - \tilde{X}$ 804–968 nm
10189(10) Ar AB[5]

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		400(5)	gas	MPD	4
			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

References

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$C_{10}H$

$^2\Pi_{3/2}$ $C_{\infty v}$

$T_0 = 14000$ gas CR[2] $^2\Pi - \tilde{X}$ 622–715 nm

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		2084(2)	gas	CR	2
			2075(2)			
			2097(5)	Ne	AB	1
	5		1520(5)T	Ne	AB	1

$B_0 = 0.010$ MW[3]

$C_{10}D$

$^2\Pi_{3/2}$ $C_{\infty v}$

$T_0 = 14020$ gas CR[2] $^2\Pi - \tilde{X}$ 621–714 nm

13866(4) Ne AB[2] $^2\Pi - \tilde{X}$ 626–722 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3		2082.2	gas	CR	2
			2094(6)	Ne	AB	2

References

[1] P. Freivogel, J. Fulara, M. Jakobi, D. Forney, and J. P. Maier, J. Chem. Phys. **103**, 54 (1995).

[2] H. Linnartz, T. Motylewski, and J. P. Maier, J. Chem. Phys. **109**, 3819 (1998).

[3] C. A. Gottlieb, M. C. McCarthy, M. J. Travers, J.-U. Grabow, and P. Thaddeus, J. Chem. Phys. **109**, 5433 (1998).

cum-$C_{10}H^-$ [a]

$\tilde{A}$

$T_0 = 27847(10)$ gas MPD[1] $\tilde{A} - \tilde{X}$ 281–359 nm

28050(15) Ne AB[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C=C stretch	1678(10)	gas	MPD	1

[a]This isomer of $C_{10}H^-$, with cumulenic bonding, lies at a somewhat higher energy than the acetylenic isomer, and either the $\tilde{X}$ or the $\tilde{A}$ state may be nonlinear.

Reference

[1] D. A. Kirkwood, M. Tulej, M. V. Pachkov, M. Schnaiter, F. Güthe, M. Grutter, M. Wyss, J. P. Maier, and G. Fischer, J. Chem. Phys. **111**, 9280 (1999).

acet-$C_{10}H^-$

$^1\Sigma^+$ $C_{\infty v}$

$T_0 = 30600(15)$ Ne AB[1,2] $^1\Sigma^+ - \tilde{X}$ 302–327 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		CC stretch	2363(15)	gas	MPD	2
			2394(20)	Ne	AB	2
		C–C stretch	480(15)	gas	MPD	2
			553(27)	Ne	AB	1,2

$\tilde{X}\ ^1\Sigma^+$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		CC stretch	2040	Ne	IR	1

References

[1] M. Grutter, M. Wyss, and J. P. Maier, J. Chem. Phys. **110**, 1492 (1999).

[2] D. A. Kirkwood, M. Tulej, M. V. Pachkov, M. Schnaiter, F. Güthe, M. Grutter, M. Wyss, J. P. Maier, and G. Fischer, J. Chem. Phys. **111**, 9280 (1999).

C_{11}

$^1\Sigma_u^+$ $D_{\infty h}$

$T_0 = 29732(20)$ Ne AB[2] $^1\Sigma_u^+ - \tilde{X}$ 323–337 nm

28248 Ar AB[7]

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

$\tilde{a}$ $D_{\infty h}$

$T^a = 9520(80)$ gas PE[6]

$\tilde{X}\ ^1\Sigma_g^+$ $D_{\infty h}$

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
			1946.0(8)	Ar	IR	4,5
			1937.3	Kr	IR	5
			1942.6	N_2	IR	5
	8	Asym. stretch	1853.4	Ne	IR	3
			1856.7(8)	Ar	IR	4,5
			1849.9	Kr	IR	5
			1854.8	N_2	IR	5
	9	Asym. stretch	1357.0w	N_2	IR	5

[a]From vertical ionization potentials.

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).
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[4] M. Grutter, P. Freivogel, D. Forney, and J. P. Maier, J. Chem. Phys. **107**, 5356 (1997).
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[6] M. Kohno, S. Suzuki, H. Shiromaru, and Y. Achiba, J. Chem. Phys. **110**, 3781 (1999).
[7] J. Szczepanski, J. Fuller, S. Ekern, and M. Vala, Spectrochim. Acta A **57**, 775 (2001).

C_{11}^-

Threshold for electron detachment from ground-state C_{11}^- = 31570(65) gas PE[1,2]

REMPD studies[5] suggest the formation of cyclic species of C_{11}^- when the anion is generated at low laser fluence.

$\tilde{D}\,^2\Pi_u$ $D_{\infty h}$
T_0 = 29884(18) Ne AB[4] $\tilde{D}-\tilde{X}$ 320–335 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	4		765(18)	Ne	AB	4
	5		344(18)	Ne	AB	4

$\tilde{C}\,^2\Pi_u$ $D_{\infty h}$
T_0 = 25151(13) Ne AB[4] $\tilde{C}-\tilde{X}$ 392–398 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	5		355(13)	Ne	AB	4

$\tilde{B}\,^2\Pi_u$ $D_{\infty h}$
T_0 = 13850(5) gas MPD[5] $\tilde{B}-\tilde{X}$ 496–722 nm
13906(4) Ne AB[4] $\tilde{B}-\tilde{X}$ 627–720 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1		2070(5)	gas	MPD	5
			2032(5)	Ne	AB	4
			1882(4)	Ne	AB	4
	5		580(5)	gas	MPD	5

$\tilde{A}\,^2\Pi_u$ $D_{\infty h}$
T_0 = 11050(10) gas MPD[3,5] $\tilde{A}-\tilde{X}$ 788–905 nm
11042(2) Ne AB[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	5		570(5)	gas	MPD	3,5

References

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[4] D. Forney, M. Grutter, P. Freivogel, and J. P. Maier, J. Phys. Chem. A **101**, 5292 (1997).
[5] M. Ohara, M. Suwa, T. Ishigaki, H. Shiromaru, Y. Achiba, and W. Krätschmer, J. Chem. Phys. **109**, 1329 (1998).

cum-$C_{11}H^-$ [a]

$^1A'$ C_s
T_0 = 26742(10) gas MPD[1]

[a]This isomer of $C_{11}H^-$, with cumulenic bonding, lies at a somewhat higher energy than the acetylenic isomer.

Reference

[1] M. Tulej, F. Güthe, M. Schnaiter, M. V. Packhov, D. A. Kirkwood, J. P. Maier, and G. Fischer, J. Phys. Chem. A **103**, 9712 (1999).

acet-$C_{11}H^-$

$^3\Sigma^-$ $C_{\infty v}$
T_0 = 24288(10) gas MPD[1] $^3\Sigma^- - \tilde{X}$ 391–412 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		CC stretch	1234(10)	gas	MPD	1
		CC stretch	725(10)	gas	MPD	1

Reference

[1] M. Tulej, F. Güthe, M. Schnaiter, M. V. Packhov, D. A. Kirkwood, J. P. Maier, and G. Fischer, J. Phys. Chem. A **103**, 9712 (1999).

$HC_{11}H$

$^3\Sigma_u^-$ $D_{\infty h}$
T_0 = 15294.9 gas CR[2] $^3\Sigma_u^- - \tilde{X}$ 579–654 nm
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	1944.5(3)	gas	CR	2
			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 = 15345.5 gas CR[2] $^3\Sigma_u^- - \tilde{X}$ 578–652 nm
15294(5) Ne AB[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+		C≡C s-stretch	1944.1(3)	gas	CR	2

References

[1] J. Fulara, P. Freivogel, D. Forney, and J. P. Maier, J. Chem. Phys. **103**, 8805 (1995).
[2] C. D. Ball, M. C. McCarthy, and P. Thaddeus, J. Chem. Phys. **112**, 10149 (2000).

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^+	7		2140.6T	Ar	IR	2
	8		2003.9T	Ne	IR	1
			1997.2	Ar	IR	2
	9		1818.0	Ar	IR	2

References

[1] P. Freivogel, M. Grutter, D. Forney, and J. P. Maier, Chem. Phys. **216**, 401 (1997).
[2] X. D. Ding, S. L. Wang, C. M. L. Rittby, and W. R. M. Graham, J. Chem. Phys. **112**, 5113 (2000).

cyc-C_{12}

(2) $^1E_{1u}$ D_{6h}
$T_0 = 30112(18)$ Ne AB[1] 290–332 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g			1882(28)	Ne	AB	1
			300(26)	Ne	AB	1

(1) $^1E_{1u}$ D_{6h}
$T_0 = 13893(4)$ Ne AB[1] 626–720 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g			2071(7)	Ne	AB	1
			1907(7)	Ne	AB	1

Reference

[1] M. Grutter, M. Wyss, E. Riaplov, J. P. Maier, S. D. Peyerimhoff, and M. Hanrath, J. Chem. Phys. **111**, 7397 (1999).

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

$\tilde{C}\,^2\Pi_u$ $D_{\infty h}$
$T_0 = 8100(100)$ gas MPD[4] $\tilde{C}-\tilde{X}$ 1100–1240 nm
8006(5) Ne AB[1] $\tilde{C}-\tilde{X}$ 1200–1250 nm
7906(10) Ar AB[5]

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).
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[3] P. Freivogel, M. Grutter, D. Forney, and J. P. Maier, J. Chem. Phys. **107**, 4468 (1997).
[4] M. Ohara, D. Kasuya, H. Shiromaru, and Y. Achiba, J. Phys. Chem. A **104**, 8622 (2000).
[5] J. Szczepanski, J. Fuller, S. Ekern, and M. Vala, Spectrochim. Acta A **57**, 775 (2001).

$C_{12}H$

$^2\Pi_{3/2}$ $C_{\infty v}$
$T_0 = 12492(5)$ 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

$B_0 = 0.0058$ MW[2]

References

[1] P. Freivogel, J. Fulara, M. Jakobi, D. Forney, and J. P. Maier, J. Chem. Phys. **103**, 54 (1995).
[2] C. A. Gottlieb, M. C. McCarthy, M. J. Travers, J.-U. Grabow, and P. Thaddeus, J. Chem. Phys. **109**, 5433 (1998).

cum-$C_{12}H^-$ [a]

$\tilde{A}$
$T_0 = 25654(10)$ gas MPD[1] $\tilde{A}-\tilde{X}$ 377–390 nm
25806(15) Ne AB[1]

[a]This isomer of $C_{12}H^-$, with cumulenic bonding, lies at a somewhat higher energy than the acetylenic isomer, and either the $\tilde{X}$ or the $\tilde{A}$ state may be nonlinear.

Reference

[1] D. A. Kirkwood, M. Tulej, M. V. Pachkov, M. Schnaiter, F. Güthe, M. Grutter, M. Wyss, J. P. Maier, and G. Fischer, J. Chem. Phys. **111**, 9280 (1999).

acet-$C_{12}H^-$

$^1\Sigma^+$ $C_{\infty v}$
$T_0 = 26802(10)$ gas MPD[2] $^1\Sigma^+ - \tilde{X}$ 339–373 nm
26961(15) Ne AB[1,2] $^1\Sigma^+ - \tilde{X}$ 315–372 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		CC stretch	2100(15)	gas	MPD	2
			2034(20)	Ne	AB	1,2
		C–C stretch	776(15)	gas	MPD	2
			737(20)	Ne	AB	1,2

$\tilde{X}\,^1\Sigma^+$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		CC stretch	1986	Ne	IR	1

References

[1] M. Grutter, M. Wyss, and J. P. Maier, J. Chem. Phys. **110**, 1492 (1999).
[2] D. A. Kirkwood, M. Tulej, M. V. Pachkov, M. Schnaiter, F. Güthe, M. Grutter, M. Wyss, J. P. Maier, and G. Fischer, J. Chem. Phys. **111**, 9280 (1999).

$HC_{12}H$

$^1\Sigma_u^+$ $D_{\infty h}$
$T_0 = 38971(30)$ Ne AB[1] $^1\Sigma_u^+ - X$ 232–257 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+		CC stretch	2029(40)	Ne	AB	1

Reference

[1] M. Grutter, M. Wyss, J. Fulara, and J. P. Maier, J. Phys. Chem. A **102**, 9785 (1998).

$HC_{12}H^-$

(3) $^2\Pi_g$ $D_{\infty h}$
$T_0 = 31506(20)$ Ne AB[1]

(2) $^2\Pi_g$ $D_{\infty h}$
$T_0 = 13526(4)$ Ne AB[1] $(2)^2\Pi_g - \tilde{X}$ 522–740 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+		CC stretch	2301(7)	Ne	AB	1
		CC stretch	2014(7)	Ne	AB	1
		C–C stretch	464(6)	Ne	AB	1

(1) $^2\Pi_g$ $D_{\infty h}$
$T_0 = 12814(3)$ Ne AB[1] $(1)^2\Pi_g - \tilde{X}$ 650–781 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+		CC stretch	2140(6)	Ne	AB	1
		CC stretch	1994(6)	Ne	AB	1
		C–C stretch	550(5)	Ne	AB	1

Reference

[1] M. Grutter, M. Wyss, J. Fulara, and J. P. Maier, J. Phys. Chem. A **102**, 9785 (1998).

C_{13}

$^1\Sigma_u^+$ $D_{\infty h}$
$T_0 = 26341(15)$ Ne AB[2] $^1\Sigma_u^+ - \tilde{X}$ 370–380 nm
24969 Ar AB[4]

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

$\tilde{a}$ $D_{\infty h}$
$T^a = 7750(80)$ gas PE[3]

$\tilde{X}\,^1\Sigma_g^+$ $D_{\infty h}$ 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]

[a] From vertical ionization potentials.

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).
[3] M. Kohno, S. Suzuki, H. Shiromaru, and Y. Achiba, J. Chem. Phys. **110**, 3781 (1999).
[4] J. Szczepanski, J. Fuller, S. Ekern, and M. Vala, Spectrochim. Acta A **57**, 775 (2001).

C_{13}^-

$\tilde{B}\,^2\Pi_g$ $D_{\infty h}$
$T_0 = 11300(100)$ gas MPD[2] $\tilde{B}-\tilde{X}$ 813–885 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			400T	gas	MPD	2

$\tilde{A}\,^2\Pi_g$ $D_{\infty h}$
$T_0 = 9500(100)$ gas MPD[2] $\tilde{A}-\tilde{X}$ 917–1053 nm
9502(2) Ne AB[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			300T	gas	MPD	2

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[1] M. Wyss, M. Grutter, and J. P. Maier, Chem. Phys. Lett. **304**, 35 (1999).
[2] M. Ohara, D. Kasuya, H. Shiromaru, and Y. Achiba, J. Phys. Chem. A **104**, 8622 (2000).

$C_{13}H$

$\tilde{X}\,^2\Pi_{1/2}$ $C_{\infty v}$
$B_0 = 0.0046$ MW[1]

Reference

[1] C. A. Gottlieb, M. C. McCarthy, M. J. Travers, J.-U. Grabow, and P. Thaddeus, J. Chem. Phys. **109**, 5433 (1998).

cum-$C_{13}H^-$ [a]

$^1A'$ C_s
$T_0 = 24726(10)$ gas MPD[1]

[a]This isomer of $C_{13}H^-$, with cumulenic bonding, lies at a somewhat higher energy than the acetylenic isomer.

Reference

[1] M. Tulej, F. Güthe, M. Schnaiter, M. V. Packhov, D. A. Kirkwood, J. P. Maier, and G. Fischer, J. Phys. Chem. A **103**, 9712 (1999).

acet-$C_{13}H^-$

$^3\Sigma^-$ $C_{\infty v}$
$T_0 = 22200(10)$ gas MPD[1] $^3\Sigma^- - \tilde{X}$ 410–450 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		C≡C stretch	2144(10)	gas	MPD	1
		C–C stretch	739(10)	gas	MPD	1
		C–C stretch	617(10)	gas	MPD	1

Reference

[1] M. Tulej, F. Güthe, M. Schnaiter, M. V. Packhov, D. A. Kirkwood, J. P. Maier, and G. Fischer, J. Phys. Chem. A **103**, 9712 (1999).

$HC_{13}H$

$^3\Sigma_u^-$ $D_{\infty h}$
$T_0 = 13916.4(3)$ gas CR[2]
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

$DC_{13}D$

$^3\Sigma_u^-$ $D_{\infty h}$
$T_0 = 13951.3(3)$ gas CR[2]

References

[1] J. Fulara, P. Freivogel, D. Forney, and J. P. Maier, J. Chem. Phys. **103**, 8805 (1995).
[2] C. D. Ball, M. C. McCarthy, and P. Thaddeus, J. Chem. Phys. **112**, 10149 (2000).

C_{14}

$\tilde{A}$
$T_0 = 19010$ N_2 LF[1] $\tilde{A}-\tilde{X}$ 526–640 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			437	N_2	LF	1
			108	N_2	LF	1

$\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2218	N_2	Ra	1
			2089	N_2	Ra	1
			1926	N_2	Ra	1
			1807	N_2	Ra	1
			1655	N_2	Ra	1
			1627	N_2	Ra	1
			1394	N_2	Ra	1
			1211	N_2	Ra	1
			851	N_2	Ra	1
			829	N_2	Ra	1
			282	N_2	Ra	1

Reference

[1] G. A. Rechtsteiner, C. Felix, A. K. Ott, O. Hampe, R. P. Van Duyne, M. F. Jarrold, and K. Raghavachari, J. Phys. Chem. A **105**, 3029 (2001).

cyc-C_{14}

$^1E_{1u}$
$T_0 = 28837(17)$ Ne AB[1]

Reference

[1] M. Grutter, M. Wyss, E. Riaplov, J. P. Maier, S. D. Peyerimhoff, and M. Hanrath, J. Chem. Phys. **111**, 7397 (1999).

C_{14}^-

(2) $^2\Pi_g$ $D_{\infty h}$
$T_0 = 10200(100)$ gas MPD[3]
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

$\tilde{C}\,^2\Pi_g$ $D_{\infty h}$
$T_0 = 6900(100)$ gas MPD[3] $\tilde{C}-\tilde{X}$ 1333–1450 nm
6849(5) Ne AB[1] $\tilde{C}-\tilde{X}$ 1402–1460 nm
6782 Ar AB[4]

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).
[3] M. Ohara, D. Kasuya, H. Shiromaru, and Y. Achiba, J. Phys. Chem. A **104**, 8622 (2000).
[4] J. Szczepanski, J. Fuller, S. Ekern, and M. Vala, Spectrochim. Acta A **57**, 775 (2001).

$C_{14}H$

$^2\Pi_{3/2}$ $C_{\infty v}$
$T_0 = 11554(5)$T Ne AB[1]
$B_0 = 0.0037$ MW[2]

References

[1] P. Freivogel, J. Fulara, M. Jakobi, D. Forney, and J. P. Maier, J. Chem. Phys. **103**, 54 (1995).
[2] C. A. Gottlieb, M. C. McCarthy, M. J. Travers, J.-U. Grabow, and P. Thaddeus, J. Chem. Phys. **109**, 5433 (1998).

cum-$C_{14}H^-$ [a]

$\tilde{A}$
$T_0 = 23763(10)$ gas MPD[1] $\tilde{A}-\tilde{X}$ 369–421 nm
23837(15) Ne AB[1] $\tilde{A}-\tilde{X}$ 361–420 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CC stretch	1996(15)	gas	MPD	1
			1982(20)	Ne	AB	1
		C=C stretch	1747(15)	gas	MPD	1
		C–C stretch	1280(15)	gas	MPD	1
			1244(20)	Ne	AB	1

[a]This isomer of $C_{14}H^-$, with cumulenic bonding, lies at a somewhat higher energy than the acetylenic isomer, and either the $\tilde{X}$ or the $\tilde{A}$ state may be nonlinear.

Reference

[1] D. A. Kirkwood, M. Tulej, M. V. Pachkov, M. Schnaiter, F. Güthe, M. Grutter, M. Wyss, J. P. Maier, and G. Fischer, J. Chem. Phys. **111**, 9280 (1999).

acet-$C_{14}H^-$

$^1\Sigma^+$ $C_{\infty v}$
$T_0 = 23763(10)$ gas MPD[1,3] $^1\Sigma^+-\tilde{X}$ 369–421 nm
23837(15) Ne AB[1–3] $^1\Sigma^+-\tilde{X}$ 360–420 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3127(7)	gas	MPD	1
			3136(20)	Ne	AB	1
	3		2276(7)	gas	MPD	1
			2238(20)	Ne	AB	1,2
			1996(15)	gas	MPD	1,3
			1982(20)	Ne	AB	1–3
		CC stretch	1838(15)	gas	MPD	3
			1597(15)	gas	MPD	3
			1280(15)	gas	MPD	1,3
			1244(20)	Ne	AB	1–3
			579(15)	gas	MPD	1,3
			539(20)	Ne	AB	1,2
			490(15)T	gas	MPD	1,3
			463(20)T	Ne	AB	1–3

$\tilde{X}\,^1\Sigma^+$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		CC stretch	1958	Ne	IR	2
		CC stretch	1888	Ne	IR	2

References

[1] D. A. Kirkwood, H. Linnartz, M. Grutter, O. Dopfer, T. Motylewski, M. Pachkov, M. Tulej, M. Wyss, and J. P. Maier, Faraday Discuss. **109**, 109 (1998).
[2] M. Grutter, M. Wyss, and J. P. Maier, J. Chem. Phys. **110**, 1492 (1999).
[3] D. A. Kirkwood, M. Tulej, M. V. Pachkov, M. Schnaiter, F. Güthe, M. Grutter, M. Wyss, J. P. Maier, and G. Fischer, J. Chem. Phys. **111**, 9280 (1999).

$HC_{14}H$

$^1\Sigma_u^+$ $D_{\infty h}$
$T_0 = 36377(37)$ Ne AB[1] $^1\Sigma_u^+ - X$ 236–275 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+		CC stretch	2040(37)	Ne	AB	1

Reference

[1] M. Grutter, M. Wyss, J. Fulara, and J. P. Maier, J. Phys. Chem. A **102**, 9785 (1998).

$HC_{14}H^-$

(3) $^2\Pi_u$ $D_{\infty h}$
$T_0 = 29070(17)$ Ne AB[1]

(2) $^2\Pi_u$ $D_{\infty h}$
$T_0 = 12309(4)$ Ne AB[1] $(2)^2\Pi_u - \tilde{X}$ 639–813 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+		CH stretch	3335(7)	Ne	AB	1
		CC stretch	2205(7)	Ne	AB	1

(1) $^2\Pi_u$ $D_{\infty h}$
$T_0 = 11633(3)$ Ne AB[1] $(1)^2\Pi_u - \tilde{X}$ 734–860 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+		CC stretch	1976(5)	Ne	AB	1

Reference

[1] M. Grutter, M. Wyss, J. Fulara, and J. P. Maier, J. Phys. Chem. A **102**, 9785 (1998).

C_{15}

$^1\Sigma_u^+$ $D_{\infty h}$
$T_0 = 23832(12)$ Ne AB[1] $^1\Sigma_u^+ - \tilde{X}$ 410–420 nm
22371 Ar AB[3]

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

$\tilde{a}$ $D_{\infty h}$
$T^a = 6370(80)$ gas PE[2]

[a]From vertical ionization potentials.

References

[1] D. Forney, P. Freivogel, M. Grutter, and J. P. Maier, J. Chem. Phys. **104**, 4954 (1996).
[2] M. Kohno, S. Suzuki, H. Shiromaru, and Y. Achiba, J. Chem. Phys. **110**, 3781 (1999).
[3] J. Szczepanski, J. Fuller, S. Ekern, and M. Vala, Spectrochim. Acta A **57**, 775 (2001).

C_{15}^-

$\tilde{B}\,^2\Pi_u$ $D_{\infty h}$
$T_0 = 10100(100)$ gas MPD[2] $\tilde{B} - \tilde{X}$ 833–990 nm

$\tilde{A}\,^2\Pi_u$ $D_{\infty h}$
$T_0 = 8300(100)$ gas MPD[2] $\tilde{A} - \tilde{X}$ 1123–1205 nm
8316 Ne AB[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			300T	gas	MPD	2

References

[1] M. Wyss, M. Grutter, and J. P. Maier, Chem. Phys. Lett. **304**, 35 (1999).
[2] M. Ohara, D. Kasuya, H. Shiromaru, and Y. Achiba, J. Phys. Chem. A **104**, 8622 (2000).

cum-$C_{15}H^-$ [a]

$^1A'$ C_s
$T_0 = 23284(10)$ gas MPD[1]

[a]This isomer of $C_{15}H^-$, with cumulenic bonding, lies at a somewhat higher energy than the acetylenic isomer.

Reference

[1] M. Tulej, F. Güthe, M. Schnaiter, M. V. Packhov, D. A. Kirkwood, J. P. Maier, and G. Fischer, J. Phys. Chem. A **103**, 9712 (1999).

acet-$C_{15}H^-$

$^3\Sigma^-$ $C_{\infty v}$
$T_0 = 19434(10)$ gas MPD[1] $^3\Sigma^- - \tilde{X}$ 498–515 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		C–C stretch	618(10)	gas	MPD	1

Reference

[1] M. Tulej, F. Güthe, M. Schnaiter, M. V. Packhov, D. A. Kirkwood, J. P. Maier, and G. Fischer, J. Phys. Chem. A **103**, 9712 (1999).

C_{16}

$\tilde{X}$ $D_{\infty h}$?

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2200	N_2	Ra	1
			2096	N_2	Ra	1
			1920	N_2	Ra	1
			1372T	N_2	Ra	1
			735	N_2	Ra	1
			646	N_2	Ra	1
			468	N_2	Ra	1
			249	N_2	Ra	1

Reference

[1] A. K. Ott, G. A. Rechtsteiner, C. Felix, O. Hampe, M. F. Jarrold, and R. P. Van Duyne, J. Chem. Phys. **109**, 9652 (1998).

C_{16}^-

(2) $^2\Pi_u$ $D_{\infty h}$
$T_0 = 9100(100)$ gas MPD[2]

(1) $^2\Pi_u$ $D_{\infty h}$
$T_0 = 5800(100)$ gas MPD[2] $^2\Pi_u - \tilde{X}$ 1587–1725 nm
5784(5) Ne AB[1] $^2\Pi_u - \tilde{X}$ 1658–1730 nm
5732(2) Ar AB[3] $^2\Pi_u - \tilde{X}$ 1668–1745 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	8		245(5)	Ne	AB	1
			263(3)	Ar	AB	3

References

[1] P. Freivogel, J. Fulara, M. Jakobi, D. Forney, and J. P. Maier, J. Chem. Phys. **103**, 54 (1995).
[2] M. Ohara, D. Kasuya, H. Shiromaru, and Y. Achiba, J. Phys. Chem. A **104**, 8622 (2000).
[3] J. Szczepanski, J. Fuller, S. Ekern, and M. Vala, Spectrochim. Acta A **57**, 775 (2001).

8.16. Non-Hydrocarbons With More Than Eight Atoms

CH_3BNCH_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2060.1	Ar	IR	1
			2058.9			

Reference

[1] D. V. Lanzisera and L. Andrews, J. Phys. Chem. A **101**, 824 (1997).

C_2H_5ZnH

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	2977.7	Ar	IR	1
		CH stretch	2974.0	Ar	IR	1
		CH stretch	2960.2	Ar	IR	1
		ZnH stretch	1869.3	Ar	IR	1
		CH_3 deform.	1465.4	Ar	IR	1
		CH_2 bend	1436.9	Ar	IR	1
		CH_3 deform.	1378.0	Ar	IR	1
		CC stretch	960.3	Ar	IR	1
		CH_2 wag	829.3	Ar	IR	1
			827.2			
		CZn stretch	545.8	Ar	IR	1

Reference

[1] V. A. Bracken, N. Legay-Sommaire, and J. G. McCaffrey, J. Phys. Chem. A **101**, 9863 (1997).

$(CH_3)_2GaH$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	GaH stretch	1869.5	Ar	IR	1
b_1	16	CH_3 umbrella	1202.5	Ar	IR	1
	18	GaC_2 a-stretch	589.5	Ar	IR	1
	19	CGaH deform.	556.0	Ar	IR	1
b_2	22	CH_3 deform.	729.0	Ar	IR	1
	23	H deform.	415.5	Ar	IR	1

Reference

[1] J. Müller, H. Sternkicker, U. Bergmann, and B. Atakan, J. Phys. Chem. A **104**, 3627 (2000).

$CH_3SiH{=}CH_2$

In the gas phase, absorption between 220 and 300 nm, with a maximum at 38460 (260 nm) has been assigned[7] to $CH_3SiH{=}CH_2$. In an argon matrix, an absorption maximum at 38460 (260 nm) has also been assigned[1,3,4] to this product.

$\tilde{X}$[a] C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CH stretch	3018w	Ar	IR	5
		CH stretch	2976w	Ar	IR	5
		SiH stretch	2181.1s	Ar	IR	1–6
		CH_3 deform.	1411.7w	Ar	IR	3,5,6
		CH_2 scissors	1297.4w	Ar	IR	1,3–6
		CH_3 deform.	1254.2s	Ar	IR	1–6
		Si=C stretch	989.1s	Ar	IR	1–6
		SiH deform.	878.4s	Ar	IR	1–3,5,6
		Deformation	810.3vs	Ar	IR	1–6
		Si–C stretch	677.9wm	Ar	IR	3,5,6
a''		CH_3 deform.	1393.6w	Ar	IR	3,5,6
		CH_2 wag	713.7m	Ar	IR	1–6
		CH deform.	615.9m	Ar	IR	1,3–6

[a]Assigned using the density functional theory calculations of Ref. 8.

References

[1] T. J. Drahnak, J. Michl, and R. West, J. Am. Chem. Soc. **103**, 1845 (1981).
[2] H. P. Reisenauer, G. Mihm, and G. Maier, Angew. Chem. **94**, 864 (1982); Angew. Chem. Int. Ed. Engl. **21**, 854 (1982).
[3] C. A. Arrington, K. A. Klingensmith, R. West, and J. Michl, J. Am. Chem. Soc. **106**, 525 (1984).
[4] G. Maier, G. Mihm, H. P. Reisenauer, and D. Littmann, Chem. Ber. **117**, 2369 (1984).
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[6] M. Trommer, W. Sander, and A. Patyk, J. Am. Chem. Soc. **115**, 11775 (1993).
[7] R. K. Vatsa, A. Kumar, P. D. Naik, H. P. Upadhyaya, U. B. Pavanaja, R. D. Saini, J. P. Mittal, and J. Pola, Chem. Phys. Lett. **255**, 129 (1996).
[8] V. N. Khabashesku, K. N. Kudin, and J. L. Margrave, J. Mol. Struct. **443**, 175 (1998).

$(CH_3)_2Si=CH_2$

$\tilde{X}$[a] C_{2v} Structure: ED[3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CH stretch	2991.6w	Ar	IR	7
		CH stretch	2968.7w	Ar	IR	7
		CH_2 scissors	1413.6w	Ar	IR	7
		CH_3 rock	1265.2w	Ar	IR	7
		Si=C stretch	1003.8s	Ar	IR	1,2,4,5,7
		CH_3 rock	818.2m	Ar	IR	1,4,5,7
		Si–C s-stretch	625.1wm	Ar	IR	7
b_1		CH stretch	2896.5w	Ar	IR	7
		CH_3 rock	1423.3wm	Ar	IR	7
		CH_2 wag	643.9m	Ar	IR	1,2,4,5,7
b_2		CH stretch	2862.0w	Ar	IR	7
		CH_3 rock	1261.6wm	Ar	IR	1,4,5,7
		Deformation	826.2vs	Ar	IR	1,2,4,5,7
		Si–C a-stretch	711.6w	Ar	IR	7

$(CD_3)_2Si=CD_2$

$\tilde{X}$[a] C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		Si=C stretch	1112.0ms	Ar	IR	6
		CD_3 deform.	1002.5sh	Ar	IR	6
		Mixed	866.5m	Ar	IR	6
		CD_3 rock	651.2m	Ar	IR	6
b_1		CD_3 rock	1028.0w	Ar	IR	6
		CD_2 wag	501.6s	Ar	IR	6
b_2		CD_3 deform.	1005.0m	Ar	IR	6
		SiC a-stretch	732.0vs	Ar	IR	6

[a]Assigned using the density functional theory calculations of Ref. 8.

References

[1] A. K. Mal'tsev, V. N. Khabashesku, and O. M. Nefedov, Dokl. Akad. Nauk SSSR **233**, 421 (1977); Dokl. Phys. Chem. **233**, 332 (1977).
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[5] L. E. Gusel'nikov, V. V. Volkova, V. G. Avakyan, and N. S. Nametkin, J. Organomet. Chem. **201**, 137 (1980).
[6] A. K. Mal'tsev, V. N. Khabashesku, and O. M. Nefedov, J. Organomet. Chem. **271**, 55 (1984).
[7] M. Trommer, W. Sander, and A. Patyk, J. Am. Chem. Soc. **115**, 11775 (1993).
[8] V. N. Khabashesku, K. N. Kudin, and J. L. Margrave, J. Mol. Struct. **443**, 175 (1998).

$(CH_3)_2Ge=CH_2$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		$=CH_2$ a-stretch	3008.0	Ar	IR	1
		CH s-stretch	2973.3	Ar	IR	1
		CH_2 scissors	1348.3	Ar	IR	1
		Mixed	847.3	Ar	IR	1
		Ge=C stretch	818.8	Ar	IR	1
		Ge–C s-stretch	576.0	Ar	IR	1
b_1		CH a-stretch	2927.9	Ar	IR	1
		CH_3 deform.	1416.8	Ar	IR	1
		CH_2 wag	596.0	Ar	IR	1
b_2		CH a-stretch	2874.0	Ar	IR	1
		CH_3 rock	1241.7	Ar	IR	1
		Deformation	804.4	Ar	IR	1
		Ge–C a-stretch	580.1	Ar	IR	1

Reference

[1] V. N. Khabashesku, K. N. Kudin, J. Tamás, S. E. Boganov, J. L. Margrave, and O. M. Nefedov, J. Am. Chem. Soc. **120**, 5005 (1998).

$(CH_3)_2Si{=}CHCH_3$

$\tilde{X}$[a] C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CH stretch	3015.3w	Ar	IR	1,2,4
		CH stretch	2980m	Ar	IR	1,2
		CH stretch	2933.1wm	Ar	IR	1,2,4
		CH stretch	2869.0wm	Ar	IR	1,2,4
		CH_3 deform.	1465.2wm	Ar	IR	1,2,4
		CH_3 deform.	1378.8wm	Ar	IR	1,2,4
		CH bend	1314.9w	Ar	IR	1,2,4
		CH_3 rock	1260.2m	Ar	IR	1,2,4
		C–C stretch	1116.1w	Ar	IR	1,2,4
		Deformation	984.9m	Ar	IR	1,2,4
		Mixed	882.7ms	Ar	IR	1,2,4
		CH_3 rock	794.5vs	Ar	IR	1–4
		Mixed	771.9wm	Ar	IR	4
		SiC a-stretch	712m	Ar	IR	1,2
			708sh			
		SiC s-stretch	607.7w	Ar	IR	1–4
		Deformation	358m	Ar	IR	1,2
a''		CH stretch	2965m	Ar	IR	1,2
		CH stretch	2901.8wm	Ar	IR	1,2,4
			2897.5wm			
		CH_3 deform.	1407.8wm	Ar	IR	1,2,4
		CH_3 rock	808	Ar	IR	1,2
		CH OPLA	645.7wm	Ar	IR	1–4
			644.1wm			

[a]Assigned using the density functional calculations of Ref. 5.

References

[1] O. L. Chapman, C.-C. Chang, J. Kolc, M. E. Jung, J. A. Lowe, T. J. Barton, and M. L. Tumey, J. Am. Chem. Soc. **98**, 7844 (1976).
[2] M. R. Chedekel, M. Skoglund, R. L. Kreeger, and H. Shechter, J. Am. Chem. Soc. **98**, 7846 (1976).
[3] A. K. Mal'tsev, V. A. Korolev, V. N. Khabashesku, and O. M. Nefedov, Dokl. Akad. Nauk SSSR **251**, 1166 (1980); Dokl. Phys. Chem. **251**, 295 (1980).
[4] M. Trommer, W. Sander, and A. Patyk, J. Am. Chem. Soc. **115**, 11775 (1993).
[5] V. N. Khabashesku, K. N. Kudin, and J. L. Margrave, J. Mol. Struct. **443**, 175 (1998).

SiC_9

$\tilde{X}\,^3\Sigma$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	4		1935.8	Ar	IR	1

Reference

[1] X. D. Ding, S. L. Wang, C. M. L. Rittby, and W. R. M. Graham, J. Chem. Phys. **110**, 11214 (1999).

FCCCF=CFCCF

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			2337.3vs	Ne	IR	1
			1678.0w	Ne	IR	1
			1072.1vs	Ne	IR	1
b_2			1398.5wm	Ne	IR	1
			912.5wm	Ne	IR	1

Reference

[1] H. H. Wenk, A. Balster, W. Sander, D. A. Hrovat, and W. T. Borden, Angew. Chem. Int. Ed. **40**, 2295 (2001).

p-$ClCC_6H_4CCl$

In an argon matrix,[2] a structured absorption maximum at 22730 (440 nm) has been assigned to *p*-$ClCC_6H_4CCl$. In a nitrogen matrix,[1] bands between 21640 (462 nm) and 24330 (411 nm) are contributed by this species.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1582s	Ar	IR	2
			1565s	N_2	IR	1
			1386w	Ar	IR	2
			1388w	N_2	IR	1
			1323w	N_2	IR	1
			1190m	Ar	IR	2
			1117w	N_2	IR	1
			1019m	Ar	IR	2
			958m	Ar	IR	2
			958m	N_2	IR	1
			939w	Ar	IR	2
			940w	N_2	IR	1
			918s	Ar	IR	2
			922m	N_2	IR	1
			918s			
			896w	Ar	IR	2
			897w	N_2	IR	1
			805m	Ar	IR	2
			809m	N_2	IR	1
			807m			
			709w	Ar	IR	2
			708m	N_2	IR	1
			689m	Ar	IR	2
			687m	N_2	IR	1
			600w	Ar	IR	2
			600m	N_2	IR	1
			464w	N_2	IR	1

References

[1] P. Zuev and R. S. Sheridan, J. Am. Chem. Soc. **115**, 3788 (1993).
[2] H. Tomioka, K. Komatsu, T. Nakayama, and M. Shimizu, Chem. Lett. 1291 (1993).

$CaOC_2H_5$

$\tilde{C}\,^2\Delta$ $C_{\infty v}^a$
$T_0 = 21650$T gas LF[2] $\tilde{C}-\tilde{X}$ 449–464 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CaO stretch	370(5)	gas	LF	2
		OCC bend	360(5)	gas	LF	2
		CaOC bend	80(5)	gas	LF	2

$\tilde{A}\,^2\Pi$ $C_{\infty v}^a$
$T_0 = 15890(5)$ gas LF[1] $\tilde{A}-\tilde{X}$ 623–635 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CaOC bend	531(5)	gas	LF	1
		CaO stretch	402(5)	gas	LF	1

$A = 63(5)$ gas LF[1]

$\tilde{X}\,^2\Sigma^+$ $C_{\infty v}^a$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CaOC bend	512(5)	gas	LF	1
		CaO stretch	385(5)	gas	LF	1
		CaOC bend	85(5)	gas	LF	1

[a]Symmetry given with respect to the spectroscopically active CaOC group.

References

[1] C. R. Brazier, L. C. Ellingboe, S. Kinsey-Nielsen, and P. F. Bernath, J. Am. Chem. Soc. **108**, 2126 (1986).
[2] M. Elhanine, R. Lawruszczuk, and B. Soep, Chem. Phys. Lett. **288**, 785 (1998).

$C_6H_5N{\equiv}N^+$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		N≡N stretch	2327vs	Ar	IR	1

Reference

[1] M. Winkler and W. Sander, Angew. Chem. Int. Ed. **39**, 2014 (2000).

$H(C{\equiv}C)_3CN^+$

$\tilde{A}\,^2\Pi$ $C_{\infty v}$
$T_0 = 14925.42$ gas AB^3
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

$B_0 = 0.0188$ AB^3

$\tilde{X}\,^2\Pi$ $C_{\infty v}$

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

$B_0 = 0.0190$ AB^3

$D(C{\equiv}C)_3CN^+$

$\tilde{A}\,^2\Pi$ $C_{\infty v}$
$T_0 = 14937.31$ gas AB^3
$B_0 = 0.0183$ AB^3

$\tilde{X}\,^2\Pi$ $C_{\infty v}$
$B_0 = 0.0183$ AB^3

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).
[3] W. E. Sinclair, D. Pfluger, D. Verdes, and J. P. Maier, J. Chem. Phys. **112**, 8899 (2000).

$H(C{\equiv}C)_3NC$

$\tilde{X}$ $C_{\infty v}$
$B_0 = 0.0194$ MW[1]

Reference

[1] P. Botschwina, Ä. Heyl, W. Chen, M. C. McCarthy, J.-U. Grabow, M. J. Travers, and P. Thaddeus, J. Chem. Phys. **109**, 3108 (1998).

C_9N

$^2\Pi$ $C_{\infty v}$
$T_0 = 14802(4)$ Ne AB^1 $^2\Pi-\tilde{X}$ 529–676 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		CC,CN stretch	2082(6)	Ne	AB	1
		C–C stretch	1480(6)	Ne	AB	1

Reference

[1] M. Grutter, M. Wyss, and J. P. Maier, J. Chem. Phys. **110**, 1492 (1999).

C_9N^-

$^1\Sigma^+$ $C_{\infty v}$
$T_0 = 30656(19)$ Ne AB[1] $^1\Sigma^+ - \tilde{X}$ 294–327 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		CC,CN stretch	2099(27)	Ne	AB	1
		C–C stretch	1283(27)	Ne	AB	1
		C–C stretch	448(27)	Ne	AB	1

$\tilde{X}\ ^1\Sigma^+$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		CC,CN stretch	2033	Ne	IR	1

Reference

[1] M. Grutter, M. Wyss, and J. P. Maier, J. Chem. Phys. **110**, 1492 (1999).

$C_{11}N$

$^2\Pi$ $C_{\infty v}$
$T_0 = 13207(4)$ Ne AB[1] $^2\Pi - \tilde{X}$ 654–758 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		CC,CN stretch	2070(6)	Ne	AB	1
		C–C stretch	1318(6)	Ne	AB	1

Reference

[1] M. Grutter, M. Wyss, and J. P. Maier, J. Chem. Phys. **110**, 1492 (1999).

$C_{11}N^-$

$^1\Sigma^+$ $C_{\infty v}$
$T_0 = 26295(14)$ Ne AB[1] $^1\Sigma - \tilde{X}$ 346–381 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		CC,CN stretch	2074(20)	Ne	AB	1
		C–C stretch	429(20)	Ne	AB	1

Reference

[1] M. Grutter, M. Wyss, and J. P. Maier, J. Chem. Phys. **110**, 1492 (1999).

$HC_{10}CN^-$

(3) $^2\Pi$ $C_{\infty v}$
$T_0 = 32895(22)$ Ne AB[1]

(2) $^2\Pi$ $C_{\infty v}$
$T_0 = 14196(4)$ Ne AB[1] $(2)^2\Pi - \tilde{X}$ 534–705 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		CH stretch	3338(9)	Ne	AB	1
		CC stretch	2297(9)	Ne	AB	1
		CC stretch	1974(9)	Ne	AB	1

(1) $^2\Pi$ $C_{\infty v}$
$T_0 = 13466(4)$ Ne AB[1] $(1)^2\Pi - \tilde{X}$ 566–743 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+			2117(7)	Ne	AB	1

Reference

[1] M. Grutter, M. Wyss, J. Fulara, and J. P. Maier, J. Phys. Chem. A **102**, 9785 (1998).

$C_{13}N$

$^2\Pi$ $C_{\infty v}$
$T_0 = 12085(3)$ Ne AB[1] $^2\Pi - \tilde{X}$ 750–828 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		C–C stretch	1238(4)	Ne	AB	1

Reference

[1] M. Grutter, M. Wyss, and J. P. Maier, J. Chem. Phys. **110**, 1492 (1999).

$C_{13}N^-$

$^1\Sigma^+$ $C_{\infty v}$
$T_0 = 22619(10)$ Ne AB[1]

Reference

[1] M. Grutter, M. Wyss, and J. P. Maier, J. Chem. Phys. **110**, 1492 (1999).

$HC_{12}CN^-$

(3) $^2\Pi$ $C_{\infty v}$
$T_0 = 29762(18)$ Ne AB[1]

(2) $^2\Pi$ $C_{\infty v}$
$T_0 = 12692(3)$ Ne AB[1] $(2)^2\Pi - \tilde{X}$ 624–788 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		CH stretch	3326(7)	Ne	AB	1
		CC stretch	2173(7)	Ne	AB	1
		CC stretch	1902(7)	Ne	AB	1

(1) $^2\Pi$ $C_{\infty v}$
$T_0 = 12038(3)$ Ne AB[1] $(1)^2\Pi - \tilde{X}$ 711–831 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		CC stretch	2019(6)	Ne	AB	1

Reference

[1] M. Grutter, M. Wyss, J. Fulara, and J. P. Maier, J. Phys. Chem. A **102**, 9785 (1998).

Cl_3TiOCH_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_3 stretch	3006	Ar	IR	1
		CH_3 stretch	2945	Ar	IR	1
		CH_3 deform.	1449	Ar	IR	1
		C–O stretch	1152vs	Ar	IR	1
		CH_3 rock	1109	Ar	IR	1
		CH_3 rock	1095	Ar	IR	1
		TiO stretch	636	Ar	IR	1
		TiCl stretch	486vs	Ar	IR	1

Cl_3TiOCD_3

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD_3 stretch	2237	Ar	IR	1
		CD_3 stretch	2086	Ar	IR	1
		C–O stretch	1196	Ar	IR	1
		CD_3 deform.	1047	Ar	IR	1
		CD_3 rock	859	Ar	IR	1
		CD_3 rock	855	Ar	IR	1
		TiO stretch	603	Ar	IR	1
		TiCl stretch	498	Ar	IR	1

Reference

[1] B. S. Ault and J. B. Everhart, J. Phys. Chem. **100**, 15726 (1996).

CH_2COCH_3

$\tilde{B}$
$T_0 = 27282.7(5)$ gas LF^{1-3} $\tilde{B}-\tilde{X}$ 331–369 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1668(25)[a]	gas	LF	3
			1303(25)[a]	gas	LF	3
			829(25)[a]	gas	LF	3
			454(25)[a]	gas	LF	3

$\tau_0 = 120(10)$ ns gas LF^1

[a] A series of low-frequency torsional transitions is superposed on each vibronic band.[3]

References

[1] S. Williams, E. Zingher, and J. C. Weisshaar, J. Phys. Chem. A **102**, 2297 (1998).
[2] N. Washida, S. Inomata, and M. Furubayashi, J. Phys. Chem. A **102**, 7924 (1998).
[3] S. Williams, L. B. Harding, J. F. Stanton, and J. C. Weisshaar, J. Phys. Chem. A **104**, 10131 (2000).

CH_3CHCHO

$\tilde{B}$
$T_0 = 29090.1(5)$T gas $LF^{1,2}$ $\tilde{B}-\tilde{X}$ 330–347 nm
$\tau_0 = 190(10)$ ns gas LF^1

References

[1] S. Williams, E. Zingher, and J. C. Weisshaar, J. Phys. Chem. A **102**, 2297 (1998).
[2] N. Washida, S. Inomata, and M. Furubayashi, J. Phys. Chem. A **102**, 7924 (1998).

n-C_3H_7O

$\tilde{B}$
$T_0 = 28634$ gas LF^{1-3} $\tilde{B}-\tilde{X}$ 335–520 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			969	gas	LF	3
		C_3 stretch	818	gas	LF	3
			796	gas	LF	3
			785	gas	LF	3
			647	gas	LF	3
		CO stretch	582	gas	LF	2,3
		CCO deformation	311	gas	LF	3
		C_3 deformation	260	gas	LF	3
		CH_3 torsion	203	gas	LF	3
		Skeletal flex	149	gas	LF	3

$\tau = 900(50)$ ns gas $LF^{1,2}$

$\tilde{X}$

Vib.	No.	Approximate	cm^{-1}	Med.	Type	Refs.
		CO stretch	1000(50)	gas	LF	1,2

References

[1] J. Bai, H. Okabe, and M. K. Emadi-Babaki, J. Photochem. Photobiol., A: Chem. **50**, 163 (1989).
[2] Ch. Mund, Ch. Fockenberg, and R. Zellner, Ber. Bunsenges. Phys. Chem. **102**, 709 (1998).
[3] C. C. Carter, J. R. Atwell, S. Gopalakrishnan, and T. A. Miller, J. Phys. Chem. A **104**, 9165 (2000).

$(CH_3)_2CHO$

$\tilde{B}$ C_s
$T_0 = 27171$ gas EM[1,4]LF[2,3,5,7] $\tilde{B}-\tilde{X}$ 330–540 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1212	gas	LF	7
			1152	gas	LF	7
			938	gas	LF	7
		C_3 stretch	860	gas	LF	7
		C–O stretch	574.4 (ω)	gas	LF	2,3,5,7
		CCO s-deformation	466	gas	LF	7
		CCO a-deform.	449	gas	LF	7
		C_3 deformation	378	gas	LF	7
		CH_3 s-torsion	357	gas	LF	7
		CH_3 a-torsion	344	gas	LF	7
			290(10)	gas	LF	5

$\tau = 0.64(9)$ μs gas EM[4]

$\tilde{A}\,^2A''$ C_s
$T_0 = 1225(65)$ gas PE[6]

$\tilde{X}\,^2A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			960(20)	gas	EM,LF PE	4–6
		Skel. s-deform.	500(15)	gas	PE	6
		CCC bend	375(25)	gas	PE	6

References

[1] K. Ohbayashi, H. Akimoto, and I. Tanaka, J. Phys. Chem. **81**, 798 (1977).
[2] R. J. Balla, H. H. Nelson, and J. R. McDonald, Chem. Phys. **99**, 323 (1985).
[3] S. C. Foster, Y.-C. Hsu, C. P. Damo, X. Liu, C.-Y. Kung, and T. A. Miller, J. Phys. Chem. **90**, 6766 (1986).
[4] J. Bai, H. Okabe, and J. B. Halpern, Chem. Phys. Lett. **149**, 37 (1988).
[5] Ch. Mund, Ch. Fockenberg, and R. Zellner, Ber. Bunsenges. Phys. Chem. **102**, 709 (1998).
[6] T. M. Ramond, G. E. Davico, R. L. Schwartz, and W. C. Lineberger, J. Chem. Phys. **112**, 1158 (2000).
[7] C. C. Carter, J. R. Atwell, S. Gopalakrishnan, and T. A. Miller, J. Phys. Chem. A **104**, 9165 (2000).

$(CH_3)_2CHO^-$

Threshold for electron detachment from ground-state $(CH_3)_2CHO^-$ = 14900(30) gas PE[1,2]

$\tilde{X}\,^1A'$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CCC bend	330(25)	gas	PE	2

References

[1] G. B. Ellison, P. C. Engelking, and W. C. Lineberger, J. Phys. Chem. **86**, 4873 (1982).
[2] T. M. Ramond, G. E. Davico, R. L. Schwartz, and W. C. Lineberger, J. Chem. Phys. **112**, 1158 (2000).

$(CH_3)_2Ge{=}O$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CH_3 rock	1239.1w	Ar	IR	1
		Ge=O stretch	943.0vs	Ar	IR	1
		CH_3 rock	857.4m	Ar	IR	1
b_1		CH_3 deform.	1441.2w	Ar	IR	1
		CH_3 rock	794.8m	Ar	IR	1
b_2		CH_3 rock	1234.0w	Ar	IR	1
		CH_3 rock	770.7m	Ar	IR	1
		GeC a-stretch	605.0s	Ar	IR	1

Reference

[1] V. N. Khabashesku, S. E. Boganov, K. N. Kudin, J. L. Margrave, and O. M. Nefedov, Organomet. **17**, 5041 (1998).

$(CH_3)_2Ge{=}S$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CH_3 deform.	1407	Ar	IR	2
	4	CH_3 deform.	1237	Ar	IR	2
	5	CH_3 rock	850s	Ar	IR	1,2
	6	Ge=S stretch	605vs	Ar	IR	1,2
	7	GeC s-stretch	516m	Ar	IR	1,2
b_1	14	CH_3 a-deform.	1390m	Ar	IR	1,2
	15	CH_3 deform.	761m	Ar	IR	1,2
b_2	21	CH_3 deform.	1229m	Ar	IR	1,2
	22	CH_3 rock	809	Ar	IR	2
	23	GeC a-stretch	574	Ar	IR	2

References

[1] J. Barrau, V. Balaji, and J. Michl, Organomet. **8**, 2034 (1989).
[2] V. N. Khabashesku, S. E. Boganov, P. S. Zuev, O. M. Nefedov, J. Tamás, A. Gömöry, and I. Besenyei, J. Organomet. Chem. **402**, 161 (1991).

$CH_3CHCOCH_3$

$\tilde{B}$

gas LF[1] $\tilde{B}-\tilde{X}$ 331–366 nm

Reference

[1] N. Washida, S. Inomata, and M. Furubayashi, J. Phys. Chem. A **102**, 7924 (1998).

$(CH_3)_2CCHO$

$\tilde{B}$

gas LF[1] $\tilde{B}-\tilde{X}$ 334–340 nm

Reference

[1] N. Washida, S. Inomata, and M. Furubayashi, J. Phys. Chem. A **102**, 7924 (1998).

$(CH_3)_2CCOCH_3$

$\tilde{B}$

gas LF[1] $\tilde{B}-\tilde{X}$ 330–364 nm

Reference

[1] N. Washida, S. Inomata, and M. Furubayashi, J. Phys. Chem. A **102**, 7924 (1998).

1-C_4H_9O

$\tilde{B}$ C_s

$T_0=28649$ gas LF[1] $\tilde{B}-\tilde{X}$ 335–350 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			710	gas	LF	1
			612	gas	LF	1
			512	gas	LF	1
			444	gas	LF	1
			334	gas	LF	1
			324	gas	LF	1
			271	gas	LF	1
		CH_3 torsion	207	gas	LF	1

Reference

[1] C. C. Carter, J. R. Atwell, S. Gopalakrishnan, and T. A. Miller, J. Phys. Chem. A **104**, 9165 (2000).

2-C_4H_9O

$\tilde{B}$

$T_0=26757$ gas LF[1,2] $\tilde{B}-\tilde{X}$ 350–380 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CC stretch	918	gas	LF	2
		CC stretch	729	gas	LF	2
		CO stretch	559	gas	LF	1,2
			470	gas	LF	2

$\tau\cong 85$ ns gas LF[1]

References

[1] C. Wang, L. G. Shemesh, W. Deng, M. D. Lilien, and T. S. Dibble, J. Phys. Chem. A **103**, 8207 (1999).
[2] C. C. Carter, J. R. Atwell, S. Gopalakrishnan, and T. A. Miller, J. Phys. Chem. A **104**, 9165 (2000).

$(CH_3)_3CO$

$\tilde{B}$ C_{3v}

$T_0=25861$ gas LF[1,2,4,5] $\tilde{B}-\tilde{X}$ 333–387 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			975	gas	LF	5
			855	gas	LF	5
			760	gas	LF	5
		CO stretch	546 (ω)	gas	LF	1,2,4,5
			311	gas	LF	1,2,4,5

$\tau\geqslant 1.5(1)$ μs gas LF[4]

$\tilde{X}\,^2E$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CO stretch	1205(15)	gas	PE	3
		C_3 umbrella	435(15)	gas	PE	3

References

[1] M. Blitz, M. J. Pilling, S. H. Robertson, and P. W. Seakins, Phys. Chem. Chem. Phys. **1**, 73 (1999).
[2] C. Wang, L. G. Shemesh, W. Deng, M. D. Lilien, and T. S. Dibble, J. Phys. Chem. A **103**, 8207 (1999).
[3] T. M. Ramond, G. E. Davico, R. L. Schwartz, and W. C. Lineberger, J. Chem. Phys. **112**, 1158 (2000).
[4] Ch. Lotz and R. Zellner, Phys. Chem. Chem. Phys. **2**, 2353 (2000).
[5] C. C. Carter, J. R. Atwell, S. Gopalakrishnan, and T. A. Miller, J. Phys. Chem. A **104**, 9165 (2000).

$(CH_3)_3CO^-$

Threshold for electron detachment from ground-state $(CH_3)_3CO^-$ = 15400(30) gas PE[1,2]

$\tilde{X}$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C_3 umbrella	440(25)	gas	PE	2

References

[1] G. B. Ellison, P. C. Engelking, and W. C. Lineberger, J. Phys. Chem. **86**, 4873 (1982).
[2] T. M. Ramond, G. E. Davico, R. L. Schwartz, and W. C. Lineberger, J. Chem. Phys. **112**, 1158 (2000).

C_9O

$\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2239.5wmT	Ar	IR	2
			2040.7vsT	Ar	IR	2

B_0 = 0.010 MW[1]

References

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[2] M. Dibben, J. Szczepanski, C. Wehlburg, and M. Vala, J. Phys. Chem. A **104**, 3584 (2000).

cyc-(N=CHN=CHC)=C=O

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	3036.1vw	Ar	IR	1
	3	CCO stretch	2152.7vs	Ar	IR	1
	4	Mixed	1493.5m	Ar	IR	1
	5	C=C stretch	1402.0vw	Ar	IR	1
	6	Mixed	1359.0m	Ar	IR	1
	7	Mixed	1278.3w	Ar	IR	1
	8	CH deform.	1197.5vw	Ar	IR	1
	9	Mixed	1177.8w	Ar	IR	1
	10	Mixed	1077.3w	Ar	IR	1
	11	Ring deform.	946.4m	Ar	IR	1
a''	18	Ring deform.	627.1vw	Ar	IR	1
	19	Ring deform.	616.3vw	Ar	IR	1
	20	CCO deform.	537.4vw	Ar	IR	1

Reference

[1] G. Maier and J. Endres, Eur. J. Org. Chem. 2535 (2000).

$Cl_2V(O)OCH_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_3 a-stretch	2940	Ar	IR	1
		CH_3 a-stretch	2933	Ar	IR	1
		CH_3 s-stretch	2827	Ar	IR	1
		CH_3 a-deform.	1447	Ar	IR	1
		CH_3 a-deform.	1444	Ar	IR	1
		CH_3 deform.	1430	Ar	IR	1
		CH_3 rock	1152	Ar	IR	1
		CH_3 rock	1121	Ar	IR	1
		C–O stretch	1069vs	Ar	IR	1
		V=O stretch	1030vs	Ar	IR	1
		V–O stretch	674s	Ar	IR	1
		VCl_2 stretch	502vs	Ar	IR	1
		VCl_2 stretch	446	Ar	IR	1

$Cl_2V(O)OCD_3$

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD_3 a-stretch	2186	Ar	IR	1
		CD_3 a-stretch	2179	Ar	IR	1
		CD_3 s-stretch	2050	Ar	IR	1
		CD_3 deform.	1085	Ar	IR	1
		C–O stretch	1066	Ar	IR	1
		CD_3 a-deform.	1050	Ar	IR	1
		V=O stretch	1030	Ar	IR	1
		CD_3 rock	897	Ar	IR	1
		CD_3 rock	887	Ar	IR	1
		V–O stretch	646	Ar	IR	1
		VCl_2 stretch	502	Ar	IR	1
		VCl_2 stretch	443	Ar	IR	1

Reference

[1] B. S. Ault, J. Phys. Chem. A **103**, 11474 (1999).

$C_2H_5O_2$

An unstructured gas-phase absorption between 200 and 290 nm, with maximum at 240 nm, has been assigned[1,3–5,7,8] to $C_2H_5O_2$.

$\tilde{A}$

T_0 = 7593(6) gas AB^2PE[9] $\tilde{A}$–$\tilde{X}$ 1175–1317 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	918(9)	gas	AB,PE	2,9
		Skel. bend	178(10)	gas	PE	9

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_2 a-stretch	3016wm	Ar	IR	6
		CH_2 scissors	1474m	Ar	IR	6
		CH_2 deform.	1451sh	Ar	IR	6
		CH_2 deform.	1389vs	Ar	IR	6
		CH_2 deform.	1380sh	Ar	IR	6
		CH_2 wag	1351m	Ar	IR	6
		CH_2 twist	1242w	Ar	IR	6
		CH_2 rock	1136m,br	Ar	IR	6
		OO stretch	1089(16)	gas	PE	9
			1112ms	Ar	IR	6
		CC stretch	1009s	Ar	IR	6
		CO stretch	838m	Ar	IR	6
		CH_2 rock	800m	Ar	IR	6
		Skel. bend	499vs	Ar	IR	6
		Skel. bend	234(9)	gas	PE	9

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$C_2H_5O_2^-$

Threshold for electron detachment from ground-state $C_2H_5O_2^- = 9570(30)$ gas PE[1]

Reference

[1] S. J. Blanksby, T. M. Ramond, G. E. Davico, M. R. Nimlos, S. Kato, V. M. Bierbaum, W. C. Lineberger, G. B. Ellison, and M. Okumura, J. Am. Chem. Soc. **123**, 9585 (2001).

t-$C_4H_9O_2$

A gas-phase absorption between 210 and 300 nm, with maximum near 240 nm, has been attributed[2] to *t*-$C_4H_9O_2$.

$\tilde{A}\ ^2A'$ C_s
$T_0 = 7800(90)$ gas PE[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		OO stretch	930(90)	gas	PE	4
			240(90)	gas	PE	4

$\tilde{X}\ ^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_3 rock	1187(2)vs	Ar	IR	3
		CH_3 rock	1139(2)m	Ar	IR	3
		OO stretch	1130(90)	gas	PE	4
			1124(2)s	Ar	IR	3
		CC stretch	808(2)ms	Ar	IR	3
			760(2)	gas	IR	1
		CO stretch	730(2)m	Ar	IR	3
			693.7(5)	gas	IR	1
		Skel. bend	539(2)ms	Ar	IR	3
		Skel. bend	403(2)wm	Ar	IR	3
		Skel. bend	361(2)m	Ar	IR	3
		Skel. bend	337(2)m	Ar	IR	3
			245(90)	gas	PE	4

References

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t-$C_4H_9O_2^-$

Threshold for electron detachment from ground-state *t*-$C_4H_9O_2^- = 9650(90)$ gas PE[1]

Reference

[1] E. P. Clifford, P. G. Wenthold, R. Gareyev, W. C. Lineberger, C. H. DePuy, V. M. Bierbaum, and G. B. Ellison, J. Chem. Phys. **109**, 10293 (1998).

(*cyc*-C_5H_4)O_2

(Cyclopentadiene Dioxirane)[a]

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1395s	Ar	IR	1,2
			1385vs	Ar	IR	1,2
			1184m	Ar	IR	1,2
			1179w	Ar	IR	1,2
			1142m	Ar	IR	1
			1023w	Ar	IR	1
			983w	Ar	IR	1
			938vw	Ar	IR	1
		C_5H_4 deform.	895vs	Ar	IR	1,2
		C_5H_4 deform.	741s	Ar	IR	1,2

[a]These absorptions were assigned by Ref. 1 to cyclopentadienone-O-oxide. However, Ref. 2 demonstrated that they are instead contributed by the dioxirane isomer.

References

[1] O. L. Chapman and T. C. Hess, J. Am. Chem. Soc. **106**, 1842 (1984).
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$O=C_6H_2=O$

(Dehydrobenzoquinone)

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C≡C stretch	2285(20)	gas	PE	1
	3		1685(15)	gas	PE	1
	4		1535(15)	gas	PE	1
	5		1240(20)	gas	PE	1
	8		465(15)	gas	PE	1
	9		405(15)	gas	PE	1

Reference

[1] G. E. Davico, R. L. Schwartz, T. M. Ramond, and W. C. Lineberger, J. Am. Chem. Soc. **121**, 6047 (1999).

$O=C_6H_2=O^-$

Threshold for electron detachment from ground-state $O=C_6H_2=O^-$ = 15000(40) gas PE[1]

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	8		460(20)	gas	PE	1
	9		260(20)	gas	PE	1

Reference

[1] G. E. Davico, R. L. Schwartz, T. M. Ramond, and W. C. Lineberger, J. Am. Chem. Soc. **121**, 6047 (1999).

CF_3OONO_2

In the gas phase,[3] the onset of continuous absorption occurs near 340 nm. The intensity of this absorption increases out to the measurement limit, near 190 nm.

$\tilde{X}$ C_1

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NO_2 a-stretch	1764s	gas	IR	1–3
			1762s	Ar	IR	3
	2	NO_2 s-stretch	1314sh	gas	IR	3
			1308m	Ar	IR	3
	3	CF_3 s-stretch	1303s	gas	IR	1–3
			1290s	Ar	IR	3
	4	CF_3 a-stretch	1243vs	gas	IR	1–3
			1238vs	Ar	IR	3
	5	CF_3 a-stretch	1192vs	gas	IR	1–3
			1187s	Ar	IR	3
	6	OO stretch	958wm	gas	IR	1–3
			960wm	Ar	IR	3
	7	CO stretch	860w	gas	IR	3
			880w	Ar	IR	3
	8	NO_2 scissors	792ms	gas	IR	1–3
			787m	Ar	IR	3
	9	ONO_2 OPLA	710wm	gas	IR	1–3
			708w	Ar	IR	3
	11	CF_3 a-deform.	674wm	gas	IR	1,3
			676w	Ar	IR	3
	12	CF_3 a-deform.	608wm	gas	IR	1,3
			609w	Ar	IR	3
	13	NO_2 rock	565w	gas	IR	1,3
			570w	Ar	IR	3
	14	N–OO stretch	495wm	gas	IR	1,3
			498w	Ar	IR	3
	15	CF_3 rock	445vw	gas	IR	1,3
			450w	Ar	IR	3
	16	CF_3 rock	380w	gas	IR	1,3
	17	OO–NO_2 deform.	286vw	gas	IR	1,3
	18	OO–CF_3 deform.	256w	gas	IR	1,3

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8.17. Molecules Related to Benzene

3,5-C_6H_3F

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CF stretch	1440vs	Ar	IR	1
		Mixed	1184ms	Ar	IR	1
		CC s-bend	884m	Ar	IR	1
b_1		CH wag	810m	Ar	IR	1
		CH wag	767wm	Ar	IR	1
		Mixed	532wm	Ar	IR	1
b_2		Mixed	949wm	Ar	IR	1
		Skel. deform.	543s	Ar	IR	1

Reference

[1] W. Sander and M. Exner, J. Chem. Soc., Perkin Trans. **2**, 2285 (1999).

o-C_6F_4

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1495.9wm	Ar	IR	1
			1459.1m	Ar	IR	1
			1289.0vw	Ar	IR	1
			1076.2m	Ar	IR	1
			1073.5wm			
b_2			1488.6vs	Ar	IR	1
			1483.4m			
			981.4wm	Ar	IR	1
			972.7ms			
			586.6w	Ar	IR	1
			465.6w	Ar	IR	1

Reference

[1] H. H. Wenk and W. Sander, Chem. Eur. J. **7**, 1837 (2001).

m-C_6F_4

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1823.8m	Ne	IR	1
			1817.7wm			
			1534.2vs	Ne	IR	1
			952.3vs	Ne	IR	1
b_1			488.2w	Ne	IR	1
b_2			1605.4vs	Ne	IR	1
			1497.0wm	Ne	IR	1
			1273.3wm	Ne	IR	1
			1268.5wm			
			992.7ms	Ne	IR	1
			981.3m			
			649.1w	Ne	IR	1
			511.6w	Ne	IR	1

Reference

[1] H. H. Wenk and W. Sander, Chem. Eur. J. **7**, 1837 (2001).

p-C_6F_4

$\tilde{X}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{1u}			1406.6m	Ne	IR	1
			1117.3ms	Ne	IR	1
b_{2u}			1516.1s	Ne	IR	1
			1501.7s			
			924.6s	Ne	IR	1

Reference

[1] H. H. Wenk, A. Balster, W. Sander, D. A. Hrovat, and W. T. Borden, Angew. Chem. Int. Ed. **40**, 2295 (2001).

2,4-C_6H_3OH

In an argon matrix,[1,2] the first absorption region has a shoulder at 28090 (356 nm), maxima at 29070 and 31450 (344 and 318 nm), and a shoulder at 32900 (304 nm). The second absorption region has maxima at 39060 (256 nm) and 42020 (238 nm).

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3612.0m	Ar	IR	1,2
	6		1516.3s	Ar	IR	1,2
	7		1429.0w	Ar	IR	1,2
	8		1368.2m	Ar	IR	1,2
	9		1290.1w	Ar	IR	1,2
	10		1259.4m	Ar	IR	1,2
	11		1209.1m	Ar	IR	1,2
	12	OH deform.	1157.6m	Ar	IR	1,2
	13		1128.6vw	Ar	IR	1,2
	14		971.0w	Ar	IR	1,2
	15		877.0w	Ar	IR	1,2
	16		641.2s	Ar	IR	1,2
	17		518.8s	Ar	IR	1,2
a''	22		694.7m	Ar	IR	1,2

References

[1] G. Bucher, W. Sander, E. Kraka, and D. Cremer, Angew. Chem. **104**, 1225 (1992); Angew. Chem. Int. Ed. Engl. **31**, 1230 (1992).
[2] W. Sander, G. Bucher, H. Wandel, E. Kraka, D. Cremer, and W. S. Sheldrick, J. Am. Chem. Soc. **119**, 10660 (1997).

m-C_6F_4I

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'			1636.8w	Ne	IR	1
			1562.3wm	Ne	IR	1
			1484.4vs	Ne	IR	1
			1416.6wm	Ne	IR	1
			1073.4ms	Ne	IR	1
			1030.4m	Ne	IR	1
			837.0wm	Ne	IR	1

Reference

[1] H. H. Wenk and W. Sander, Chem. Eur. J. **7**, 1837 (2001).

p-C_6F_4I

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1574.4w	Ne	IR	1
			1428.3wm	Ne	IR	1
			1352.2vw	Ne	IR	1
			1188.1wm	Ne	IR	1
			833.6wm	Ne	IR	1
b_2			1471.7vs	Ne	IR	1
			1259.4w	Ne	IR	1
			1138.4vw	Ne	IR	1
			941.9m	Ne	IR	1
			692.9wm	Ne	IR	1

Reference

[1] H. H. Wenk, A. Balster, W. Sander, D. A. Hrovat, and W. T. Borden, Angew. Chem. Int. Ed. **40**, 2295 (2001).

$C_6H_5F^+$

$\tilde{H},\tilde{I}\,^2B_2$, $^2B_1$ C_{2v}
$T^a = 57900(1000)$ gas PE[2]

$\tilde{G}\,^2A_1$ C_{2v}
$T^a = 48250(1000)$ gas PE[2]

$\tilde{F}\,^2B_2$ C_{2v}
$T^a = 43400(1000)$ gas PE[2]

$\tilde{E}\,^2B_2$ C_{2v}
$T_0 = 37680(160)$ gas PE[2]

$\tilde{D}\,^2A_1$ C_{2v}
$T^a = 30500(1000)$ gas PE[2]

$\tilde{C}\,^2B_1$ C_{2v}
$T^a = 24800(1000)$ gas PE[2]
$T_0 = 23220$ Ar AB[1,3] $\tilde{C}-\tilde{X}$ 410–435 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			510	Ar	AB	3

$\tilde{B}\,^2B_1$ C_{2v}
$T_0 = 21075$ gas PE[2]PF[4]PRI[8] $\tilde{B}-\tilde{X}$ 440–490 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	9a		1152	gas	PF,PRI	4,8
	12		695	gas	PRI	8
	6a		458	gas	PF,PRI	4,8
a_2	16a		236	gas	PRI	8
b_1			366	gas	PRI	8
	11		207	gas	PRI	8
b_2	6b		520	gas	PRI	8
	18b		430	gas	PRI	8

$\bar{A}\,^2A_2$ C_{2v}
$T^a = 4680(1000)$ gas PE[2]

$\tilde{X}\,^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	8a		1619	gas	MPI,TPE	5,6
			1370(40)	gas	PE	2
	9a		1164(2)	gas	MPI,TPE,TPI	5–7
	1		983	gas	MPI,TPE	5,6
	18a		959	gas	MPI,TPE,TPI	5–7
	12		795(2)	gas	MPI,TPE,TPI	4–7
	6a		500(2)	gas	TPE,TPI	2,4,6,7
a_2	16a		341	gas	TPI	8
b_1	11		181(2)	gas	TPI	7
b_2	6b		505(2)	gas	MPI,TPE,TPI	5–7
	18b		400(2)	gas	MPI,TPE,TPI	5–7

[a] From vertical ionization potential.

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$C_6H_5Cl^+$

$\tilde{K}\,^2A_1$ C_{2v}
$T_0 = 63450(25)$ gas PE[16]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CH stretch	2905(10)	gas	PE	16
	(1)		970(10)	gas	PE	16
	(12)		565T	gas	PE	16

$\tilde{J}\,^2A_1$ C_{2v}
$T^a = 55950(800)$ gas PE[16]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CH stretch	2820(10)	gas	PE	16

$\tilde{I}\,^2B_2$ C_{2v}
$T^a = 50700(100)$ gas PE[16]

$\tilde{H}\,^2B_2$ C_{2v}
$T^a = 45460(800)$ gas PE[16]

$\tilde{G}\,^2A_1$ C_{2v}
$T^a = 42150(100)$ gas PE[16]

$\tilde{F}\,^2B_1$ C_{2v}
$T^a = 33520(100)$ gas PE[3,16]
$T_0 = 33410(10)$ 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}
$T^a = 30930(800)$ gas PE[3,16]

$\tilde{D}\,^2A_1$ C_{2v}
$T^a = 25850(100)$ gas PE[1,3,16]

$\tilde{C}\,^2B_1$ C_{2v}
$T^0 = 21240(25)$ gas PE[1,3,16]
20750(10) Ar AB[4,6] $\tilde{C}-\tilde{X}$ 434–482 nm
Photodissociation into $C_6H_5^+ + Cl$ occurs.[2,7,8,10]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1370(10)	Ar	AB	6
	(1)		936(10)	gas	PE	3,16
			900(10)	Ar	AB	6
	(12)		734(10)	gas	PE	16
			370(10)	Ar	AB	6

$\tilde{B}\,^2B_1$ C_{2v}
$T^0 = 18270(25)$ gas PE[1,3,16]PF[7,8,10]MPI[15] $\tilde{B}-\tilde{X}$ 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	5 (19a)		1488	gas	PRI	15
	6 (9a)		1263	gas	PRI	15
	7 (7a)		1131	gas	PRI	15
	8 (1)		1010	gas	PRI	15
			970(10)	gas	PE,PF	3,7,16
			930(10)	Ar	AB	6
	9 (18a)		866	gas	PRI	15
	10 (12)		636	gas	PF,PRI	7,15
	11 (6a)		340(10)	gas	PE,PF,PRI	3,7,15,16
a_2	14 (16a)		223	gas	PRI	15
b_1	15 (5)		730	gas	PRI	15
	19 (16b)		218	gas	PRI	15
b_2	29 (6b)		562	gas	PRI	15
	30 (18b)		329	gas	PRI	15

$\tilde{A}\,^2A_2$ C_{2v}
$T^a = 5170(25)$ gas PE[1,3,16]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	(1)		1000(10)	gas	PE	3,16

$\tilde{X}\,^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	(8a)		1540(10)	gas	PE	16
	5 (19a)		1429(2)	gas	PE,TPE	3,13
	6 (9a)		1200(2)	gas	MPI,TPE,TPI	9,12–14
	7 (7a)		1116(2)	gas	MPI,TPE,TPI	9,12–14,16
	8 (18a)		995(2)	gas	MPI,TPE,TPI	9,12–14
	9 (1)		975(2)	gas	MPI,TPE,TPI	9,12–14
	10 (12)		716(2)	gas	MPI,TPE,TPI	9,12–14
	11 (6a)		422(2)	gas	TPE,PF,MPI	3,5,7 11–14,16
a_2	14 (16a)		348(2)	gas	MPI,PE	11–14
b_1	15 (5)		909(20)	gas	TPE	12
	16		812(20)	gas	TPE	12
	17 (10b)		603(20)	gas	TPE	12
	18 (4)		558(20)	gas	TPE	12
	19 (16b)		394(2)	gas	TPE,TPI	12–14
	20		154(10)	gas	MPI,PE	11,12
b_2	29 (6b)		531(2)	gas	MPI,PE	9,11–14
	30 (18b)		311(2)	gas	MPI,PE	11–13

$C_6D_5Cl^+$

$\tilde{X}\,^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	11		413(20)	gas	TPE	12

[a]From vertical ionization potential.

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$C_6H_5Br^+$

$\tilde{K}\,^2A_1$ C_{2v}
$T_0 = 63170(100)$ gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1		920(10)	gas	PE	2

$\tilde{J}\,^2A_1$ C_{2v}
$T^a = 53300T$ gas PE[2]

$\tilde{I}\,^2B_2$ C_{2v}
$T^a = 49530(100)$ gas PE[2]

$\tilde{H}\,^2B_2$ C_{2v}
$T^a = 44690(100)$ gas PE[2]

$\tilde{G}\,^2A_1$ C_{2v}
$T^a = 40980(100)$ gas PE[2]

$\tilde{F}\,^2B_1$ C_{2v}
$T^a = 31540T$ gas PE[2]

$\tilde{E}\,^2B_2$ C_{2v}
$T^a = 29760(100)$ gas PE[2]

$\tilde{D}\,^2A_1$ C_{2v}
$T^a = 24040(100)$ gas PE[2]

$\tilde{C}\,^2B_1$ C_{2v}
$T_0 = 17730(25)$ gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	12		605(10)	gas	PE	2
	6a		234(10)	gas	PE	2

$\tilde{B}\,^2B_2$ C_{2v}
$T_0 = 13250(25)$ gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1		968(10)	gas	PE	2
	12		621(10)	gas	PE	2

$\tilde{A}\,^2A_2$ C_{2v}
$T_0 = 5420(25)$ gas PE[2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	12		775(10)	gas	PE	2
	6a		258(10)	gas	PE	2

$\tilde{X}\,^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	8a		1530(30)	gas	MPI,PE	1
	1		1017(10)	gas	MPI,PE	1,2
	18a		980(30)	gas	MPI,PE	1
	6a		331(10)	gas	MPI,PE	1,2
b_2	9b		1080(30)	gas	MPI,PE	1
	6b		540(30)	gas	MPI,PE	1

[a]From vertical ionization potential.

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[1] K. Walter, K. Scherm, and U. Boesl, J. Phys. Chem. **95**, 1188 (1991).
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$C_6H_5I^+$

$\tilde{K}\,^2A_1$ C_{2v}
$T^a = 64110(100)$ gas PE[1]

$\tilde{J}\,^2B_2$ C_{2v}
$T^a = 53620(800)$ gas PE[1]

$\tilde{I}\,^2A_1$ C_{2v}
$T^a = 50640(100)$ gas PE[1]

$\tilde{H}\,^2B_2$ C_{2v}
$T^a = 45470(100)$ gas PE[1]

$\tilde{G}\,^2A_1$ C_{2v}
$T^a = 39340(100)$ gas PE[1]

$\tilde{F}\,^2B_1$ C_{2v}
$T^a = 31840(800)$ gas PE[1]

$\tilde{E}\,^2B_2$ C_{2v}
$T^a = 29340(100)$ gas PE[1]

$\tilde{D}\,^2A_1$ C_{2v}
$T^a = 23280(100)$ gas PE[1]

$\tilde{C}\,^2B_1$ C_{2v}
$T_0 = 14420(25)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	12		637(10)	gas	PE	1
	6a		202(10)	gas	PE	1

$\tilde{B}\,^2B_2$ C_{2v}
$T_0 = 8200(25)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1		968(10)	gas	PE	1
	12		621(10)	gas	PE	1

$\tilde{A}\,^2A_2$ C_{2v}
$T_0 = 6060(25)$ gas PE[1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	12		686(10)	gas	PE	1
	6a		210(10)	gas	PE	1

$\tilde{X}\,^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	7a		1017(10)	gas	PE	1
	6a		282(10)	gas	PE	1

[a]From vertical ionization potential.

Reference

[1] D. M. P. Holland, D. Edvardsson, L. Karlsson, R. Maripuu, K. Siegbahn, A. W. Potts, and W. von Niessen, Chem. Phys. **253**, 133 (2000).

1,2,3,4-$C_6H_2F_4^+$

$\tilde{B}\,^2B_1$ C_{2v}

T_0=23291.7 gas EF[1]EM[2]LF[3,7] $\tilde{B}-\tilde{X}$ 415–465 nm
23192 Ne LF[4] $\tilde{B}-\tilde{X}$ 387–480 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		1539	Ne	LF	4
	4		1355	Ne	LF	4
	6		1172	Ne	LF	4
	7		1060	Ne	LF	4
	8		654	gas	LF	3
			668	Ne	LF	4
	9		433	gas	EM,LF	2,3,10
			442	Ne	LF	4
	10		324	gas	LF	7,10
			324	Ne	LF	4
	11		271	gas	EM,LF	2,3,10
			277	Ne	LF	4

τ_0=50(3) ns gas EF[1]PIFCO[5]PEFCO[6]
44(2) ns Ne LF[9]

$\tilde{A}\,^2A_2$ C_{2v}

T_0=gas PE[1] $\tilde{B}-\tilde{A}$ 520–600 nm
2767T Ne LF[8]

$\tilde{X}\,^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		1665	gas	EM,EF	2,7
			1665	Ne	LF	4
			1228	gas	EM	2
	6		1198	Ne	LF	4
	7		1083	gas	EF	7
			1082	Ne	LF	4
	8		678	gas	EF	7
			680	Ne	LF	4
			593	gas	EM	2
	9		444	gas	EM,LF,EF	2,3,7,10
			443	Ne	LF	4
	10		343	gas	EF,LF	7,10
			340	Ne	LF	4
	11		271	gas	EM,LF,EF	2,3,7,10
			273	Ne	LF	4

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1,2,3,5-$C_6H_2F_4^+$

$\tilde{B}\,^2B_1$ C_{2v}

T_0=23323.7 gas EF[1]EM[2]LF[3,8] $\tilde{B}-\tilde{X}$ 400–470 nm
23232 Ne LF[5] $\tilde{B}-\tilde{X}$ 400–502 nm
22903 Ar LF[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		1580	Ne	LF	5
			1582	Ar	LF	4
	3		1445T	Ne	LF	5
			1536T	Ar	LF	4
	5		1264	gas	LF	3
			1259	Ne	LF	5
			1263	Ar	LF	4
	6		1140	Ne	LF	5
	8		783	Ne	LF	5
			783	Ar	LF	4
	9		569	gas	LF	3,11
			573	Ne	LF	5
			576	Ar	LF	4
	10		424	gas	EM,LF	2,3,11
			428	Ne	LF	5
			431	Ar	LF	4
	11		301	gas	EM,LF	2,3,11
			305	Ne	LF	5
			307	Ar	LF	4

τ_0=50(3) ns gas EF[1]PIFCO[6]PEFCO[7]
43(2) ns Ne LF[10]

$\tilde{A}\,^2A_2$ C_{2v}

T_0=gas EF[1] $\tilde{B}-\tilde{A}$ 520–600 nm
2442 Ne LF[9]

$\tilde{X}\,^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		1650	gas	EM,EF,LF	2,8,11
			1647	Ne	LF	5
	3		1458	gas	EF	8
			1449	Ne	LF	5
	5		1318	gas	EM,EF	2,8
			1305	Ne	LF	5
	8		785	Ne	LF	5
	9		584	gas	EF,LF	8,11
			581	Ne	LF	5
			586	Ar	LF	4
	10		424	gas	EM,EF,LF	2,8,11
			426	Ne	LF	5
			429	Ar	LF	4
	11		305	gas	EM,EF,LF	2,8,11
			303	Ne	LF	5
			307	Ar	LF	4

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1,2,4,5-$C_6H_2F_4^+$

$\tilde{B}\,^2B_{1u}$ D_{2h}
T_0 = 24443.5 gas EF[1]EM[2]LF[3,8,12]PI[11] $\tilde{B}$–$\tilde{X}$ 385–500 nm
24352 Ne LF[5] B̃–X̃ 385–510 nm
24072 Ar LF[4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2		1536	Ne	LF	5
			1536	Ar	LF	4
	3		1392	Ar	LF	4
	4		725	Ne	LF	5
			722	Ar	LF	4
	5		460	gas	LF	3,12
			465	Ne	LF	5
			470	Ar	LF	4
	6		274	gas	LF	3,12
			276	Ne	LF	5
			279	Ar	LF	4

τ_0 = 32(2) ns gas EF[1]PIFCO[6]PEFCO[7]
30(2) ns Ne LF[10]

$\tilde{A}\,^2B_{3g}$ D_{2h}
T_0 = gas EF[1] $\tilde{B}$–$\tilde{A}$ 550–650 nm
6115 Ne LF[9] $\tilde{B}$–$\tilde{A}$ 545–625 nm

$\tilde{X}\,^2B_{2g}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2		1558	gas	EF,LF	8,12
			1558	Ne	LF	5
	3		1477	gas	EF	8
			1476	Ne	LF	5
	4		726	Ne	LF	5
	5		482	gas	EM,EF,PI,LF	2,8,11,12
			485	Ne	LF	5
			480	Ar	LF	4
	6		287	gas	EF,LF	8,12
			287	Ne	LF	5
			289	Ar	LF	4
b_{1u}			183H	gas	PI	11

1,2,4,5-$C_6D_2F_4^+$

$\tilde{B}\,^2B_{1u}$ D_{2h}
T_0 = 24400 Ne LF[5] $\tilde{B}$–$\tilde{X}$ 370–465 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2		1531	Ne	LF	5
	3		1383T	Ne	LF	5
	4		722	Ne	LF	5
	5		466	Ne	LF	5
	6		276	Ne	LF	5

τ_0 = 38(3) ns gas PEFCO[7]

$\tilde{X}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2		1542	Ne	LF	5
	3		1472	Ne	LF	5
	4		706	Ne	LF	5
	5		480	Ne	LF	5
	6		286	Ne	LF	5

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[7] J. P. Maier and F. Thommen, Chem. Phys. **57**, 319 (1981).
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[9] V. E. Bondybey, C. R. Vaughn, T. A. Miller, J. H. English, and R. H. Shiley, J. Chem. Phys. **74**, 6584 (1981).
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C_6H_5CHCl

T_0 = 22044.5 gas LF[1]MPI[1] 431–467 nm

$\tilde{X}\,^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	6b		612.0	gas	MPI	1
	6a		358.4	gas	MPI	1

Reference

[1] J. Yao and E. R. Bernstein, J. Chem. Phys. **107**, 3352 (1997).

C_6H_5CHBr

$T_0 = 21952.6$ gas LF[1] 444–456 nm

Reference

[1] J. Yao and E. R. Bernstein, J. Chem. Phys. **107**, 3352 (1997).

$C_6H_5CCl_2$

gas LF[1]MPI[1] 439–466 nm

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	6a		406.3	gas	MPI	1
b_2	6b		639.3	gas	MPI	1

Reference

[1] J. Yao and E. R. Bernstein, J. Chem. Phys. **107**, 3352 (1997).

$(2\text{-}FC_6H_4)CH_2$

$\tilde{A}$

$T_0 = 21924$ gas EM[1,4]LF[2] $\tilde{A}-\tilde{X}$ 435–524 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

$\tau_0 = 1220(40)$ ns gas LF[2]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	7 (8a)	C–CH_2 stretch	1570	gas	PE,EM	3,4
	13 (14)		1285	gas	EM	4
	14 (7a)		1264	gas	PE,EM	3,4
	15 (13)		1208	gas	EM	4
	17 (18a)		1119	gas	EM	4
	18 (18b)		1033	gas	EM	4
	20		882	gas	LF	2
	21 (1)	Ring breathing	757	gas	PE,EM	3,4
	22 (6a)	Ring deform.	575	gas	PE,EM	3,4
	23 (6b)	Ring deform.	516	gas	EM	4
	24 (9b)	CH_2 rock	436	gas	PE,EM	3,4
	25 (15)		304	gas	EM	4
a''	(5)		969	gas	EM	4
	(16a)		535	gas	EM	4
	(16b)		424	gas	EM	4
	(10a)		266	gas	EM	4

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$(3\text{-}FC_6H_4)CH_2$

$\tilde{A}$

$T_0 = 21691$ gas EM[1,4]LF[2] $\tilde{A}-\tilde{X}$ 445–498 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			734	gas	LF	2
			466	gas	LF	2

$\tau_0 = 597(15)$ ns gas LF[2]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	7 (19b)	C–CH_2 stretch	1599	gas	PE,EM	3,4
	9 (8b)		1567	gas	EM	4
	10 (8a)		1557	gas	EM	4
	11 (19a)		1428	gas	EM	4
	14 (14)		1288	gas	EM	4
	16 (9b)		1142	gas	EM	4
	19 (12)		998	gas	EM	4
	20 (7b)		930	gas	EM	4
	21 (1)		741	gas	LF,PE,EM	2–4
	22 (6a)		530	gas	EM	4
	23 (6b)	Ring deform.	506	gas	EM,LF,PE	1–4
	24 (15)		453	gas	EM	4

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$(4\text{-}FC_6H_4)CH_2$

$\tilde{A}\,^2A_2$ C_{2v}

$T_0 = 21524.0(2)$ gas EM[1,3,5,6]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

$\tau_0 = 532(5)$ ns gas LF[2,4]

$\tilde{X}\,^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4 (8a)	C–CH_2 stretch	1568	gas	EM,PE	6,7
	(7a)		1262	gas	EM	6
	(13)		1243	gas	EM	6
	11 (1)		835	gas	EM,LF	3,4,6
	12 (12)		754	gas	EM	6
	13 (6a)	Ring deform.	453	gas	EM,LF,PE	1–4,6,7
b_2	(6b)		632T	gas	EM	6
	(9b)		420T	gas	EM	6
	(15)		323T	gas	EM	6

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[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] C. Cossart-Magos and D. Cossart, Mol. Phys. **65**, 627 (1988).
[4] M. Fukushima and K. Obi, J. Chem. Phys. **93**, 8488 (1990).
[5] D. Y. Baek and S. K. Lee, Bull. Korean Chem. Soc. **19**, 1359 (1998).
[6] S. K. Lee and D. Y. Baek, Chem. Phys. Lett. **301**, 407 (1999).
[7] J. B. Kim, P. G. Wenthold, and W. C. Lineberger, J. Phys. Chem. A **103**, 10833 (1999).

$(2\text{-}ClC_6H_4)CH_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	7	C–CH_2 stretch	1540(40)	gas	PE	1
	13	Deformation	1250(40)	gas	PE	1
	22	Ring deform.	560(20)	gas	PE	1

Reference

[1] J. B. Kim, P. G. Wenthold, and W. C. Lineberger, J. Phys. Chem. A **103**, 10833 (1999).

$(3\text{-}ClC_6H_4)CH_2$

$\tilde{A}$ C_s

$T_0 = 21194.8$ gas EM^2 $\tilde{A}–\tilde{X}$ 471–503 nm

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	7	C–CH_2 stretch	1520(40)	gas	PE	1
	13 (3)		1287	gas	EM	2
	14 (13)		1237	gas	EM	2
	18 (12)		984	gas	EM	2
	19 (5)		959	gas	EM	2
	21 (1)		686	gas	PE,EM	1,2
	22 (6a)	Ring deform.	525	gas	PE,EM	1,2
	23 (7b)		413	gas	EM	2
	24 (15)		394	gas	EM	2

References

[1] J. B. Kim, P. G. Wenthold, and W. C. Lineberger, J. Phys. Chem. A. **103**, 10833 (1999).
[2] S. K. Lee and S. Y. Chae, J. Phys. Chem. A **105**, 5808 (2001).

$(4\text{-}ClC_6H_4)CH_2$

$\tilde{B}\,^2B_1$ C_{2v}

$T_0 = 21733.8(5)$ gas LF^1EM^3 $\tilde{A},\tilde{B}–\tilde{X}$ 436–515 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}

$T_0 = 21638.7(5)$ gas LF^1EM^3 $\tilde{A},\tilde{B}–\tilde{X}$ 436–515 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	4 (8a)	C–CH_2 stretch	1544	gas	LF,EM,PE	2–4
	(1)		1079	gas	LF,EM	2,3
	(6a)		811	gas	LF,EM	2,3
	(12)		638	gas	LF,EM	1,3
			559	gas	LF	2
	13 (7a)	Ring deform.	380	gas	EM,PE	3,4
b_2	8b		1529	gas	EM	3
	3		1306	gas	EM	3
	15		257	gas	EM	3
			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).
[3] S. K. Lee and D. Y. Baek, Chem. Phys. Lett. **304**, 39 (1999).
[4] J. B. Kim, P. G. Wenthold, and W. C. Lineberger, J. Phys. Chem. A **103**, 10833 (1999).

$(2\text{-}BrC_6H_4)CH_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	7	C–CH_2 stretch	1540(40)	gas	PE	1
	13	Deformation	1230(40)	gas	PE	1
	22	Ring deform.	550(20)	gas	PE	1

Reference

[1] J. B. Kim, P. G. Wenthold, and W. C. Lineberger, J. Phys. Chem. A **103**, 10833 (1999).

$(3\text{-}BrC_6H_4)CH_2$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	7	C–CH_2 stretch	1520(40)	gas	PE	1
	22	Ring deform.	525(20)	gas	PE	1

Reference

[1] J. B. Kim, P. G. Wenthold, and W. C. Lineberger, J. Phys. Chem. A **103**, 10833 (1999).

$(4\text{-}BrC_6H_4)CH_2$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4	C–CH_2 stretch	1510(40)	gas	PE	1
	13	Ring deform.	290(20)	gas	PE	1

Reference

[1] J. B. Kim, P. G. Wenthold, and W. C. Lineberger, J. Phys. Chem. A **103**, 10833 (1999).

$(2,6\text{-}F_2C_6H_3)CH_2$

$\tilde{A}\,^2A_2$ C_{2v}

$T_0 = 21774$ gas EM[1] $\tilde{A}$–$\tilde{X}$ 459–488 nm

$\tilde{X}\,^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1		696	gas	EM	1
	6a		470	gas	EM	1
	9a		332	gas	EM	1
b_2	14		1268	gas	EM	1

Reference

[1] S. K. Lee and D. Y. Baek, J. Phys. Chem. A **104**, 5219 (2000).

$C_6F_5CH_2$

$\tilde{A}\,^2A_2$ C_{2v}

$T_0 = 21857$ gas EM[1] $\tilde{A}$–$\tilde{X}$ 457–473 nm

$\tilde{X}\,^2B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1		550	gas	EM	1
	6a		456	gas	EM	1
	18a		334	gas	EM	1
	9a		277	gas	EM	1
b_1	4		727	gas	EM	1
	16b		584	gas	EM	1
	11		219	gas	EM	1

Reference

[1] S. K. Lee and D. Y. Baek, Chem. Phys. Lett. **311**, 36 (1999).

$(2\text{-}FC_6H_4)CH_2^-$

Threshold for electron detachment from ground-state $(2\text{-}FC_6H_4)CH_2^-$ = 8800(65) gas PE[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	24	CH_2 rock	425(40)	gas	PE	1

Reference

[1] J. B. Kim, P. G. Wenthold, and W. C. Lineberger, J. Phys. Chem. A **103**, 10833 (1999).

$(3\text{-}FC_6H_4)CH_2^-$

Threshold for electron detachment from ground-state $(3\text{-}FC_6H_4)CH_2^-$ = 9465(65) gas PE[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	22	Ring deform.	510(20)	gas	PE	1

Reference

[1] J. B. Kim, P. G. Wenthold, and W. C. Lineberger, J. Phys. Chem. A **103**, 10833 (1999).

$(4\text{-}FC_6H_4)CH_2^-$

Threshold for electron detachment from ground-state $(4\text{-}FC_6H_4)CH_2^-$ = 7560(65) gas PE[1]

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	13	Ring deform.	420(20)	gas	PE	1

Reference

[1] J. B. Kim, P. G. Wenthold, and W. C. Lineberger, J. Phys. Chem. A **103**, 10833 (1999).

$(2\text{-}ClC_6H_4)CH_2^-$

Threshold for electron detachment from ground-state $(2\text{-}ClC_6H_4)CH_2^-$ = 10140(65) gas PE[1]

Reference

[1] J. B. Kim, P. G. Wenthold, and W. C. Lineberger, J. Phys. Chem. A **103**, 10833 (1999).

$(3\text{-}ClC_6H_4)CH_2^-$

Threshold for electron detachment from ground-state $(3\text{-}ClC_6H_4)CH_2^-$ = 10260(65) gas PE[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	22	Ring deform.	490(20)	gas	PE	1

Reference

[1] J. B. Kim, P. G. Wenthold, and W. C. Lineberger, J. Phys. Chem. A **103**, 10833 (1999).

$(4\text{-}ClC_6H_4)CH_2^-$

Threshold for electron detachment from ground-state $(4\text{-}ClC_6H_4)CH_2^-$ = 9470(65) gas PE[1]

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	13	Ring deform.	365(20)	gas	PE	1

Reference

[1] J. B. Kim, P. G. Wenthold, and W. C. Lineberger, J. Phys. Chem. A **103**, 10833 (1999).

$(2\text{-}BrC_6H_4)CH_2^-$

Threshold for electron detachment from ground-state $(2\text{-}BrC_6H_4)CH_2^-$ = 10550(65) gas PE[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	22	Ring deform.	530(30)	gas	PE	1

Reference

[1] J. B. Kim, P. G. Wenthold, and W. C. Lineberger, J. Phys. Chem. A **103**, 10833 (1999).

$(3\text{-}BrC_6H_4)CH_2^-$

Threshold for electron detachment from ground-state $(3\text{-}BrC_6H_4)CH_2^-$ = 10545(65) gas PE[1]

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	22	Ring deform.	500(20)	gas	PE	1

Reference

[1] J. B. Kim, P. G. Wenthold, and W. C. Lineberger, J. Phys. Chem. A **103**, 10833 (1999).

$(4\text{-}BrC_6H_4)^-$

Threshold for electron detachment from ground-state $(4\text{-}BrC_6H_4)CH_2^-$ = 9915(65) gas PE[1]

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	13	Ring deform.	265(40)	gas	PE	1

Reference

[1] J. B. Kim, P. G. Wenthold, and W. C. Lineberger, J. Phys. Chem. A **103**, 10833 (1999).

$(4\text{-}NC\text{-}C_6H_4)CH_2$

$\tilde{A}\,^2B_1$ C_{2v}

T_0 = 20743.9 gas LF[1]EM[2] $\tilde{A}$–$\tilde{X}$ 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	20a	CH stretch	3133	gas	EM	2
		CN stretch	2225	gas	LF,EM	1,2
	8a		1563	gas	LF,EM	1,2
	7a		1210	gas	EM	2
	9a		1149	gas	LF,EM	1,2
	1		825	gas	LF,EM	1,2
			513	gas	LF	1
	6a		407	gas	EM	2
a_2	17a		951	gas	EM	2
b_1	16b		427	gas	EM	2
b_2	8b		1521	gas	EM	2
	6b		642	gas	LF,EM	1,2
	9b		355	gas	EM	2

$A_0 = 0.182$; $B_0 = 0.032$; $C_0 = 0.028$ LF[1]

References

[1] M. Fukushima, K. Saito, and K. Obi, J. Mol. Spectrosc. **180**, 389 (1996).
[2] S. K. Lee and B. U. Ahn, Chem. Phys. Lett. **320**, 601 (2000).

p-$(CF_2)_2C_6H_4$

In an argon matrix, *p*-$(CF_2)_2C_6H_4$ has prominent absorption maxima at 36100 (277 nm), 37600 (266 nm), and 50500 (198 nm).[1] When irradiated at 248 nm, rearrangement to 4,5-$F_2C_7H_4{=}CF_2$ occurs.

$\tilde{X}$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{1u}			1693vs	Ar	IR	1
			1423wm	Ar	IR	1
			1080ms	Ar	IR	1
			956w	Ar	IR	1
			678wm	Ar	IR	1
b_{2u}			1590vw	Ar	IR	1
			1341m	Ar	IR	1
			1267ms	Ar	IR	1
			1118w	Ar	IR	1
b_{3u}			800w	Ar	IR	1

Reference

[1] H. H. Wenk, W. Sander, A. Leonov, and A. de Meijere, Eur. J. Org. Chem. 3287 (1999).

4,5-$F_2C_7H_4{=}CF_2$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1698s	Ar	IR	1
			1608vs	Ar	IR	1
			1217s	Ar	IR	1
			1046s	Ar	IR	1
			870wm	Ar	IR	1
			693m	Ar	IR	1
b_1			777wm	Ar	IR	1
b_2			1442m	Ar	IR	1
			1345wm	Ar	IR	1
			1293s	Ar	IR	1
			1070wm	Ar	IR	1
			719m	Ar	IR	1

Reference

[1] H. H. Wenk, W. Sander, A. Leonov, and A. de Meijere, Eur. J. Org. Chem. 3287 (1999).

$C_6H_5NH_2^+$

$\tilde{A}\,^2A_2$ 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			1635	Ar	IR	8
	8a[a]		1594	gas	TPE	2,5,6
			1515	Ar	IR	8
			1483	Ar	IR	8
	19a		1436(10)T	gas	PE	2
	13		1385	gas	TPE	2,5,6
	9a		1188	gas	TPE,PI	2,4–6,9
	18a		996	gas	TPE,TPI	5,6,9
	12	Ring s-stretch	982	gas	PI,TPE	1,2,4–6,9
	1		814	gas	PI,TPE	1,2,4,6,9
	6a	N-ring s-str.	522	gas	PI,TPE	1–6,9
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
			785	Ar	IR	8
		Inversion	658	gas	PI,TPE	2,3,5,6,9
			656(2)	Ar	IR	8
	16b		629	gas	TPE	6
	4	Ring deform.	445	gas	TPE,TPI	6,9
	10b		179	gas	PI,TPE	3,5,6,9
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.
a_1	8a		1563	gas	TPI	9
	12		948	gas	TPI	9
	18a		847	gas	TPI	9
	1		738	gas	TPI	9
	6a		513	gas	TPI	9
a_2	16a		309	gas	TPI	9
b_1	5		831	gas	TPI	9
		Inversion	465(10)	gas	PI	3
	10b		157	gas	TPI	9
b_2	14		1341	gas	TPI	9

[a]Vibrational numbering and assignments parallel those given by Chernoff and Rice [J. Chem. Phys. **70**, 2511 (1979)] for aniline.
[b]From combination band.

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[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).
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[8] Ch. Gée, S. Douin, C. Crépin, and Ph. Bréchignac, Chem. Phys. Lett. **338**, 130 (2001).
[9] J. L. Lin and W. B. Tzeng, J. Chem. Phys. **115**, 743 (2001).

o-$C_6H_4FNH_2^+$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CH deform.	1243(10)	gas	TPI	1
	7a	CF stretch	1209(10)	gas	TPI	1
	9a	CH deform.	1145(25)	gas	TPI	1
	18b	CH deform.	1093(20)	gas	TPI	1
	18a	CH deform.	988(10)	gas	TPI	1
	5	CH deform.	962(10)	gas	TPI	1
	12	C_3 deform.	855(10)	gas	TPI	1
	1	Ring breathing	754(10)	gas	TPI	1
	6a	C_3 deform.	515(10)	gas	TPI	1
	9b	CF deform.	421(10)	gas	TPI	1
	15	CN deform.	308(10)	gas	TPI	1
a''	17a	CH deform.	920(10)	gas	TPI	1
		NH_2 wag	716(10)	gas	TPI	1
	11	CF deform.	682(10)	gas	TPI	1
	10a	CH deform.	562(10)	gas	TPI	1
	4	C_3 deform.	466(10)	gas	TPI	1
	16a	C_3 deform.	256(10)	gas	TPI	1
	10b	CN deform.	154(10)	gas	TPI	1

Reference

[1] J. L. Lin and W. B. Tzeng, Phys. Chem. Chem. Phys. **2**, 3759 (2000).

p-$C_6H_4FNH_2^+$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		NH_2 scissors	1730(10)	gas	TPI	1
	8a	Ring stretch	1615(10)	gas	TPI	1
	13	CN stretch	1471(10)	gas	TPI	1
	7a	CF stretch	1352(10)	gas	TPI	1,2
	18a	CH deform.	968(10)	gas	TPI	1,2
	12	C_3 deform.	836(10)	gas	TPI	1,2
	1	Ring breathing	763(10)	gas	TPI	1,2
	6a	C_3 deform.	452(10)	gas	TPI	1,2
a_2	17b	CH deform.	867(10)	gas	TPI	1
b_1	5	CH deform.	939(10)	gas	TPI	1
		NH_2 wag	737(10)	gas	TPI	1,2
	16b	C_3 deform.	502(10)	gas	TPI	1
b_2	19b	Ring stretch	1512	gas	TPI	1,2
	3	CH deform.	1410(10)	gas	TPI	1
	18b	CH deform.	1165(10)	gas	TPI	1,2
	6b	C_3 deform.	634(10)	gas	TPI	1,2
	15	CN deform.	371(10)	gas	TPI	1,2

References

[1] W. B. Tzeng and J. L. Lin, J. Phys. Chem. A **103**, 8612 (1999).
[2] J. L. Lin and W. B. Tzeng, J. Chem. Phys. **115**, 743 (2001).

p-$C_6H_4ClNH_2^+$

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	9a	CH deform.	1195(10)	gas	TPI	1
	1	C_3 deform.	1136(10)	gas	TPI	1
	18a	CH deform.	1005(10)	gas	TPI	1
	6a	C_3 deform.	821(10)	gas	TPI	1
	12	C_3 deform.	664(10)	gas	TPI	1
	7a	Mixed	380(10)	gas	TPI	1
b_1		NH deform.	1041(10)	gas	TPI	1
	5	CH deform.	976(10)	gas	TPI	1
	17b	CH deform.	842(10)	gas	TPI	1
		NH_2 wag	724(10)	gas	TPI	1
	16b	C_3 deform.	494(10)	gas	TPI	1
b_2	14	CC stretch	1269(10)	gas	TPI	1
	6b	C_3 deform.	621(10)	gas	TPI	1

Reference

[1] J. L. Lin and W. B. Tzeng, J. Chem. Phys. **113**, 4109 (2000).

C_6H_5O

$\tilde{E}\,^2B_1$ C_{2v}

In the gas phase, a prominent absorption maximum near 43100 (232 nm) has been attributed[5,8,9] to C_6H_5O.

$T_0 = 41800$ Ar AB[11]

$\tilde{D}\,^2A_1$ C_{2v}

In the gas phase, a broad band between about 33300 (300 nm) and 37000 (270 nm) has been attributed[5,8,9] to C_6H_5O.

$T_0=33900$ Ar AB[11]

$\tilde{C}\,^2B_1$ C_{2v}

gas AB[1,2] $\tilde{C}-\tilde{X}$ 380–395 nm

$T_0=25175(10)$ Ar AB[4,6,10,11] $\tilde{C}-\tilde{X}$ 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

$\tilde{B}\,^2A_1$ C_{2v}

$T_0\cong16360$ gas AB[2,3] $\tilde{B}-\tilde{X}$ 559–612 nm

15930(10) Ar AB[4,6,10,11] $\tilde{B}-\tilde{X}$ 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

$\tilde{A}\,^2B_2$ C_{2v}

$T_0=8550(40)$ gas PE[7]

8900T Ar AB[11]

$\tilde{X}\,^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1 (20a)	CH stretch	3090vw	Ar	IR	10
	2 (13)	CH stretch	3065w	Ar	IR	10
	3 (2)	CH stretch	3018vw	Ar	IR	10
	4 (8a)	CC stretch	1550ms	Ar	IR	10
	5 (7a)	CO stretch	1490(25)	gas	PE	7
			1481m	Ar	IR	10
	6 (19a)	Mixed	1397w	Ar	IR	10
	7 (9a)	CH bend	1167w	Ar	IR	10
	8 (12)	Mixed	1038vw	Ar	IR	10
	9 (18a)	CCC bend	977w	Ar	IR	10
	10 (1)	Mixed	813w	Ar	IR	10
	11 (6a)	CCC bend	515(15)	gas	PE	7
			520w	Ar	IR	10
b_1	15 (5)	HCCH torsion	1016vw	Ar	IR	10
	16 (17b)	Mixed	898wm	Ar	IR	10
	17 (4)	Mixed	784s	Ar	IR	10
	18 (11)	Mixed	635vs	Ar	IR	10
	19 (16b)	Mixed	472vw	Ar	IR	10
b_2	21 (20b)	CH stretch	3074wm	Ar	IR	10
	22 (7b)	CH stretch	3054vw	Ar	IR	10
	23 (19b)	Mixed	1515m	Ar	IR	10
	24 (8b)	Mixed	1441vw	Ar	IR	10
	25 (14)	Mixed	1318wm	Ar	IR	10
	26 (3)	Mixed	1266wm	Ar	IR	10
	27 (15)	Mixed	1140w	Ar	IR	10
	28 (9b)	Mixed	1072m	Ar	IR	10
	29 (6b)	CCC bend	616w	Ar	IR	10
	30 (18b)	CO bend	446wm	Ar	IR	10

C_6D_5O

$\tilde{C}\,^2B_1$ C_{2v}

$T_0=25240(10)$ Ar AB[4,10] $\tilde{C}-\tilde{X}$ 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

$\tilde{B}\,^2A_1$ C_{2v}

$T_0=15973(10)$ Ar AB[11]

$\tilde{X}\,^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1 (20a)	CD stretch	2331vw	Ar	IR	10
	2 (13)	CD stretch	2298w	Ar	IR	10
	3 (2)	CD stretch	2284vw	Ar	IR	10
	4 (8a)	CC stretch	1509s	Ar	IR	10
	5 (7a)	CO stretch	1467ms	Ar	IR	10
	6 (19a)	Mixed	1244wm	Ar	IR	10
	7 (18a)	CCC bend	944w	Ar	IR	10
	8 (12)	Mixed	902vw	Ar	IR	10
	9 (9a)	CD bend	844vw	Ar	IR	10
	10 (1)	Mixed	724w	Ar	IR	10
	11 (6a)	CCC bend	505w	Ar	IR	10
b_1	15 (5)	DCCD torsion	860w	Ar	IR	10
	16 (17b)	Mixed	775wm	Ar	IR	10
	17 (4)	Mixed	660m	Ar	IR	10
	18 (11)	Mixed	489s	Ar	IR	10
	19 (16b)	Mixed	406w	Ar	IR	10
b_2	21 (20b)	CD stretch	2326vw	Ar	IR	10
	22 (7b)	CD stretch	2281vw	Ar	IR	10
	23 (19b)	Mixed	1449wm	Ar	IR	10
	24 (8b)	Mixed	1334wm	Ar	IR	10
	25 (14)	Mixed	1255m	Ar	IR	10
	26 (3)	Mixed	1032w	Ar	IR	10
	27 (15)	Mixed	836w	Ar	IR	10
	28 (9b)	Mixed	824w	Ar	IR	10
	30 (18b)	CO bend	423w	Ar	IR	10

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1,2-C_6F_4>CO

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1			1904.4m	Ar	IR	1
			1610.5w	Ar	IR	1
			1470.7s	Ar	IR	1
			1288.7w	Ar	IR	1
			1108.4wm	Ar	IR	1
			884.6w	Ar	IR	1
			548.1w	Ar	IR	1
b_1			580.6vw	Ar	IR	1
b_2			1605.6w	Ar	IR	1
			1494.4vs	Ar	IR	1
			1050.2wm	Ar	IR	1
			818.1wm	Ar	IR	1
			691.0w	Ar	IR	1
			623.2w	Ar	IR	1

Reference

[1] H. H. Wenk and W. Sander, Chem. Eur. J. **7**, 1837 (2001).

o-$C_6H_4(OH)_2^+$

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	18b		987	gas	TPI	1
	1		755	gas	TPI	1
	6a		585	gas	TPI	1
	6b		507	gas	TPI	1
a''		Torsion	504H	gas	TPI	1

Reference

[1] M. Gerhards, S. Schumm, C. Unterberg, and K. Kleinermanns, Chem. Phys. Lett. **294**, 65 (1998).

m-$C_6H_4(OH)_2^+$ (C_s)

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		OH stretch	3582	gas	PIR	1
		OH stretch	3569	gas	PIR	1
	12		974	gas	TPI	1
	7b		926	gas	TPI	1
	1		736	gas	TPI	1
	6a		522	gas	TPI	1
	6b		489	gas	TPI	1
	15		441	gas	TPI	1
	9a		343	gas	TPI	1
a''	16a		638	gas	TPI	1
	4		597	gas	TPI	1
		Torsion	577	gas	TPI	1
		Torsion	540	gas	TPI	1
	16b		395H	gas	TPI	1
	10a		198H	gas	TPI	1
	10b		187	gas	TPI	1

Reference

[1] M. Gerhards, C. Unterberg, and S. Schumm, J. Chem. Phys. **111**, 7966 (1999).

m-$C_6H_4(OH)_2^+$ (C_{2v})

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	12		971	gas	TPI	1
	1		733	gas	TPI	1
	6a		526	gas	TPI	1
	9a		343	gas	TPI	1
a_2	16a		629	gas	TPI	1
	10a		196H	gas	TPI	1
b_1	4		592	gas	TPI	1
	16b		392H	gas	TPI	1
	10b		185	gas	TPI	1
b_2		OH stretch	3576	gas	PIR	1
	7b		917	gas	TPI	1
	6b		495	gas	TPI	1
	15		427	gas	TPI	1

Reference

[1] M. Gerhards, C. Unterberg, and S. Schumm, J. Chem. Phys. **111**, 7966 (1999).

p-$C_6H_4(OH)_2^+$ (C_{2v})

$\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	13	CO stretch	1292T	gas	TPI	1
	9a	CH deform.	1174	gas	TPI	1
	18b	Mixed	1055T	gas	TPI	1
	17b	CH deform.	875T	gas	TPI	1
	1	Ring breathing	834	gas	TPI	1
	12	Ring deform.	724T	gas	TPI	1
	6a	Ring deform.	456	gas	TPI	1
	15	CO deform.	365	gas	TPI	1

Reference

[1] J. L. Lin, L. C. L. Huang, and W. B. Tzeng, J. Phys. Chem. A **105**, 11455 (2001).

p-$C_6H_4(OH)_2^+$ (C_{2h})

$\tilde{X}$ C_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	13	CO stretch	1294T	gas	TPI	1
	9a	CH deform.	1175	gas	TPI	1
	17b	CH deform.	882T	gas	TPI	1
	1	Ring breathing	837	gas	TPI	1
	6a	Ring deform.	459	gas	TPI	1
	9b	CO deform.	439	gas	TPI	1

Reference

[1] J. L. Lin, L. C. L. Huang, and W. B. Tzeng, J. Phys. Chem. A **105**, 11455 (2001).

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 Supplement A,[6] and numbers prefixed by "B" give the page number in the present work.

Formula	*Structure/Name*	*References*
AgAuCu	CuAgAu	60
$AgCu_2$	Cu_2Ag	59
AgHO	AgOH	B28
$AgNO^+$	$AgNO^+$	B78
AgNO	AgNO	B93
$AgNO^-$	$AgNO^-$	B102
AgO_2	AgOO	A178,B108
AgO_2^-	$AgOO^-$	B118
Ag_2O	AgOAg	B55
Ag_3	Ag_3	60,A161,B52
Ag_4	Ag_4	B200
Ag_5	Ag_5	B277
Ag_8	Ag_8	B360
$AlBr_2$	$AlBr_2$	A193
$AlBr_2H$	$HAlBr_2$	B194
$AlBr_3^+$	$AlBr_3^+$	203
AlClO	OAlCl	85
$AlCl_2$	$AlCl_2$	90,A193
$AlCl_2H$	$HAlCl_2$	169,B193
$AlCl_3^+$	$AlCl_3^+$	203
AlFO	FAlO	85
$AlFO_2$	$FAlO_2$	B232
$AlFO_4$	$FAl(O_2)_2$	B330
AlF_2	AlF_2	A192,B134
AlF_3^+	AlF_3^+	202
AlHO	AlOH	36,A143
AlH_2	AlH_2	17,A129
AlH_2N	$AlNH_2$	B168
AlH_2O	HAlOH	139
AlH_3	AlH_3	A212
AlH_3N^+	$AlNH_3^+$	B251
AlH_3N	$AlNH_3$	B251
AlH_3N	$HAlNH_2$	B252
AlH_3P	$AlPH_3$	B253
AlH_3P	$HAlPH_2$	B253
AlH_3P	H_2AlPH	B254
AlH_4^-	AlH_4^-	A266
AlH_4N	H_2AlNH_2	B310
AlH_4Si	SiH_3AlH	307
AlI_2	AlI_2	A193
AlNO	NAlO	B111
AlNO	AlNO	B111
AlNO	AlON	B111
$AlNO^-$	$AlNO^-$	B120
AlN_2	NAlN	B97
AlN_3	AlNNN	B222
AlOSi	AlOSi	B98
AlO_2	*cyc*-AlO_2	75
AlO_2	OAlO	75,A183
AlO_2^-	$OAlO^-$	A189
AlO_3	OAlOO	190
AlP_2	*cyc*-AlP_2	B98
AlP_2^-	*cyc*-AlP_2^-	B111
Al_2H_2	*cyc*-Al_2H_2	A219
Al_2H_2	(*cyc*-AlHAl)	A219
Al_2H_2	HAlAlH	A220
Al_2N	AlNAl	B63
Al_2N_2	Al_2N_2	B213
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
$Al_2O_5^-$	$Al_2O_5^-$	B347
Al_2P	Al_2P	B63
Al_2P^-	Al_2P^-	B80
Al_2P_2	Al_2P_2	B213
$Al_2P_2^-$	$Al_2P_2^-$	B217
Al_2S_3	Al_2S_3	A297
Al_3	Al_3	62,A162
Al_3Ge	*cyc*-$GeAl_3$	B202
Al_3Ge^-	*cyc*-$GeAl_3^-$	B208
Al_3N	NAl_3	B208
Al_3N^-	Al_3N^-	B209
Al_3O	Al_3O	B210
Al_3O^-	Al_3O^-	B214
Al_3O_2	Al_3O_2	B283
$Al_3O_2^-$	$Al_3O_2^-$	B288
Al_3O_3	Al_3O_3	B329
$Al_3O_3^-$	$Al_3O_3^-$	B329
Al_3O_4	Al_3O_4	B345
$Al_3O_4^-$	$Al_3O_4^-$	B345
Al_3Pb	*cyc*-$PbAl_3$	B202
Al_3Pb^-	*cyc*-$PbAl_3^-$	B208
Al_3Si	*cyc*-$SiAl_3$	B202
Al_3Si^-	*cyc*-$SiAl_3^-$	B208
Al_3Sn	*cyc*-$SnAl_3$	B202
Al_3Sn^-	*cyc*-$SnAl_3^-$	B208
Al_4Ge	Al_4Ge	B278
Al_4Ge^-	Al_4Ge^-	B279
Al_4N	Al_4N	B279
Al_4N^-	$Al_4N^-(D_{4h})$	B279
Al_4N^-	$Al_4N^-(C_{2v})$	B279
Al_4Si	Al_4Si	B278
Al_4Si^-	Al_4Si^-	B278
Al_5	Al_5	B278
Al_5^-	Al_5^-	B278

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
ArBeO	ArBeO	A188	$BClH^+$	$HBCl^+$	B32
$ArBeO_2$	$ArBeO_2$	A253	$BClH_2$	H_2BCl	142
ArBrKr	ArKrBr	123	$BClN_2$	(*cyc*-NNB)Cl	B228
ArBrXe	ArXeBr	123	BClO	ClBO	84,A189,B130
ArClKr	ArKrCl	122	$BClS^+$	$ClBS^+$	74,A183
ArDKr	ArKrD	57	BClS	ClBS	85,A189,B130
ArFH	HArF	B47	BCl_2^+	BCl_2^+	A189
ArFKr	ArKrF	121,A210	BCl_2	BCl_2	89,A192,B133
ArFXe	ArXeF	121	BCl_2H^+	$HBCl_2^+$	166
ArHXe	ArXeH	57	BCl_2H	$HBCl_2$	A238
Ar_2Cl	Ar_2Cl	122	$BCl_2H_2N^+$	$NH_2BCl_2^+$	332
Ar_2H^+	HAr_2^+	56,A159,B48	BCl_2N	ClBNCl	B232
Ar_2H	Ar_2H	56	BCl_3^+	BCl_3^+	201,A255,B234
Ar_2F	Ar_2F	121,A210	BCl_3^-	BCl_3^-	A261
$AsBr_3^+$	$AsBr_3^+$	221	BCl_4^-	BCl_4^-	302
AsClO	ClAsO	104	BFH^+	HBF^+	37
$AsCl_3^+$	$AsCl_3^+$	221	BFH_2	H_2BF	142
$AsFH_2$	AsH_2F	152	BFO	FBO	84,A188
AsF_2	AsF_2	109,A203	BFS^+	FBS^+	74
AsF_2H	$HAsF_2$	179	BFS	FBS	85,B130
AsF_2H_3	AsH_3F_2	325	BF_2^+	BF_2^+	A189
AsF_3^+	AsF_3^+	221	BF_2	BF_2	89,A191
$AsGa_2$	Ga_2As	A165,B64	BF_2H^+	HBF_2^+	165
$AsGa_2^-$	Ga_2As^-	B80	BF_2H	HBF_2	A238
$AsHO_3$	$HOAsO_2$	273	BF_2HO	BF_2OH	B274
AsH_2	AsH_2	23,B20	$BF_2H_2N^+$	$NH_2BF_2^+$	332
AsH_3^+	AsH_3^+	129	BF_2O	F_2BO	200
AsH_3O	H_3AsO	243	BF_3^+	BF_3^+	201,A255,B234
AsH_3O	H_2AsOH	243	BF_3^-	BF_3^-	A261
$AsIn_2$	In_2As	A165	BF_4^-	BF_4^-	302
As_2Ga	*cyc*-$GaAs_2$	A172,B98	$BGaH_6^+$	$GaBH_6^+$	A332
As_2Ga^-	*cyc*-$GaAs_2^-$	B111	$BGaH_6$	$GaBH_6$	B348
As_3	As_3	B127	BHN	HNB	31,A141
As_3Ga_2	Ga_2As_3	B282	BHO	HBO	35,B32
$As_3Ga_2^-$	$Ga_2As_3^-$	B288	BHO_2	HOBO	162
As_4^+	As_4^+	187	BHS^+	HBS^+	31,A141
As_4O	As_4O	284	BHS	HBS	35
As_4O	br-As_4O	284	BH_2	BH_2	17
$AuCu_2$	Cu_2Au	60	BH_2N	HBNH	137,A222
AuH_3	$HAu(H_2)$	B154	BH_2N	H_2NB	A223
AuO_2	AuOO	A178,B108	BH_3	BH_3	124,A212
AuO_2	OAuO	B108	BH_3^-	BH_3^-	125
Au_3	Au_3	60,A161	BH_3N	$HBNH_2$	A269
$BBrH^+$	$HBBr^+$	B32	BH_3O	H_2BOH	233
$BBrH_2$	H_2BBr	142	BH_3O_3	$B(OH)_3$	A326
BBrO	BrBO	85,B130	BH_3S	H_2BSH	233
BBrS	BrBS	85	BH_4^-	BH_4^-	A266
BBr_2^+	BBr_2^+	A189	BH_4K	KBH_4	A308
BBr_2	BBr_2	89,A192	BH_4Li	$LiBH_4$	305,A307
BBr_2H^+	$HBBr_2^+$	166	BH_4N^+	$H_2BNH_2^+$	307
BBr_2H	$HBBr_2$	A238	BH_4N	H_2BNH_2	309
$BBr_2H_2N^+$	$NH_2BBr_2^+$	332	BH_4Na	$NaBH_4$	305,A307
BBr_3^+	BBr_3^+	202,B235	BH_4Sr	$SrBH_4$	306
$BCaH_4$	$CaBH_4$	305	BI_2	BI_2	89
$BClF_3^-$	BF_3Cl^-	302	BI_3^+	BI_3^+	202,B236

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
BNSi	BNSi	B79	BeO_3	BeO_3	A250
BN_2	NBN	67	BeO_4	O_2BeO_2	A297
BN_2	BNN	69	Be_2H	BeBeH	A136
BN_3	NNBN	184,B222	Be_2H_2	HBeBeH	A217
BO_2	BO_2	73,B120	Be_2H_2O	HBeOBeH	A275
BO_2^-	BO_2^-	84	Be_2H_3	HBeHBeH	A267
BO_2S	OBSO	190	Be_2H_4	$HBeH_2BeH$	A308
BS_2	BS_2	74,A182	Be_2NO_2	BeOBeNO	B281
$B_2Cl_4^+$	$B_2Cl_4^+$	348	Be_2N_2	BeBeNN	A242
$B_2F_4^+$	$B_2F_4^+$	347	Be_2N_2	BeNNBe	A242
B_2HN	HBNB	A232	Be_2N_2	$(BeN)_2$	A242
B_2H_2	HBBH	A219	Be_2N_4	NNBeBeNN	A317
$B_2H_2N_2$	HNBBNH	A315	Be_2O	BeOBe	A163
B_2H_3N	H_2BNBH	A311	Be_2O_2	*cyc*-$(BeO)_2$	A242
$B_2H_4^+$	$B_2H_4^+$	306	Be_2O_2	BeOBeO	A242
$B_2H_5^+$	$B_2H_5^+$	359	Be_2O_3	OBeOBeO	A294
$B_2H_6^+$	$B_2H_6^+$	A332	BiHO	BiOH	B42
B_2H_7N	$B_2H_5NH_2$	398	Bi_3	Bi_3	82
B_2N	BNB	62,A165,B62	Bi_4	Bi_4	189
B_2N^-	BNB^-	63,A165,B78	Bi_4^-	Bi_4^-	197
B_2N_2	BBNN	181	$BrClH^-$	$ClHBr^-$	54
B_2N_2	BNBN	181	BrClO	BrClO	A209
B_2N_2	*cyc*-$(BN)_2$	181	BrClO	ClBrO	A209
B_2O	BBO	63	BrClO	BrOCl	A207,B151
B_2O	BOB	63	$BrClO_2$	$BrClO_2$	A263
$B_2O_2^+$	$B_2O_2^+$	183	$BrClO_2$	BrOClO	A264
B_2O_2	B_2O_2	184	$BrClO_2$	ClOBrO	A264
B_3	B_3	A162	BrClS	ClSBr	B152
$B_3F_3H_3N_3^+$	*cyc*-$(FBNH)_3^+$	399	$BrCl_2^-$	$ClBrCl^-$	119
B_3N	BNBB	B207	$BrCl_2^-$	$ClClBr^-$	119
B_3N^-	$BNBB^-$	B209	$BrFH^-$	$FHBr^-$	54
BaHO	BaOH	30,B24	BrFS	FSBr	A208
BaH_2N	$BaNH_2$	133	BrF_2	BrF_2	117
BaH_2O	HBaOH	135	BrF_2^-	$FBrF^-$	118
BaH_2O_2	$Ba(OH)_2$	251	BrF_2^-	$FFBr^-$	118
BaO_2	OBaO	A175	BrF_2P^+	PF_2Br^+	220
BaO_2	*cyc*-BaO_2	A175	BrF_3^+	BrF_3^+	226
Ba_2O_2	*cyc*-$(BaO)_2$	A243	BrF_3Si^+	SiF_3Br^+	295
Ba_2O_2	BaOBaO	A243	BrF_5^+	BrF_5^+	358
$BeBr_2$	$BeBr_2$	84	BrFeH	HFeBr	35
$BeCl_2$	$BeCl_2$	84	BrGeH	HGeBr	45,B41
BeF_2	BeF_2	83	$BrGeH_2$	H_2GeBr	150
BeHO	BeOH	A138	$BrGeH_3^+$	GeH_3Br^+	241
BeH_2	BeH_2	A125	$BrHI^-$	$BrHI^-$	55
BeH_2O	HBeOH	A222	$BrHO^+$	$HOBr^+$	A155
BeH_2O_2	$Be(OH)_2$	A281	BrHO	HOBr	52,A156,B45
BeI_2	BeI_2	84	BrHSi	HSiBr	44,A151,B40
BeKrO	KrBeO	A188	BrHXe	HXeBr	A158,B47
BeNO	BeNO	B87	BrH_2N^+	H_2NBr^+	152
BeN_2O_2	$NNBeO_2$	A296	BrH_2P	H_2PBr	A229
BeN_4	NNBeNN	A294	BrH_3Si^+	SiH_3Br^+	241
BeN_4	NN(*cyc*-BeN_2)	A294	BrKrXe	KrXeBr	123
BeOXe	XeBeO	A188	$BrKr_2$	Kr_2Br	123
BeO_2^+	$OBeO^+$	A171	$BrNO^+$	$BrNO^+$	94
BeO_2	OBeO	A174	BrNO	BrON	B143

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
$BrNO_2$	$BrNO_2$	213,A260,B239	CAlSi	AlCSi	B63
$BrNO_2$	*c*-BrONO	B239	$CAlSi^-$	$AlCSi^-$	B78
$BrNO_2$	*t*-BrONO	213,A260,B240	$CAlSi_2$	$CAlSi_2$	B210
$BrNO_3^+$	$BrONO_2^+$	A301	$CAlSi_2^-$	*cis*-$CAlSi_2^-$	B213
$BrNO_3$	$BrONO_2$	289,A303	CAl_2	Al_2C	A164
$BrNS^+$	$NSBr^+$	95	CAl_3	CAl_3	B201
BrNS	NSBr	104	CAl_3^-	CAl_3^-	B208
BrN_3^+	BrN_3^+	197	CAl_3Ge	CAl_3Ge	B279
BrNeXe	NeXeBr	123	CAl_3Ge^-	CAl_3Ge^-	B280
BrOP	BrPO	103,B142	CAl_3Si	CAl_3Si	B279
BrOPS	BrP(O)S	214	CAl_3Si^-	CAl_3Si^-	B279
BrO_2	BrOO	110,A204,B147	CAl_4	Al_4C	B278
BrO_2	OBrO	114,A206,B150	CAl_4^-	Al_4C^-	B278
BrO_2P	PO_2Br	214	Al_5C	Al_5C	B325
BrPS	BrPS	104	Al_5C^-	Al_5C^-	B325
BrS_2	SSBr	111	CAsN	AsCN	71
$BrXe_2$	Xe_2Br	123	CAsO	AsCO	B123
Br_2Cl^-	$BrClBr^-$	119	$CAsO^-$	$AsCO^-$	B131
Br_2Cl^-	$ClBrBr^-$	119	$CAuO^+$	$AuCO^+$	B62
Br_2F	BrBrF	117	CAuO	AuCO	B68
Br_2F_2	Br_2F_2	227	CBF_2NO	F_2BNCO	A321
Br_2GaH	$HGaBr_2$	B194	CBN	BCN	B78
Br_2Ge^+	$GeBr_2^+$	92	CBN	BNC	B78
$Br_2GeH_2^+$	$GeH_2Br_2^+$	263	CBO	BCO	68
Br_2H^-	$BrHBr^-$	55,A157	CBO_2	OBCO	186
Br_2HN^+	$HNBr_2^+$	179	CBS_2	SBCS	A249
$Br_2H_2^+$	$HBrBrH^+$	B179	CB_2	*cyc*-B_2C	B55
$Br_2H_2Si^+$	$SiH_2Br_2^+$	262	CBaN	BaNC	B60
Br_2Li	BrLiBr	B115	CBeN	BeCN	B58
Br_2N	NBr_2	108	CBeN	BeNC	B58
Br_2Na	BrNaBr	B116	$CBeO_2$	OCBeO	A247
Br_2O	BrOBr	114,A207,B151	$CBeO_2$	COBeO	A248
Br_2O	BrBrO	116,A209,B153	CBe_2O	BeBeCO	A241
Br_2OP	$OPBr_2$	221	$CBrCl^+$	$CClBr^+$	91,B135
Br_2P	PBr_2	109,A203	CBrCl	CClBr	99,B139
Br_2S^+	SBr_2^+	112	$CBrCl_2^+$	CCl_2Br^+	211
Br_2S	SBr_2	115	$CBrCl_2$	CCl_2Br	218
$Br_2S_2^+$	$S_2Br_2^+$	224	$CBrClF_2^-$	CF_2ClBr^-	303
Br_2S_2	$SSBr_2$	226	CBrF	CFBr	98,B138
Br_2Se^+	$SeBr_2^+$	113	$CBrF_2^+$	CF_2Br^+	210
Br_2Si	$SiBr_2$	101	$CBrF_2$	CF_2Br	216
Br_3^-	Br_3^-	119	$CBrF_2^-$	CF_2Br^-	225
Br_3P^+	PBr_3^+	221,B242	$CBrF_3^+$	CF_3Br^+	291
Br_3PO^+	Br_3PO^+	299	$CBrF_3^-$	CF_3Br^-	303
Br_3PS^+	Br_3PS^+	299	$CBrF_4$	CF_3BrF	356
Br_3Sb^+	$SbBr_3^+$	222	$CBrN^+$	$BrCN^+$	80,A187
Br_4Ge^+	$GeBr_4^+$	297	CBrN	BrNC	88
Br_4Si^+	$SiBr_4^+$	296,B305	$CBrNO^+$	$BrCNO^+$	A252
CAgN	AgCN	B60	$CBrNO^+$	$BrNCO^+$	193
$CAgN^-$	$AgCN^-$	B64	CBrNO	BrCNO	199,A253,B233
$CAgO^+$	$AgCO^+$	B62	CBrNO	BrNCO	198
CAlN	AlCN	B79	$CBrNS^+$	$BrSCN^+$	194
CAlN	AlNC	B79	CBrNS	BrSCN	199
CAlO	AlCO	68,A172	$CBrNSe^+$	$BrSeCN^+$	195
$CAlO^-$	$AlCO^-$	B111	CBr_2^+	CBr_2^+	91

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
CBr_2	CBr_2	100,B139	CCl_3F^-	$CFCl_3^-$	303
CBr_2^-	CBr_2^-	B145	CCl_3NO^+	CCl_3NO^+	353
CBr_2Cl^+	$CClBr_2^+$	211	CCl_3NO_4	CCl_3OONO_2	426
CBr_2Cl	$CClBr_2$	218	CCl_3O_2	CCl_3O_2	354
CBr_2F^+	$CFBr_2^+$	210	CCl_4^+	CCl_4^+	294,A305
CBr_2F	$CFBr_2$	216	CCl_4	$Cl_2CCl\text{-}Cl$	302,B306
$CBr_2F_2^+$	$CF_2Br_2^+$	292	CCl_4^-	$Cl_2CCl\text{-}Cl^-$	B307
$CBr_2F_2^-$	$CF_2Br_2^-$	303	CCl_4^-	CCl_4^-	B307
CBr_3^+	CBr_3^+	211	$CCoO^+$	$CoCO^+$	B61
CBr_3	CBr_3	218	CCoO	CoCO	A167,B67
CBr_3F^+	$CFBr_3^+$	293	$CCoO^-$	$CoCO^-$	B86
CBr_3F^-	$CFBr_3^-$	303	$CCoO_2$	OCoCO	B221
CBr_4^+	CBr_4^+	294	$CCoO_2^-$	$OCoCO^-$	B224
CCaN	CaNC	62,A164,B59	$CCoO_2^-$	$CoCO_2^-$	B224
CCaNO	CaNCO	182	CCrO	CrCO	A166,B65
CClF	CFCl	98,B138	$CCrO_2^+$	$OCrCO^+$	B217
CClFOS	ClFCSO (I)	288	$CCrO_2$	OCrCO	B220
CClFOS	ClFCSO (II)	288	$CCrO_2$	CrOCO	B221
$CClFS^+$	$FClCS^+$	205	$CCrO_2^-$	$OCrCO^-$	B224
$CClF_2^+$	CF_2Cl^+	210	CCuN	CuCN	B60
$CClF_2$	CF_2Cl	216	$CCuN^-$	$CuCN^-$	B64
$CClF_2NO^+$	CF_2ClNO^+	353	$CCuN^-$	$CuNC^-$	B64
$CClF_2NO_4$	$CF_2ClOONO_2$	425	$CCuO^+$	$CuCO^+$	B62
$CClF_3^+$	CF_3Cl^+	290,B303	CCuO	CuCO	A167,B68
$CClF_3^-$	CF_3Cl^-	303	$CCuO^-$	$CuCO^-$	B86
$CClF_4$	CF_3ClF	356	$CCuO_2^-$	$OCuCO^-$	B225
$CClN^+$	$ClCN^+$	79,B126	$CCuO_2^-$	$CuCO_2^-$	B225
CClN	ClNC	88	CFI	CFI	99
$CClNO^+$	$ClCNO^+$	B232	CFI_2^+	CFI_2^+	210
$CClNO^+$	$ClNCO^+$	193	CFI_2	CFI_2	217
CClNO	ClCNO	199,B233	CFN^+	FCN^+	79
CClNO	ClNCO	198	CFN	FNC	88
$CClNS^+$	$ClSCN^+$	194	CFNO	FNCO	198,A253
CClNS	ClSCN	198	$CFNO_5$	$FC(O)OONO_2$	A342
$CClNSe^+$	$ClSeCN^+$	195	$CFNS^+$	$FSCN^+$	193
CClO	ClCO	90,B135	CFN_2	FNCN	192
$CClP^+$	$ClCP^+$	81	CFO^+	FCO^+	86
CClP	ClCP	A190	CFO	FCO	90,A193,B134
CClS	ClCS	105	CFO_2	FCO_2	203,A256
CCl_2^+	CCl_2^+	91,B135	CFO_2^-	FCO_2^-	212,A259
CCl_2	CCl_2	99,B138	CFO_3	*c*-FC(O)OO	B300
CCl_2^-	CCl_2^-	107,B145	CFO_3	*t*-FC(O)OO	287,B301
CCl_2F^+	$CFCl_2^+$	210	CFP^+	FCP^+	81
CCl_2F	$CFCl_2$	216	CFP	FCP	A190
CCl_2FNO^+	$CFCl_2NO^+$	353	CFS	FCS	A194
CCl_2FNO_4	$CFCl_2OONO_2$	426	CF_2^+	CF_2^+	91
$CCl_2F_2^+$	$CF_2Cl_2^+$	292,A304	CF_2	CF_2	97,A196,B137
$CCl_2F_2^-$	$CF_2Cl_2^-$	303	CF_2^-	CF_2^-	107,B145
CCl_2I	CCl_2I	218	CF_2I^+	CF_2I^+	210
CCl_2O^+	Cl_2CO^+	204	CF_2I	CF_2I	216
CCl_2S^+	Cl_2CS^+	206	CF_2N	F_2CN	204
CCl_2Se	Cl_2CSe	212	CF_2NOP^+	PF_2NCO^+	349
CCl_3^+	CCl_3^+	210,B238	CF_2NP^+	PF_2CN^+	285
CCl_3	CCl_3	217,B240	CF_2NPS^+	PF_2NCS^+	350
CCl_3F^+	$CFCl_3^+$	293	$CF_2N_2^+$	$CF_2N_2^+$	285

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
CF_2O^+	F_2CO^+	204	$CHCaO_2$	HCOOCa	268
CF_2OS	F_2CSO	288	$CHCl^+$	$HCCl^+$	B36
CF_2O_2	*cyc*-F_2CO_2	A302	CHCl	HCCl	42,A149,B37
CF_2S^+	F_2CS^+	205	$CHCl^-$	$HCCl^-$	47
CF_2Se^+	F_2CSe^+	206	$CHClF^+$	$HCFCl^+$	171
CF_3^+	CF_3^+	210,A258	CHClF	HCFCl	176
CF_3	CF_3	215,A261	$CHClF_2^+$	HCF_2Cl^+	275
CF_3^-	CF_3^-	A263	$CHClO^+$	$HCOCl^+$	169
CF_3I^+	CF_3I^+	291	CHClO	HCOCl	170,A239,B194
CF_3I^-	CF_3I^-	303	$CHCl_2^+$	$HCCl_2^+$	171,B195
CF_3IO	CF_3IO	356	$CHCl_2$	$HCCl_2$	177,B199
CF_3IO	CF_3OI	356	$CHCl_2F^+$	$HCFCl_2^+$	275
CF_3N	CF_3N	B301	$CHCl_2NO_4$	$CHCl_2OONO_2$	425
CF_3NO^+	CF_3NO^+	353	$CHCl_3^+$	$HCCl_3^+$	275
CF_3NO_3	CF_3ONO_2	382,A342	$CHCl_3O$	CCl_3OH	B324
CF_3NO_4	CF_3OONO_2	A368,B395	CHF^+	HCF^+	41
CF_3O	CF_3O	289,A303,B302	CHF	HCF	42,A148,B36
CF_3O^-	CF_3O^-	302	CHF^-	HCF^-	47
CF_3O_2	CF_3O_2	354,B332	$CHFI^+$	$HCFI^+$	171
CF_3S	CF_3S	A303,B302	CHFI	HCFI	177
CF_4^+	CF_4^+	290,A303,B303	CHFN	HFCN	168,B193
CF_4I	CF_3IF	356	CHFN	FCNH	B193
CF_4O^+	CF_3OF^+	355	$CHFO^+$	$HFCO^+$	168
CF_4OS	CF_3OSF	372	$CHFS^+$	$HFCS^+$	A237
CFeN	FeNC	B60	CHF_2^+	HCF_2^+	170
$CFeO^+$	$FeCO^+$	B61	CHF_2	HCF_2	176,B199
CFeO	FeCO	63,A167,B66	CHF_2N^+	CF_2NH^+	A289
$CFeO^-$	$FeCO^-$	67,B85	CHF_2N	$CF_2{=}NH$	270,A289
$CFeO_2$	OFeCO	B221	CHF_2N	*c*-HFC=NF	271
$CFeO_2^-$	$OFeCO^-$	B224	CHF_2P	$CF_2{=}PH$	271
CFe_2O	Fe_2CO	B204	CHF_3^+	HCF_3^+	274,B276
CGaN	GaCN	B79	CHGe	HCGe	B30
CGaN	GaNC	B79	CHI	HCI	43
CGaO	GaCO	B97	CHI^-	HCI^-	48
CGeO	GeCO	A180,B112	CHIO	HCOI	A240
$CGeO^-$	$GeCO^-$	B121	CHI_2	HCI_2	178
CHBBr	HCBBr	B188	CHK	KCH	B22
CHBCl	HCBCl	B187	CHKrN	HKrCN	B195
CHBF	HCBF	B187	CHN^+	HCN^+	33,B31
CHBN	HBCN	B183	CHN^+	HNC^+	34
CHBN	HBNC	B183	CHN	HNC	38,A145,B33
CHBN	*cyc*-HB(CN)	B183	$CHNO^+$	$HNCO^+$	160
CHBeN	HBeCN	B182	$CHNO^+$	$HCNO^+$	161
CHBeN	HBeNC	B182	CHNO	HNCO	163,A236,B190
CHBr	HCBr	43,A149,B38	CHNO	HOCN	163,B191
$CHBr^-$	$HCBr^-$	47	CHNO	HCNO	164,B191
$CHBrCl^+$	$HCClBr^+$	171,B195	CHNOXe	HXeNCO	B276
CHBrCl	HCClBr	178,B199	CHNP	HPCN	160
$CHBrClF^+$	$HCFClBr^+$	A292	$CHNS^+$	$HNCS^+$	160
$CHBrF^+$	$HCFBr^+$	171	CHNS	HSCN	B192
CHBrF	HCFBr	177	CHNS	HSNC	B192
CHBrO	HCOBr	170,A239	CHNSi	HCNSi	B186
$CHBr_2^+$	$HCBr_2^+$	172	CHNSi	*cyc*-(HCSiN)	B186
$CHBr_2$	$HCBr_2$	178	CHNSi	HSiNC	B187
$CHBr_3^+$	$HCBr_3^+$	276	CHNSi	HSiCN	B187

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
CHNXe	HXeCN	B196	CH_2ClN	$CH_2{=}NCl$	258
CHNXe	HXeNC	B196	CH_2ClNO_4	$CH_2ClOONO_2$	425
CHN_2	HCNN	161,A235,B189	CH_2ClP	$CH_2{=}PCl$	258
CHN_2	HNCN	160,A235,B188	$CH_2Cl_2^+$	$CH_2Cl_2^+$	261,A285
CHN_2^-	$HCNN^-$	B190	CH_2Cl_2	$H_2CCl\text{-}Cl$	263,B269
CHN_2^-	$HNCN^-$	B190	CH_2Cl_2O	$HCCl_2OH$	339,B322
CHNa	NaCH	B22	$CH_2Cl_2O_2$	$CHCl_2OOH$	368
CHO^+	HCO^+	37,A145,B33	CH_2Cl_2Si	$CH_2{=}SiCl_2$	337,B322
CHO^+	HOC^+	39,B34	CH_2Co	$CoCH_2$	A219
CHO	HCO	40,A146,B34	CH_2Cr	$CrCH_2$	A218
CHOP	HPCO	165	CH_2Cu	$CuCH_2$	132
$CHOS^+$	$HOCS^+$	165,A236	CH_2F^+	H_2CF^+	147
CHO_2^+	$HOCO^+$	165	CH_2F	H_2CF	149,B176
CHO_2	*c*-HOCO	167	CH_2FI^+	CH_2FI^+	261
CHO_2	*t*-HOCO	167,A236	CH_2FMg	CH_2MgF	B263
CHO_2	HCO_2	A237	CH_2FO_2	CH_2FO_2	339
CHO_2^-	HCO_2^-	A230	$CH_2F_2^+$	$CH_2F_2^+$	260,A284
CHO_2Sr	HCOOSr	268	CH_2Fe	$FeCH_2$	131
CHO_3	HC(O)OO	270	CH_2Fe	HFeCH	132
CHP^+	HCP^+	34	CH_2Ge	H_2CGe	B170
CHS^+	HCS^+	38,A145	CH_2I	H_2CI	150
CHS	HCS	B36	$CH_2I_2^+$	$CH_2I_2^+$	262
CHS	HSC	B36	CH_2I_2	$H_2CI\text{-}I$	265
CHS_2	*t*-HSCS	167	CH_2Mg	$MgCH_2$	B162
CHS_2	HCS_2	168	CH_2N^+	$HCNH^+$	138,B170
CHSi	HCSi	B30	CH_2N	H_2CN	140,B171
CHTi	TiCH	A137	CH_2N	HCNH	B171
CHV	VCH	A137	CH_2N^-	H_2CN^-	143
CHW	WCH	A137	CH_2NO	H_2NCO	B268
CH_2^+	CH_2^+	18	CH_2NO	H_2CNO	A283
CH_2	CH_2	18,A130,B16	CH_2NOSr	HCONHSr	326
CH_2^-	CH_2^-	21	CH_2NO_2	CH_2NO_2	331,A316
CH_2B	HBCH	A221	$CH_2NO_2^-$	$CH_2NO_2^-$	337
CH_2BBr	H_2CBBr	B266	$CH_2N_2^+$	$CH_2N_2^+$	253
CH_2BCl	H_2CBCl	B266	$CH_2N_2^+$	*cyc*-$CH_2N_2^+$	254
CH_2BF	H_2CBF	B266	$CH_2N_2^+$	NH_2CN^+	253
CH_2BN	BH_2CN	B262	CH_2N_2	$HN{=}C{=}NH$	254,A282,B266
CH_2BN	CH_2NB	B262	CH_2N_2	HCNNH	A282
CH_2BO	CH_2BO	B263	CH_2N_2O	H_2NNCO	331
CH_2B_2	HBCBH	245,A275	CH_2Ni	$NiCH_2$	A219
CH_2Be	HCBeH	B162	CH_2O^+	H_2CO^+	140,A223,B172
CH_2Br^+	H_2CBr^+	147	CH_2OS^+	H_2CSO^+	258
CH_2Br	H_2CBr	150,A228	CH_2OS	H_2CSO	259,A284
CH_2BrCl	$H_2CCl\text{-}Br$	264,B269	$CH_2O_2^+$	$HCOOH^+$	257,B268
CH_2BrF^+	CH_2FBr^+	261	CH_2O_2	*cyc*-H_2CO_2	A283
CH_2BrI	$H_2CBr\text{-}I$	265	CH_2O_3	HC(O)OOH	336
CH_2BrMg	CH_2MgBr	B263	CH_2P	H_2CP	B171
$CH_2Br_2^+$	$CH_2Br_2^+$	261	CH_2S^+	H_2CS^+	141
CH_2Br_2	$H_2CBr\text{-}Br$	264	CH_2S	H_2CS	143,A224,B173
CH_2CaNO	HCONHCa	326	CH_2S^-	H_2CS^-	149
CH_2Cl^+	H_2CCl^+	147	CH_2S_2	H_2CSS	B269
CH_2Cl	H_2CCl	149,A228,B176	CH_2S_2	*cyc*-H_2CS_2	B269
CH_2ClF^+	CH_2FCl^+	261	CH_2S_2	*t*-HCSSH	259
CH_2ClI	$H_2CCl\text{-}I$	264	CH_2S_2	*c*-HCSSH	259
CH_2ClMg	CH_2MgCl	B263	CH_2Se^+	H_2CSe^+	141

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
CH_2Se	H_2CSe	145,A226,B174	CH_3IO	ICH_2OH	323
CH_2Si	H_2CSi	138,A223,B169	CH_3In	$InCH_3$	B250
CH_2Zn	$ZnCH_2$	131	CH_3K	KCH_3	230,B247
CH_2Zn	HZnCH	131	CH_3Li	$LiCH_3$	B247
CH_3^+	CH_3^+	124,A213,B156	CH_3Mg^+	$MgCH_3^+$	B248
CH_3	CH_3	125,A214,B156	CH_3Mg	$MgCH_3$	A267,B249
CH_3^-	CH_3^-	129	CH_3N^+	CH_2NH^+	233
CH_3Al	$AlCH_3$	A268	CH_3N	CH_3N	234,A269,B256
CH_3B	$H_2C{=}BH$	A268	CH_3N	CH_2NH	234
CH_3BBr	CH_3BBr	B316	CH_3NO^+	CH_3NO^+	318
CH_3BCl	CH_3BCl	B316	CH_3NO^+	CH_2NOH^+	318
CH_3BN	CH_2BNH	B314	CH_3NO^+	$HCONH_2^+$	318
CH_3BN	CH_3NB	B314	CH_3NO	CH_3NO	320
CH_3BO^+	BH_3CO^+	312	CH_3NO	CH_2NOH	320,A314
CH_3BO	CH_3BO	B315	CH_3NO_2	*c*-$CH_2(NO)OH$	367
CH_3BO	CH_2BOH	B316	CH_3NO_2	*t*-$CH_2(NO)OH$	367
CH_3Ba	$BaCH_3$	B249	CH_3NO_4	CH_3OONO_2	425
CH_3BaO	$BaOCH_3$	315	CH_3NO_5	$HOCH_2OONO_2$	425
CH_3Be	$BeCH_3$	B248	CH_3NS^+	$HCSNH_2^+$	319
CH_3Be	CH_2BeH	B248	CH_3Na	$NaCH_3$	229,B247
CH_3Br^+	CH_3Br^+	239,A274	CH_3O^+	CH_3O^+	235,B256
CH_3Br^+	H_2CBrH^+	A274	CH_3O^+	CH_2OH^+	235,A270
CH_3BrF	CH_3BrF	324	CH_3O	CH_3O	236,A271,B257
CH_3BrMg	CH_3MgBr	B318	CH_3O	CH_2OH	237,A272,B258
CH_3Ca	$CaCH_3$	230,A267,B249	CH_3O^-	CH_3O^-	242,B260
CH_3CaO	$CaOCH_3$	314,B315	CH_3OSr	$SrOCH_3$	315
CH_3CaS	$CaSCH_3$	315	CH_3O_2	CH_3O_2	321,B320
CH_3Cd^+	$CdCH_3^+$	B248	$CH_3O_2^-$	$CH_3O_2^-$	B321
CH_3Cd	$CdCH_3$	231,A268,B250	CH_3O_3	$HOCH_2O_2$	368
CH_3Cl^+	CH_3Cl^+	239,A273,B259	CH_3P^+	CH_2PH^+	233
CH_3Cl^+	H_2CClH^+	A274	CH_3S^+	CH_3S^+	235,A270,B257
CH_3ClF	CH_3ClF	324	CH_3S^+	CH_2SH^+	235
CH_3ClMg	CH_3MgCl	B318	CH_3S	CH_3S	237,A272,B259
CH_3ClMg	$HMgCH_2Cl$	B318	CH_3S	CH_2SH	238
CH_3ClO^+	CH_3OCl^+	322	CH_3S^-	CH_3S^-	242,B261
CH_3ClO	$ClCH_2OH$	323,B321	CH_3SSr	$SrSCH_3$	315
CH_3ClO_2	CH_2ClOOH	368	$CH_3S_2^+$	$CH_3S_2^+$	B320
CH_3ClS^+	CH_3SCl^+	B320	CH_3S_2	CH_3S_2	322
CH_3ClS	CH_3SCl	B321	$CH_3S_2^-$	$CH_3S_2^-$	322
CH_3ClSi	$CH_2{=}SiHCl$	321	CH_3Si	CH_2SiH	232
CH_3ClSi	CH_3SiCl	321	CH_3Si	CH_3Si	232
$CH_3Cl_2O_2V$	$Cl_2V(O)OCH_3$	B393	CH_3Si^-	CH_2SiH^-	233
CH_3Cl_3OTi	Cl_3TiOCH_3	B390	CH_3Si^-	CH_3Si^-	233
CH_3F^+	CH_3F^+	238	CH_3Sr	$SrCH_3$	230,A267
CH_3F^+	H_2CFH^+	A273	CH_3Te	CH_3Te	238
CH_3FI	CH_3IF	324	CH_3Zn^+	$ZnCH_3^+$	B247
CH_3FMg	CH_3MgF	B317	CH_3Zn	$ZnCH_3$	230,A267,B249
CH_3FMg	$HMgCH_2F$	B318	CH_4^+	CH_4^+	227,B246
CH_3FO^+	CH_3OF^+	322	CH_4B	H_2CBH_2	A309
CH_3FO	CH_3OF	322	CH_4B	CH_3BH	A310
CH_3Ga	$GaCH_3$	B250	CH_4BN	CH_3BNH	B336
CH_3I^+	CH_3I^+	239,B260	CH_4BN	CH_3NBH	B336
CH_3IMg	CH_3MgI	B318	CH_4BN	CH_2BNH_2	B336
CH_3IO	CH_3IO	323	CH_4Be	CH_3BeH	B308
CH_3IO	CH_3OI	323	CH_4Cd	CH_3CdH	A309

Formula	*Structure/Name*	*References*
CH_4Co	CH_3CoH	A308
CH_4Fe	CH_3FeH	306
CH_4Ga	CH_3GaH	307,A310,B309
CH_4Ge	CH_3GeH	B312
CH_4Hg	CH_3HgH	A309,B309
CH_4In	CH_3InH	B310
CH_4Mg	CH_3MgH	B308
CH_4N^+	$CH_2NH_2^+$	310
CH_4N	CH_2NH_2	B312
CH_4Ni	CH_3NiH	306
CH_4NiO	$HNiOCH_3$	362
CH_4NiO	CH_3NiOH	362
CH_4O^+	CH_3OH^+	310
CH_4OSi	HCH_3SiO	363
CH_4OSi	*t*-CH_3OSiH	B338
CH_4OSi	*c*-CH_3OSiH	B338
CH_4O_2	$CH_2(OH)_2$	A325
CH_4O_3	HO_2CH_2OH	379
CH_4S^+	CH_3SH^+	310,B312
CH_4Si^+	$CH_2{=}SiH_2^+$	308
CH_4Si	$CH_2{=}SiH_2$	309,A310,B311
CH_4Si	CH_3SiH	309
CH_4Zn	CH_3ZnH	A309
CH_5^+	CH_5^+	B308
CH_5BO	$H_2B{=}OCH_3$	374
CH_5BS	H_2BSCH_3	A335
CH_5Ga	CH_3GaH_2	B333
CH_5GaN^+	$GaNH_2CH_3^+$	B350
CH_5GaN	$GaNH_2CH_3$	B350
CH_6BN	$H_2B{=}NHCH_3$	398
CH_6OSi	CH_3SiH_2OH	416
CHfO	HfCO	B65
CIN^+	ICN^+	81
CIN	INC	A191
$CINO^+$	$INCO^+$	193
CINO	INCO	198
$CINS^+$	$ISCN^+$	195
CINS	ISCN	199
CI_2	CI_2	B140
CI_2^-	CI_2^-	B145
CI_3	CI_3	218
CInN	InCN	B79
CInN	InNC	B79
CInO	InCO	B98
$CIrO^+$	$IrCO^+$	B61
CIrO	IrCO	B67
$CIrO^-$	$IrCO^-$	B86
CMgN	MgCN	A164
CMgN	MgNC	62,A164,B59
CMnO	MnCO	B66
$CMnO^-$	$MnCO^-$	B85
$CMnO_2^+$	$OMnCO^+$	B217
$CMnO_2$	OMnCO	B221
$CMnO_2^-$	$OMnCO^-$	B224
CMoO	MoCO	B66
$CMoO_2$	OMoCO	B221
CNO^+	NCO^+	71
CNO	CNO	82
CNO	NCO	76,A184,B122
CNO^-	NCO^-	85,B131
CNOP	NCPO	B229
CNOSr	SrNCO	182
CNO_3^-	O_2CNO^-	B299
CNP	PCN	70
$CNPd^-$	$PdCN^-$	B64
CNS	NCS	77,B123
CNS^-	NCS^-	86
CNSi	SiCN	B100
CNSi	SiNC	B101
CNSn	SnCN	B101
$CNSn^-$	$SnCN^-$	B115
CNSr	SrNC	62,B59
CNTl	TlCN	B80
CNTl	TlNC	B80
CN_2	NCN	70,A180,B113
CN_2	CNN	71,B114
CN_2^-	NCN^-	B121
CN_2^-	CNN^-	B126
CN_2O^+	$ONCN^+$	186
CN_2O	NCNO	188,B229
CN_2O	NOCN	B228
CN_2O	CNNO	B229
CN_2S^+	$NSCN^+$	A249
CN_2S	NSCN	A252
CN_4^+	N_3CN^+	278
CNbO	CNbO	B65
CNbO	NbCO	B65
$CNbO^-$	$NbCO^-$	B85
$CNbO_2$	ONbCO (I)	B220
$CNbO_2$	ONbCO (II)	B220
$CNiO^+$	$NiCO^+$	B61
CNiO	NiCO	A167,B67
$CNiO^-$	$NiCO^-$	A171,B86
$CNiO_2$	ONiCO	B221
$CNiO_2^-$	$ONiCO^-$	B224
$CNiO_2^-$	$NiCO_2^-$	B224
$COOs^+$	$OsCO^+$	B61
COOs	OsCO	B66
$COOs^-$	$OsCO^-$	B85
COP	PCO	77
$COPd^+$	$PdCO^+$	B61
COPd	PdCO	A167,B67
$COPd^-$	$PdCO^-$	B86
$COPt^+$	$PtCO^+$	B62
COPt	PtCO	A167,B67
$COPt^-$	$PtCO^-$	B86
$CORe^+$	$ReCO^+$	B61
CORe	ReCO	B66
$CORe^-$	$ReCO^-$	B85
$CORh^+$	$RhCO^+$	B61

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
CORh	RhCO	B67	CO_2V	*cyc*-(COV)O	B220
$CORh^-$	$RhCO^-$	B86	CO_2W	OWCO	B221
$CORu^+$	$RuCO^+$	B61	CO_2Y^+	$OYCO^+$	B216
CORu	RuCO	B66	CO_2Y^+	$OYOC^+$	B216
$CORu^-$	$RuCO^-$	B85	CO_2Y^+	$YOCO^+$	B216
COS^+	OCS^+	78,A185,B124	CO_2Y	OYCO	B219
COS^-	OCS^-	B135	CO_2Y	*cyc*-(YOC)O	B219
$COSc^+$	$ScCO^+$	B60	CO_2Y	*cyc*-(COY)O	B219
COSc	ScCO	A166,B64	CO_2Zn^-	$OZnCO^-$	B225
$COSc^-$	$ScCO^-$	B84	CO_2Zr	OZrCO	B220
COSi	SiCO	70,B112	CO_3	CO_3	199
$COSi^-$	$SiCO^-$	B121	CO_3^-	CO_3^-	203
COSn	SnCO	A180,B112	CO_3Ti	O_2TiCO	A296
$COSn^-$	$SnCO^-$	B121	CO_3U	O_2UCO	A297
COTa	TaCO	A166,B65	CO_4^-	CO_4^-	287,B300
$COTa^-$	$CTaO^-$	B85	CS_2^+	CS_2^+	79,A186,B125
$COTa^-$	$TaCO^-$	B85	CS_2	*cyc*-CS_2	B131
COTe	OCTe	B131	CS_2^-	CS_2^-	A194,B135
COTh	ThCO	B68	CSi_2	Si_2C	67
COTh	CThO	B68	CSi_3	Si_3C	181
$COTh^-$	$CThO^-$	B86	$C_2AgO_2^+$	$Ag(CO)_2^+$	B282
$COTi^+$	$TiCO^+$	B60	C_2AgO_2	$Ag(CO)_2$	B286
COTi	TiCO	A166,B65	C_2Al	AlCC	B63
$COTi^-$	$TiCO^-$	B84	C_2Al^-	$AlCC^-$	B78
COU	CUO	A168,B68	C_2AlO_2	$Al(CO)_2$	B291
COU	UCO	A168,B68	$C_2AlO_2^-$	$Al(CO)_2^-$	B295
COU^-	CUO^-	B87	C_2Al_2	AlCCAl	A242,B207
COU^-	UCO^-	B87	$C_2Al_2^-$	$AlCCAl^-$	B210
COV	VCO	A166,B65	$C_2Al_2^-$	*cyc*-$Al_2C_2^-$	B210
COV^-	VCO^-	B84	$C_2AuO_2^+$	$Au(CO)_2^+$	B282
COW	WCO	B66	C_2AuO_2	$Au(CO)_2$	B287
COY^+	YCO^+	B60	C_2B	*cyc*-BCC	62,A164,B62
COY	YCO	B64	C_2B^-	BCC^-	B78
COZr	ZrCO	B65	$C_2BFN_2O_2$	$FB(NCO)_2$	A341
CO_2^+	CO_2^+	77,A185,B123	C_2B_2	BCCB	B207
CO_2^-	CO_2^-	90,A193,B134	C_2BeO_2	$Be(CO)_2$	A293
CO_2Sc^+	$OScCO^+$	B216	C_2BrCl^+	$ClCCBr^+$	191
CO_2Sc^+	$OScOC^+$	B216	C_2BrF_3	CF_3CBr	354
CO_2Sc^+	$ScOCO^+$	B216	C_2BrN	BrCNC	B230
CO_2Sc	OScCO	B219	C_2BrN	BrCCN	189,B230
CO_2Sc	*cyc*-(ScOC)O	B219	$C_2Br_2^+$	$C_2Br_2^+$	191
CO_2Sc	*cyc*-(COSc)O	B219	$C_2ClF_3^+$	$CF_2{=}CFCl^+$	352
CO_2Ta	OTaCO	B220	C_2ClF_3	CF_3CCl	354
CO_2Ta^-	$OTaCO^-$	B224	C_2ClN	ClCNC	B229
CO_2Th^+	$OThCO^+$	B217	C_2ClN	ClCCN	189,B230
CO_2Th	OThCO	B221	$C_2Cl_2^+$	$C_2Cl_2^+$	190
CO_2Ti^+	$OTiCO^+$	B216	$C_2Cl_2F_2^+$	$CF_2{=}CCl_2^+$	352
CO_2Ti^+	$OTiOC^+$	B217	$C_2Cl_2O^+$	Cl_2CCO^+	285
CO_2Ti	OTiCO	A248,B219	C_2Cl_2O	Cl_2CCO	285
CO_2Ti	*cyc*-(COTi)O	B220	$C_2Cl_2O_2^+$	*t*-$(ClCO)_2^+$	348
CO_2U^+	$OUCO^+$	B217	$C_2Cl_4^+$	$C_2Cl_4^+$	353
CO_2U	OUCO	A248,B222	C_2Co	CoCC	B57
CO_2V^+	$OVCO^+$	B217	C_2Co^-	$CoCC^-$	B58
CO_2V^+	$OVOC^+$	B217	$C_2CoO_2^+$	$Co(CO)_2^+$	B281
CO_2V	OVCO	B220	C_2CoO_2	$Co(CO)_2$	B285

Formula	*Structure/Name*	*References*
$C_2CoO_2^-$	$Co(CO)_2^-$	B290
C_2Cr	CrCC	B57
C_2Cr^-	$CrCC^-$	B58
$C_2CuO_2^+$	$Cu(CO)_2^+$	B282
C_2CuO_2	$Cu(CO)_2$	B286
$C_2CuO_2^-$	$Cu(CO)_2^-$	B291
$C_2F_2^+$	$C_2F_2^+$	190
C_2F_2	FCCF	197
C_2F_2	$F_2C{=}C{:}$	197,B232
$C_2F_2^-$	$F_2C{=}C{:}^-$	203
$C_2F_2N_2$	$F_2C{=}C{=}N{=}N$	347
C_2F_2O	F_2CCO	B299
$C_2F_2O_2^+$	t-$(FCO)_2^+$	348
C_2F_3	C_2F_3	287
C_2F_3O	CF_3CO	A322
$C_2F_4^+$	$C_2F_4^+$	351,B331
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,B57
C_2Fe^-	$FeCC^-$	A164,B58
$C_2FeO_2^+$	$Fe(CO)_2^+$	B281
C_2FeO_2	$Fe(CO)_2$	B285
$C_2FeO_2^-$	$Fe(CO)_2^-$	B290
C_2DFe	FeCCD	A232
C_2GaO_2	$Ga(CO)_2$	B292
C_2GeO_2	$Ge(CO)_2$	B295
C_2H^+	HCC^+	B23
C_2H	HCC	32,A142,B28
C_2H^-	HCC^-	37,B32
C_2HAl	HCCAl	A233
C_2HB	HBCC	A232,B183
C_2HB	HCCB	A232
C_2HB	cyc-HBC_2	A232
C_2HBe	BeCCH	A231
C_2HBr^+	$HCCBr^+$	158
C_2HCa	CaCCH	155,A231,B181
C_2HCl^+	$HCCCl^+$	158
C_2HClFO	CHClCFO	B323
$C_2HClF_2^+$	$CHCl{=}CF_2^+$	340
C_2HClO	HClCCO	269,B273
$C_2HCl_3^+$	$CHCl{=}CCl_2^+$	341
C_2HF^+	$HCCF^+$	158
C_2HF	$HFC{=}C{:}$	162
C_2HF^-	$HFC{=}C{:}^-$	168
C_2HFO	HFCCO	269,A288
C_2HF_2O	c-CHFCFO	B323
C_2HF_2O	t-CHFCFO	B323
$C_2HF_3^+$	$CHF{=}CF_2^+$	340
C_2HFe^-	$FeCCH^-$	A232
C_2HI^+	$HCCI^+$	159
C_2HK	KCCH	B180
C_2HLi	LiCCH	B180
C_2HMg	MgCCH	A231,B180
C_2HN	HCCN	156,A234,B185
C_2HN	HCNC	B185
C_2HN	cyc-$HC{=}NC{:}$	B186
C_2HNO	HCOCN	269,A287
C_2HNO_2	$O{=}C{=}C{=}NOH$	A317
C_2HNPd	PdCCNH	B271
C_2HNPd^-	$PdCCNH^-$	B271
C_2HNS^+	$HCSCN^+$	A287
C_2HNS	HCSCN	A288
$C_2HN_2^+$	$HNCCN^+$	268,B273
C_2HNa	NaCCH	B180
C_2HO	HCCO	156,A234,B188
C_2HO^-	$HCCO^-$	B189
C_2HP	HCCP	B187
C_2HPd	PdCCH	B181
C_2HPd^-	$PdCCH^-$	B182
C_2HS	HCCS	157,A234
C_2HS	HSCC	157
C_2HSi	HCCSi	A233,B184
C_2HSr	SrCCH	155,A231,B181
C_2HYb^+	$YbCCH^+$	B180
C_2HYb	YbCCH	B181
$C_2H_2^+$	$HCCH^+$	133,A221,B164
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_2ClO	t-CHClCHO	B322
$C_2H_2Cl_2^+$	$CH_2{=}CCl_2^+$	335
$C_2H_2Cl_2^+$	c-$CHCl{=}CHCl^+$	335
$C_2H_2Cl_2^+$	t-$CHCl{=}CHCl^+$	336
C_2H_2F	$CH_2{=}CF$	B267
C_2H_2F	c-$CHF{=}CH$	257,B267
$C_2H_2FN^+$	CH_2FCN^+	330
C_2H_2FO	CH_2CFO	A316,B321
$C_2H_2FO^-$	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,B264
C_2H_2N	H_2CNC	250
$C_2H_2N^-$	H_2CCN^-	252

Formula	*Structure/Name*	*References*
$C_2H_2N^-$	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
$C_2H_2N_2$	$H_2C{=}NCN$	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_2O	*cyc*-H_2COC:	B266
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_2P	H_2CCP	B265
$C_2H_2S^+$	H_2CCS^+	253
C_2H_2S	H_2CCS	255,A282
C_2H_2S	HCCSH	256
C_2H_2S	*cyc*-C_2H_2S	256
$C_2H_2S_2$	$HS{-}CH{=}C{=}S$	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	A249
$C_2H_3^+$	$C_2H_3^+$	232,A268
C_2H_3	C_2H_3	232,A269,B255
C_2H_3As	$HCCAsH_2$	A313
C_2H_3As	CH_3CAs	A313
C_2H_3B	*cyc*-$(CH)_2BH$	B312
C_2H_3B	H_2BCCH	B313
C_2H_3B	$HBCCH_2$	B313
$C_2H_3CaO_2$	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,B338
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,B317
$C_2H_3O^-$	CH_2CHO^-	320,A314,B319
$C_2H_3O_2Sr$	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_3Si	SiH_2CCH	B314
$C_2H_4^+$	$C_2H_4^+$	307
C_2H_4Al	AlC_2H_4	361
C_2H_4B	*cyc*-$BHCHCH_2$	B334
C_2H_4B	H_2BCCH_2	B334
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,B336
$C_2H_4O^+$	CH_3CHO^+	B336
$C_2H_4O^+$	$CH_2{=}CHOH^+$	362,A324
C_2H_4O	syn-$CH_2{=}CHOH$	363,B337
C_2H_4O	anti-$CH_2{=}CHOH$	B338
$C_2H_4O_3$	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*-$CHCHSiH_2$	A324
C_2H_4Si	*cyc*-CH_2CH_2Si	B335
C_2H_4Si	$H_2CCHSiH$	B336
C_2H_4Si	H_2CCSiH_2	B336
$C_2H_4Si_2$	H_3Si(*cyc*-CSiCH)	B357
$C_2H_4Si_2$	$HSiCCSiH_3$	B358
$C_2H_4Si_2$	$HCCSiSiH_3$	B358
$C_2H_5^+$	$C_2H_5^+$	359
C_2H_5	C_2H_5	359,A323,B334
C_2H_5B	$H_2BC_2H_3$	B349
C_2H_5B	$CH_3B{=}CH_2$	B349
C_2H_5BrS	CH_3SBrCH_2	418
C_2H_5CaO	$CaOC_2H_5$	B388
C_2H_5Cd	CdC_2H_5	B349
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,B352
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
$C_2H_5O^+$	CH_3CHOH^+	B352
$C_2H_5O^+$	$CH_3CH_2O^+$	B352
C_2H_5O	C_2H_5O	376,A337,B353
C_2H_5O	CH_3CHOH	376

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
C_2H_5O	$HOCH_2CH_2$	376,A337	$C_2N_2^+$	$NCCN^+$	183
$C_2H_5O^-$	$C_2H_5O^-$	B353	$C_2N_2^+$	$CNCN^+$	184
$C_2H_5O_2$	$C_2H_5O_2$	420,B393	C_2N_2	CNCN	185,A248
$C_2H_5O_2^-$	$C_2H_5O_2^-$	B394	C_2N_2	CNNC	185
$C_2H_5O_3$	$HOCH_2CH_2O_2$	424	$C_2N_2O^+$	$NCCNO^+$	A295
$C_2H_5S^+$	$CH_3SCH_2^+$	A336	$C_2N_2O^+$	$NCNCO^+$	279
$C_2H_5S^+$	$C_2H_5S^+$	B352	C_2N_2O	NCCNO	283,A297,B295
C_2H_5S	C_2H_5S	376,A337,B353	C_2N_2O	NCNCO	283
$C_2H_5Zn^+$	$ZnC_2H_5^+$	B349	$C_2N_2O_2^+$	$ONCCNO^+$	A320
C_2H_5Zn	ZnC_2H_5	B349	$C_2N_2O_2$	ONCCNO	A321
C_2H_6BN	CH_3BNCH_3	B385	$C_2N_2O_2$	OCNNCO	B329
C_2H_6Ge	$(CH_3)_2Ge$	400	$C_2N_2S^+$	$S(CN)_2^+$	280
C_2H_6GeO	$(CH_3)_2Ge{=}O$	B391	$C_2N_2S^+$	$NCNCS^+$	280
C_2H_6GeS	$(CH_3)_2Ge{=}S$	B391	C_2N_2S	NCNCS	284
C_2H_6Hg	C_2H_5HgH	A357	$C_2N_2S_2^+$	$(SCN)_2^+$	346
$C_2H_6N_2O$	CH_3NHCH_2NO(A)	424	$C_2N_2Se^+$	$Se(CN)_2^+$	281
$C_2H_6N_2O$	CH_3NHCH_2NO(B)	424	C_2N_2Sn	$Sn(CN)_2$	B289
C_2H_6OSi	$(CH_3)_2SiO$	416	$C_2N_2Sn^-$	$Sn(CN)_2^-$	B292
C_2H_6OSi	$CH_2{=}Si(OH)CH_3$	417	C_2Nb	NbCC	B56
C_2H_6OSi	CH_3OSiCH_3	417	C_2Nb^-	$NbCC^-$	B58
C_2H_6OSi	$CH_3OSiH{=}CH_2$	417	C_2NbO_2	$Nb(CO)_2$	B284
$C_2H_6O_2Si$	$(CH_3O)_2Si$	421	C_2NbO_2	ONbCCO	B284
$C_2H_6O_2Si$	$CH_3SiOOCH_3$	421	$C_2NbO_2^-$	$Nb(CO)_2^-$	B289
$C_2H_6O_2Si$	$CH_3SiHOHCHO$	A365	$C_2Nb_3^+$	$Nb_3C_2^+$	B277
$C_2H_6O_3$	$HOCH_2CH_2OOH$	424	C_2Nb_3	Nb_3C_2	B277
$C_2H_6O_4$	$CH_3O_4CH_3$	424	$C_2NiO_2^+$	$Ni(CO)_2^+$	B282
C_2H_6Si	$(CH_3)_2Si$	399	C_2NiO_2	$Ni(CO)_2$	B286
C_2H_6Si	$CH_3SiH{=}CH_2$	399,B385	$C_2NiO_2^-$	$Ni(CO)_2^-$	B291
C_2H_6Sn	$(CH_3)_2Sn$	400	C_2O	CCO	69,A179,B111
$C_2H_6Zn^+$	$(CH_3)_2Zn^+$	A357	C_2O^-	CCO^-	76,A183,B121
C_2H_6Zn	C_2H_5ZnH	B385	C_2OS	OCCS	B228
$C_2H_7^+$	$C_2H_7^+$	383	$C_2O_2^+$	*t*-$OCCO^+$	186,B225
$C_2H_7^+$	*br*-$C_2H_7^+$	383	$C_2O_2^-$	*t*-$OCCO^-$	190,B232
C_2H_7BO	$H_2B{=}OC_2H_5$	408	C_2O_2Os	$Os(CO)_2$	B285
C_2H_7BS	$H_2BSC_2H_5$	A361	$C_2O_2Os^-$	$Os(CO)_2^-$	B290
C_2H_7Ga	$(CH_3)_2GaH$	B385	$C_2O_2Pd^+$	$Pd(CO)_2^+$	B282
C_2H_8BN	$H_2B{=}N(CH_3)_2$	399	C_2O_2Pd	$Pd(CO)_2$	B286
C_2H_8OSi	$(CH_3)_2SiHOH$	417	$C_2O_2Pd^-$	$Pd(CO)_2^-$	B291
C_2HfO_2	$Hf(CO)_2$	B284	$C_2O_2Pt^+$	$Pt(CO)_2^+$	B282
C_2HfO_2	OHfCCO	B284	C_2O_2Pt	$Pt(CO)_2$	B286
$C_2HfO_2^-$	$Hf(CO)_2^-$	B289	$C_2O_2Pt^-$	$Pt(CO)_2^-$	B291
$C_2I_2^+$	$C_2I_2^+$	192	C_2O_2Re	$Re(CO)_2$	B285
C_2InO_2	$In(CO)_2$	B292	$C_2O_2Re^-$	$Re(CO)_2^-$	B290
$C_2IrO_2^+$	$Ir(CO)_2^+$	B282	$C_2O_2Rh^+$	$Rh(CO)_2^+$	B281
C_2IrO_2	$Ir(CO)_2$	B286	C_2O_2Rh	$Rh(CO)_2$	B286
$C_2IrO_2^-$	$Ir(CO)_2^-$	B290	$C_2O_2Rh^-$	$Rh(CO)_2^-$	B290
C_2Mn	MnCC	B57	C_2O_2Ru	$Ru(CO)_2$	B285
C_2Mn^-	$MnCC^-$	B58	$C_2O_2Ru^-$	$Ru(CO)_2^-$	B290
C_2MnO_2	$Mn(CO)_2$	B285	$C_2O_2Sc^+$	$Sc(CO)_2^+$	B281
$C_2MnO_2^-$	$Mn(CO)_2^-$	B289	C_2O_2Sc	$Sc(CO)_2$	B283
C_2N^+	CCN^+	B84	C_2O_2Si	$Si(CO)_2$	283,B295
C_2N^+	CNC^+	67,B84	C_2O_2Sn	$Sn(CO)_2$	B295
C_2N	CCN	68,A173,B99	C_2O_2Ta	$Ta(CO)_2$	B284
C_2N	CNC	69,B100	C_2O_2Ta	OTaCCO	B285
C_2NP	NCCP	B223	$C_2O_2Ta^-$	$Ta(CO)_2^-$	B289

Formula	*Structure/Name*	*References*
C_2O_2Th	$Th(CO)_2$	B287
C_2O_2Th	OThCCO	B287
$C_2O_2Th^-$	$Th(CO)_2^-$	B291
C_2O_2Ti	$Ti(CO)_2$	B283
$C_2O_2Ti^-$	$Ti(CO)_2^-$	B289
C_2O_2U	$U(CO)_2$	B287
C_2O_2U	OUCCO	B287
$C_2O_2U^-$	$U(CO)_2^-$	B291
C_2O_2V	$V(CO)_2$	B284
$C_2O_2V^-$	$V(CO)_2^-$	B289
C_2O_2Zr	$Zr(CO)_2$	B284
C_2O_2Zr	OZrCCO	B284
$C_2O_2Zr^-$	$Zr(CO)_2^-$	B289
$C_2O_3^-$	$C_2O_3^-$	B298
$C_2O_4^+$	$O_2CCO_2^+$	B329
$C_2O_4^-$	$O_2CCO_2^-$	B330
C_2S	CCS	70,B113
C_2S_2	SCCS	188
C_2S_3	$S(CS)_2$	284
$C_2S_4^+$	$S_2CCS_2^+$	B330
C_2Sc	ScCC	B56
C_2Sc^-	$ScCC^-$	B58
C_2Si	SiCC	66,A170
C_2Si_2	Si_2C_2	181,A245
C_2Si_3	Si_3C_2	A293
C_2Ti	TiCC	B56
C_2Ti^-	$TiCC^-$	B58
C_2V	VCC	B56
C_2V^-	VCC^-	B58
C_2Xe	XeC_2	B133
C_2Y	YCC	A164
$C_2Y_3^+$	$Y_3C_2^+$	B277
C_2Y_3	Y_3C_2	B277
C_3	C_3	65,A168,B81
C_3^-	C_3^-	68,A173,B99
C_3B	BCCC	B210
C_3BrN^+	$BrCCCN^+$	282
C_3ClN^+	$ClCCCN^+$	281
C_3Cl_2	*cyc*-C_3Cl_2	A299
C_3Cl_2	ClCCCCl	A299
C_3Cl_2	$Cl_2C{=}C{=}C$:	A299
C_3Co	*cyc*-CoC_3	B204
C_3Co^-	*cyc*-CoC_3^-	B209
C_3Cr	*cyc*-CrC_3	B203
C_3Cr^-	*cyc*-CrC_3^-	B209
C_3FN^+	$FCCCN^+$	281
C_3F_2	*cyc*-C_3F_2	A299
C_3F_2	FCCCF	A299
C_3F_2	$F_2C{=}C{=}C$:	A299
C_3F_2O	$F_2C{=}C{=}C{=}O$	347
C_3F_2O	*cyc*-(CF=CFC)=O	347
$C_3F_6^+$	$C_3F_6^+$	405
C_3F_7	*n*-C_3F_7	405
C_3F_7	*i*-C_3F_7	406
C_3Fe	*cyc*-FeC_3	A242,B203
C_3Fe^-	*cyc*-FeC_3^-	A242,B209
C_3Ge_2	GeCCCGe	B281
C_3H	HC_3	156,A233,B183
C_3H	*cyc*-HC_3	156,A233
C_3HCl	*cyc*-C_3HCl	A288
C_3HCl	HCCCCl	A288
C_3HCl	$HClC{=}C{=}C$:	A288
C_3HFe	$FeC{=}C{=}CH$	A286
C_3HFe	FeCCCH	A286
C_3HFe^-	$FeC{=}C{=}CH^-$	A286
C_3HFe^-	$FeCCCH^-$	A286
C_3HN^+	$HCCCN^+$	266,B272
C_3HN^+	$HCCNC^+$	267
C_3HN	HNCCC	267,B273
C_3HN	HCCNC	267,B273
C_3HNO	$NCCH{=}C{=}O$	B323
C_3HF_3S	CF_3H(*cyc*-CCS)	381
C_3HO	HCCCO	268,A286
C_3HS	HCCCS	A287
$C_3H_2^+$	*cyc*-$C_3H_2^+$	248
C_3H_2	HCCCH	249,A278
C_3H_2	*cyc*-C_3H_2	248,B262
C_3H_2	$H_2C{=}C{=}C$:	248,A277,B262
C_3H_2	$HCCH{=}C$:	249
$C_3H_2^-$	$H_2C{=}C{=}C{:}^-$	A280,B264
$C_3H_2N^+$	$HCCCNH^+$	326,A315,B321
$C_3H_2N_2$	*cyc*-(HC=CHN=C=N)	B340
$C_3H_2N_2$	(*cyc*-HC=CHN)CN	B340
$C_3H_2N_2$	$H_2C{=}C{=}NCN$	B340
$C_3H_2N_2$	*cyc*-(C=NCHNCH)	B341
$C_3H_2N_2$	HC-N=CHCN	B341
$C_3H_2N_2$	*cyc*-(HC=NCH)CN	B341
$C_3H_2N_2$	$HNC{=}C{=}CHCN$	B341
$C_3H_2O^+$	$H_2C{=}C{=}C{=}O^+$	327
C_3H_2O	$HOCH{=}C{=}C$:	328,B321
C_3H_2O	$H_2C{=}C{=}C{=}O$	328
$C_3H_2O_2$	*t*-HCCCHOO	A327
$C_3H_2O_2$	*c*-HCCCHOO	A327
$C_3H_2O_2$	HCC(*cyc*-CHOO)	A328
$C_3H_2O_3$	*cyc*-(HOC=COHC)=O	A340
C_3H_2S	$H_2C{=}C{=}C{=}S$	329
C_3H_2Se	$H_2C{=}C{=}C{=}Se$	329
C_3H_2Se	HCC–CHSe	329
$C_3H_3^+$	*cyc*-$C_3H_3^+$	B313
$C_3H_3^+$	CH_2CCH^+	312,B313
C_3H_3	CH_2CCH	312,A311,B314
$C_3H_3^-$	CH_2CCH^-	A311,B316
$C_3H_3^-$	CH_3CC^-	A312
$C_3H_3Br^+$	CH_3CCBr^+	365
$C_3H_3Cl^+$	CH_3CCCl^+	365
$C_3H_3N^+$	$C_2H_3CN^+$	A325
C_3H_3N	$H_2C{=}$(*cyc*-CN=CH)	A326
$C_3H_4^+$	$H_2CCCH_2^+$	362,A323,B335
$C_3H_4^+$	CH_3CCH^+	B335
C_3H_4	H_2CCHCH:	B335

Formula	*Structure/Name*	*References*
C_3H_4Fe	$HFeCH{=}C{=}CH_2$	B354
C_3H_4Fe	$HCCCH_2FeH$	B354
C_3H_4Fe	$HFeCCCH_3$	B354
C_3H_4Fe	CH_3FeCCH	B355
C_3H_4Li	CH_3CCHLi	377
$C_3H_4NO_2$	$CH_3C(=NO)CHO$	A367
C_3H_4O	*cyc*-$(H_2COC){=}CH_2$	379
C_3H_4O	CH_3CCOH	A338
C_3H_4S	HCH_3(*cyc*-CCS)	379
C_3H_4Si	H_3C(*cyc*-CSiCH)	B356
C_3H_4Si	*cyc*-$CH_2CHCHSi$	B356
C_3H_4Si	$H_3CCHCSi$	B356
C_3H_4Si	$H_2CCHCHSi$	B356
C_3H_4Si	$H_3CCCSiH$	B356
C_3H_4Si	$H_3CSiCCH$	B357
C_3H_4Si	$H_2CCCHSiH$	B357
C_3H_4Si	$H_2CSiHCCH$	B357
$C_3H_5^+$	$CH_2CHCH_2^+$	372,B350
$C_3H_5^+$	*cyc*-$C_3H_5^+$	372
C_3H_5	CH_2CHCH_2	372,A334,B350
$C_3H_5^-$	$CH_2CHCH_2^-$	A335
C_3H_5N	$H_2C{=}CH{-}CH{=}NH$	408
C_3H_5N	$H_2C{=}C{=}NCH_3$	408
C_3H_5N	$H_2C{=}CHN{=}CH_2$	409
C_3H_5N	*cyc*-C_3H_5N	409
C_3H_5O	CH_2COCH_3	B390
C_3H_5O	CH_3CHCHO	B390
C_3H_6O	*t*-CH_3C-OCH_3	415
C_3H_6O	*c*-CH_3C-OCH_3	415
C_3H_6S	$(CH_3)_2CS$	415
$C_3H_7^+$	1-$C_3H_7^+$	383
$C_3H_7^+$	2-$C_3H_7^+$	383
C_3H_7	$CH_3CH_2CH_2$	383
C_3H_7	$(CH_3)_2CH$	383
C_3H_7N	$CH_3CH{=}CHNH_2$	409
C_3H_7N	$C_2H_3NHCH_3$	409
C_3H_7O	*n*-C_3H_7O	416,B390
C_3H_7O	$(CH_3)_2CHO$	416,B391
$C_3H_7O^-$	$(CH_3)_2CHO^-$	B391
$C_3H_7O_2$	$(CH_3)_2CHO_2$	420
C_3H_8Ge	$(CH_3)_2Ge{=}CH_2$	B386
$C_3H_8O_2Si$	$(CH_3)_2SiOHCHO$	A365
$C_3H_8Si^+$	$(CH_3)_2Si$-CH_2^+	400
C_3H_8Si	$(CH_3)_2Si{=}CH_2$	401,B386
C_3H_9Al	$(CH_3)_3Al$	400
C_3H_9NSi	$(CH_3)_3SiN$	410
C_3IN^+	$ICCCN^+$	282
C_3Mn	*cyc*-MnC_3	B203
C_3Mn^-	*cyc*-MnC_3	B209
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_3Nb	*cyc*-NbC_3	B203
C_3Nb^-	*cyc*-NbC_3^-	B209
C_3Ni	*cyc*-NiC_3	B204
C_3Ni^-	*cyc*-NiC_3^-	B209
C_3O	CCCO	186,B223
$C_3O_2^+$	$C_3O_2^+$	279
C_3S	CCCS	186,A249,B223
C_3Sc	*cyc*-ScC_3	B202
C_3Sc^-	*cyc*-ScC_3^-	B209
C_3Si	SiC_3	B214
C_3Si	*cyc*-SiC_3 (prolate)	B215
C_3Si	*cyc*-SiC_3 (oblate)	B215
C_3Si^-	SiC_3^-	B218
C_3Si_2	SiCCCSi	278,A293,B280
$C_3Si_2^-$	$SiCCCSi^-$	B283
C_3Ti	*cyc*-TiC_3	B202
C_3Ti^-	*cyc*-TiC_3^-	B209
C_3V	*cyc*-VC_3	B203
C_3V^-	*cyc*-VC_3^-	B209
C_4	C_4	181,A245,B214
C_4^-	C_4^-	183,A246,B217
$C_4Br_2^+$	$Br(CC)_2Br^+$	345
$C_4Cl_2^+$	$Cl(CC)_2Cl^+$	345
$C_4F_2^+$	$F(CC)_2F^+$	344
C_4F_4	$F_2C{=}C{=}CFCF$:	B363
C_4F_4	$F_2C{=}$(*cyc*-C_3F_2)	B363
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,B271
C_4H^-	C_4H^-	B272
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_4HN	CCCHCN	B323
C_4HN	HCCCCN	B323
C_4HN	(*cyc*-HC_3)CN	B323
C_4HO	HCCCCO	A316
C_4HS	HCCCCS	A317
C_4HSi	SiCCCCH	B323
$C_4H_2^+$	$C_4H_2^+$	325
C_4H_2	H_2CCCC:	326,A315
$C_4H_2F_2$	$F_2C{=}$(*cyc*-C_3H_2)	B359
$C_4H_2F_2$	$F_2C{=}CHCCH$	B359
$C_4H_2F_2$	$F_2C{=}C{=}C{=}CH_2$	B359
C_4H_2N	H_2CCCCN	B340
$C_4H_2N_2O$	*cyc*-(N=CHN=CHC) =C=O	B393
C_4H_2Si	HSiCCCCH	B339
C_4H_2Si	$Si(CCH)_2$	B339
$C_4H_4^+$	*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,B355
C_4H_4	$H_2C{=}$(*cyc*-C_3H_2)	377
C_4H_4	$C_2H_3CH{=}C$:	A338

Formula	*Structure/Name*	*References*
C_4H_4	$H_2C{=}C{=}CHCH$:	B355
$C_4H_4^-$	$C_2H_3CH{=}C{:}^-$	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	$H_2C{=}(cyc\text{-}CN{=}CCH_3)$	A361
$C_4H_6^+$	$t\text{-}H_2C{=}CH{-}CH{=}CH_2^+$	A342,B363
C_4H_6	$H_2CCHC(CH_3)$:	B364
C_4H_6	$C(CH_2)_3$	A343
$C_4H_6^-$	$C(CH_2)_3^-$	A343
C_4H_6Ge	$cyc\text{-}C_4H_4GeH_2$	A359
C_4H_6Ge	$cyc\text{-}C_4H_6Ge$:	A359
C_4H_6Ge	$cyc\text{-}C_4H_5GeH$ (1,3)	A360
C_4H_6Ge	$cyc\text{-}C_4H_5GeH$ (1,4)	A360
C_4H_6S	$(CH_3)_2(cyc\text{-}CCS)$	419
C_4H_6Si	$cyc\text{-}C_4H_4SiH_2$	A358
C_4H_6Si	$cyc\text{-}C_4H_6Si$:	A358
C_4H_6Si	$cyc\text{-}C_4H_5SiH$ (1,3)	A358
C_4H_6Si	$cyc\text{-}C_4H_5SiH$ (1,4)	A359
$C_4H_7^+$	$H_2CC(CH_3)CH_2^+$	A343
$C_4H_7^+$	$cyc\text{-}C_4H_7^+$	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_7O	$CH_3CHCOCH_3$	B392
C_4H_7O	$(CH_3)_2CCHO$	B392
C_4H_8Si	$cyc\text{-}C_2H_2Si(CH_3)_2$	A358
$C_4H_9^+$	$t\text{-}C_4H_9^+$	384
C_4H_9	$n\text{-}C_4H_9$	384,A344
C_4H_9	$i\text{-}C_4H_9$	384
C_4H_9	$t\text{-}C_4H_9$	384
C_4H_9O	$1\text{-}C_4H_9O$	B392
C_4H_9O	$2\text{-}C_4H_9O$	B392
C_4H_9O	$(CH_3)_3CO$	B392
$C_4H_9O^-$	$(CH_3)_3CO^-$	B393
$C_4H_9O_2$	$t\text{-}C_4H_9O_2$	421,B394
$C_4H_9O_2^-$	$t\text{-}C_4H_9O_2^-$	B394
$C_4H_{10}Si$	$(CH_3)_2Si{=}CHCH_3$	401,B387
$C_4I_2^+$	$I(CC)_2I^+$	345
$C_4N_2^+$	$NCC{\equiv}CCN^+$	343,A319,B327
C_4N_2	NCCCNC	343,A320,B328
C_4N_2	CNCCNC	343
C_4N_2O	$(CN)_2CCO$	A330
C_4O	C_4O	278,A294
C_4O^-	C_4O^-	B292
C_4OS	C_4OS	344
C_4O_2	C_4O_2	344
C_4S	C_4S	278,A294,B288
C_4S_2	C_4S_2	344
C_4Si	C_4Si	277,A293,B280
C_4Si_2	SiC_4Si	A318,B326
$C_4Si_2^-$	SiC_4Si^-	B327
C_4Ti	TiC_4	B279
C_4Ti^-	TiC_4^-	B279
C_5	C_5	277,A292,B280
C_5^-	C_5^-	278,A293,B283
C_5Br_4	$cyc\text{-}C_5Br_4$	A357
$C_5Br_4O_2$	$cyc\text{-}C_5Br_4O\text{-}1\text{-}O$	A366
C_5Cl_4	$cyc\text{-}C_5Cl_4$	A357
$C_5Cl_4O_2$	$cyc\text{-}C_5Cl_4O\text{-}1\text{-}O$	A365
$C_5F_4^+$	$CF_3(CC)_2F^+$	407
C_5F_6O	$(CF_3)_2(cyc\text{-}CCO)$	418
C_5F_8O	$CF_3(cyc\text{-}CCO)C_2F_5$	419
C_5H	C_5H	A316,B322
C_5HN^+	$H(C{\equiv}C)_2CN^+$	369,A328,B342
C_5HN	$H(C{\equiv}C)_2NC$	B343
C_5HSi	SiC_5H	B342
$C_5H_2^+$	$C_5H_2^+$	A327
C_5H_2	HC_5H	A327,B338
C_5H_2	$(cyc\text{-}HC{=}CHC){=}C{=}C$:	B338
C_5H_2	$HCCCH{=}C{=}C$:	B339
C_5H_2	H_2C_5:	B339
C_5H_2	$(cyc\text{-}HC_3)CCH$	B339
C_5H_3	H_2C_5H	B358
$C_5H_3Br^+$	$CH_3(CC)_2Br^+$	406
$C_5H_3Cl^+$	$CH_3(CC)_2Cl^+$	406
$C_5H_3F_2N^+$	$cyc\text{-}C_5H_3F_2N^+$	412
C_5H_3N	$cyc\text{-}C_5H_3N$	412
$C_5H_4^+$	$CH_3(CC)_2H^+$	385
C_5H_4	$cyc\text{-}C_5H_4$	385
C_5H_4Cl	$cyc\text{-}C_5H_4Cl$	407
C_5H_4F	$cyc\text{-}C_5H_4F$	407
C_5H_4O	$(cyc\text{-}C_5H_4)O$	419
$C_5H_4O_2$	$(cyc\text{-}C_5H_4)O_2$	B394
$C_5H_4O_2$	$cyc\text{-}C_5H_4O\text{-}1\text{-}O$	422,A365
C_5H_5	$cyc\text{-}C_5H_5$	385,A344,B364
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
$C_5H_6^+$	$cyc\text{-}C_5H_6^+$	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_9O	$(CH_3)_2CCOCH_3$	B392
C_5H_{11}	$n\text{-}C_5H_{11}$	386,A346
C_5H_{11}	$(CH_3)_3CCH_2$	386
C_5N	C_5N	A319,B327
C_5N^-	C_5N^-	B328
C_5N_2	C_5N_2	A330,B344
C_5O	C_5O	A320,B328
C_5OS	C_5OS	370
C_5O_2	C_5O_2	370
C_5S	C_5S	343,B328

Formula	*Structure/Name*	*References*
C_5S_2	C_5S_2	370
C_5Ti	TiC_5	B325
C_5Ti^-	TiC_5^-	B325
C_6	C_6	342,A317,B325
C_6	*cyc*-C_6	B326
C_6^-	C_6^-	342,A318,B326
$C_6Br_3F_3^+$	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_4	*o*-C_6F_4	B396
C_6F_4	*m*-C_6F_4	B396
C_6F_4	*p*-C_6F_4	B396
C_6F_4	FCCCF=CFCCF	B387
C_6F_4I	*m*-C_6F_4I	B396
C_6F_4I	*p*-C_6F_4I	B397
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,B341
C_6H^-	C_6H^-	B343
$C_6HF_5^+$	$C_6HF_5^+$	437
$C_6HF_5O^+$	$C_6F_5OH^+$	445
C_6HN^+	HC_5CN^+	A340
C_6HN	HC_6N	B360
C_6HN	(*cyc*-HC_3)CCCN	B360
C_6HSi	SiC_6H	B359
$C_6H_2^+$	$C_6H_2^+$	380,A339,B358
C_6H_2	H_2C_6:	A340,B359
$C_6H_2F_4^+$	1,2,3,4-$C_6H_2F_4^+$	435,B400
$C_6H_2F_4^+$	1,2,3,5-$C_6H_2F_4^+$	436,B400
$C_6H_2F_4^+$	1,2,4,5-$C_6H_2F_4^+$	437,B401
$C_6H_2F_4O^+$	2,3,5,6-$F_4C_6HOH^+$	445
$C_6H_2O_2$	O=C_6H_2=O	B395
$C_6H_2O_2^-$	O=C_6H_2=O^-	B395
$C_6H_3ClF_2^+$	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	3,5-C_6H_3F	B395
$C_6H_3F_2N$	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,B364
C_6H_4	*m*-C_6H_4	A346,B365
C_6H_4	*p*-C_6H_4	B366
$C_6H_4^-$	*o*-$C_6H_4^-$	387,B366
$C_6H_4^-$	*m*-$C_6H_4^-$	B367
$C_6H_4^-$	*p*-$C_6H_4^-$	B367
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,B396
$C_6H_4S_2$	*p*-$C_6H_4S_2$	422
$C_6H_5^+$	$C_6H_5^+$	387,B367
C_6H_5	C_6H_5	388,A346,B367
$C_6H_5^-$	$C_6H_5^-$	388
$C_6H_5Br^+$	$C_6H_5Br^+$	B399
$C_6H_5Cl^+$	$C_6H_5Cl^+$	428,A368,B397
$C_6H_5F^+$	$C_6H_5F^+$	428,B397
$C_6H_5I^+$	$C_6H_5I^+$	B399
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
$C_6H_5N_2^+$	$C_6H_5NN^+$	B388
C_6H_5O	C_6H_5O	443,A372,B407
$C_6H_5O^-$	$C_6H_5O^-$	446
C_6H_5S	C_6H_5S	443
$C_6H_6^+$	$C_6H_6^+$	388,A347,B368
$C_6H_6^+$	$CH_3(CC)_2CH_3^+$	390
$C_6H_6ClN^+$	*p*-$C_6H_4ClNH_2^+$	B407
C_6H_6F	C_6H_6F	440
$C_6H_6FN^+$	*o*-$C_6H_4FNH_2^+$	B407
$C_6H_6FN^+$	*p*-$C_6H_4FNH_2^+$	B407
C_6H_6Li	LiC_6H_6	440
C_6H_6N	C_6H_5NH	443
$C_6H_6O^+$	$C_6H_5OH^+$	444,A373
$C_6H_6O_2^+$	*o*-$C_6H_4(OH)_2^+$	B409
$C_6H_6O_2^+$	*m*-$C_6H_4(OH)_2^+(C_s)$	B409
$C_6H_6O_2^+$	*m*-$C_6H_4(OH)_2^+(C_{2v})$	B409
$C_6H_6O_2^+$	*p*-$C_6H_4(OH)_2^+(C_{2v})$	B409
$C_6H_6O_2^+$	*p*-$C_6H_4(OH)_2^+(C_{2h})$	B409
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,B406

Formula	*Structure/Name*	*References*
$C_6H_8^+$	t-$CH_2(CH)_4CH_2^+$	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,B362
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
C_6Si	C_6Si	B343
C_7	C_7	369,A329,B343
C_7^-	C_7^-	370,A329,B344
C_7F_4O	1,2-$C_6F_4{>}CO$	B409
$C_7F_8^+$	$C_6F_5CF_3^+$	442
C_7H	C_7H	A340,B359
C_7HN^+	$H(C{\equiv}C)_3CN^+$	A362,B388
C_7HN^+	$H(C{\equiv}C)_3NC$	B388
$C_7H_2^+$	$C_7H_2^+$	A349
C_7H_2	HC_7H	A349,B370
C_7H_2	(cyc-HC_3)$(C{\equiv}C)_2H$	B370
$C_7H_2F_5$	$C_6F_5CH_2$	B404
$C_7H_3F_5^+$	$C_6F_5CH_3^+$	441
C_7H_4O	(cyc-C_5H_4)CCO	419
C_7H_4O	cyc-$C_6H_4C{=}O$	419
C_7H_5Cl	C_6H_5CCl	441
C_7H_5Cl	(2-ClC_6H_4)CH	441
C_7H_5Cl	cyc-1-C_7H_5Cl	408
C_7H_5ClO	C_6H_5OCCl	446
$C_7H_5Cl_2$	$C_6H_5CCl_2$	B402
C_7H_5F	C_6H_5CF	440
C_7H_5F	cyc-1-C_7H_5F	407
$C_7H_5F_2$	(2,6-$F_2C_6H_3$)CH_2	B404
$C_7H_5F_3^+$	sym-$C_6H_2F_3CH_3^+$	441
$C_7H_5N^+$	$C_2H_5(CC)_2CN^+$	414
C_7H_6	3,5-$C_6H_3CH_3$	B370
C_7H_6	C_6H_5CH	391,B370
C_7H_6	cyc-C_7H_6	391,B371
C_7H_6	cyc-C_7H_6:	392
C_7H_6Br	C_6H_5CHBr	B402
C_7H_6Br	(2-BrC_6H_4)CH_2	B403
C_7H_6Br	(3-BrC_6H_4)CH_2	B404
C_7H_6Br	(4-BrC_6H_4)CH_2	B404
$C_7H_6Br^-$	(2-BrC_6H_4)CH_2^-	B405
$C_7H_6Br^-$	(3-BrC_6H_4)CH_2^-	B405
$C_7H_6Br^-$	(4-BrC_6H_4)CH_2^-	B405
C_7H_6Cl	C_6H_5CHCl	B401
C_7H_6Cl	(2-ClC_6H_4)CH_2	B403
C_7H_6Cl	(3-ClC_6H_4)CH_2	B403
C_7H_6Cl	(4-ClC_6H_4)CH_2	A370,B403
$C_7H_6Cl^-$	(2-ClC_6H_4)CH_2^-	B405
$C_7H_6Cl^-$	(3-ClC_6H_4)CH_2^-	B405
$C_7H_6Cl^-$	(4-ClC_6H_4)CH_2^-	B405
C_7H_6F	(2-FC_6H_4)CH_2	A369,B402
C_7H_6F	(3-FC_6H_4)CH_2	A369,B402
C_7H_6F	(4-FC_6H_4)CH_2	A370,B402
$C_7H_6F^-$	(2-FC_6H_4)CH_2^-	B404
$C_7H_6F^-$	(3-FC_6H_4)CH_2^-	B404
$C_7H_6F^-$	(4-FC_6H_4)CH_2^-	B405
$C_7H_7^+$	cyc-$C_7H_7^+$	392
$C_7H_7^+$	$C_6H_5CH_2^+$	392,A349
C_7H_7	$C_6H_5CH_2$	392,A349,B372
C_7H_7	cyc-C_7H_7	394
$C_7H_7^-$	$C_6H_5CH_2^-$	394,B373
$C_7H_8^+$	$C_6H_5CH_3^+$	394
C_7N	C_7N	B362
C_7N^-	C_7N^-	B362
$C_7N_2^+$	NCC_5CN^+	A362
C_7O	C_7O	A341,B362
C_7O_2	C_7O_2	422
C_7Si	SiC_7	B362
C_8	C_8	381,A340,B360
C_8	cyc-C_8	B361
C_8^-	C_8^-	381,A340,B361
C_8H	C_8H	A351,B373
C_8H^-	C_8H^-	B374
C_8HN^+	HC_7CN^+	A362
$C_8H_2^+$	$C_8H_2^+$	A351,B374
$C_8H_4Cl_2$	p-$ClCC_6H_4CCl$	B387
$C_8H_4F_4$	p-$(CF_2)_2C_6H_4$	B406
$C_8H_4F_4$	4,5-$F_2C_7H_4{=}CF_2$	B406
C_8H_6	p-$HC{=}C_6H_4{=}CH$	B375
C_8H_6	cyc-C_8H_6	B374
$C_8H_6^-$	cyc-$C_8H_6^-$	B375
C_8H_6N	(4-$NC{-}C_6H_4$)CH_2	A370,B405
C_8H_8	o-$(CH_2)_2C_6H_4$	396
C_8H_8	m-$(CH_2)_2C_6H_4$	A351
C_8H_8	p-$(CH_2)_2C_6H_4$	A352
C_8H_8	$C_6H_5CCH_3$	396
C_8H_8	m-$CH_3C_6H_4CH$:	395
C_8H_8	o-$CH_3C_6H_4CH$:	395
C_8H_8	p-$CH_3C_6H_4CH$:	395
C_8H_8	1-CH_3(cyc-C_7H_5)	396
C_8H_8	4-CH_3(cyc-C_7H_5)	397
C_8H_8	5-CH_3(cyc-C_7H_5)	397
$C_8H_8^-$	m-$(CH_2)_2C_6H_4$	A352
$C_8N_2^+$	$NC(C{\equiv}C)_3CN^+$	A362
C_8O	C_8O	A364
C_9	C_9	398,A352,B375
C_9^-	C_9^-	398,A352,B376
C_9H	C_9H	A353
C_9H^-	cum-C_9H^-	B376
C_9H^-	$acet$-C_9H^-	B376
C_9HN^+	$H(C{\equiv}C)_4CN^+$	A362
$C_9H_2^+$	$C_9H_2^+$	A353
C_9H_2	HC_9H	A353,B376
C_9H_2	(cyc-HC3)$(C{\equiv}C)_3H$	B377
C_9N	C_9N	B388
C_9N^-	C_9N^-	B389
$C_9N_2^+$	NCC_7CN^+	A363
C_9O	C_9O	A364,B393

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
C_9Si	SiC_9	B387	$C_{15}H^-$	*cum*-$C_{15}H^-$	B384
C_{10}	C_{10}	A353,B377	$C_{15}H^-$	*acet*-$C_{15}H^-$	B384
C_{10}	*cyc*-C_{10}	B377	C_{16}	C_{16}	B385
C_{10}^-	C_{10}^-	A354,B377	C_{16}^-	C_{16}^-	A358,B385
$C_{10}H$	$C_{10}H$	A354,B378	CaHO	CaOH	27,A139
$C_{10}H^-$	*cum*-$C_{10}H^-$	B378	CaHS	CaSH	28,A140
$C_{10}H^-$	*acet*-$C_{10}H^-$	B378	CaH_2	CaH_2	14
$C_{10}HN^+$	HC_9CN^+	A363	CaH_2N	$CaNH_2$	132,A220,B163
$C_{10}H_2^+$	$C_{10}H_2^+$	A354	CaH_2O	HCaOH	134
$C_{10}N_2^+$	$NC(C{\equiv}C)_4CN^+$	A363	CaH_2O_2	$Ca(OH)_2$	251
C_{11}	C_{11}	398,A354,B378	CaN_3	CaN_3	182
C_{11}^-	C_{11}^-	398,B379	CaO_2	OCaO	A174
$C_{11}H$	$C_{11}H$	A354	CaO_2	*cyc*-CaO_2	A174
$C_{11}H^-$	*cum*-$C_{11}H^-$	B379	CaO_4	O_2CaO_2	A298
$C_{11}H^-$	*acet*-$C_{11}H^-$	B379	Ca_2H_2	Ca_2H_2	130
$C_{11}HN^+$	$H(C{\equiv}C)_5CN^+$	A363	Ca_2H_2O	HCaOCaH	246
$C_{11}HN^-$	$HC_{10}CN^-$	B389	Ca_2H_2O	HCa_2OH	247
$C_{11}H_2^+$	$C_{11}H_2^+$	A355	Ca_2H_4	$HCaH_2CaH$	305
$C_{11}H_2$	$HC_{11}H$	A355,B379	Ca_2O_2	*cyc*-$(CaO)_2$	A243
$C_{11}N$	$C_{11}N$	B389	Ca_2O_2	CaOCaO	A243
$C_{11}N^-$	$C_{11}N^-$	B389	Ca_3H_2	Ca_3H_2	244
$C_{11}N_2^+$	NCC_9CN^+	A363	CdH_2	CdH_2	A127
C_{12}	C_{12}	A355,B380	CdH_2O	HCdOH	A222
C_{12}	*cyc*-C_{12}	B380	CdO_2	OCdO	A179
C_{12}^-	C_{12}^-	A355,B380	Cd_2H	CdCdH	A136
$C_{12}H$	$C_{12}H$	A355,B380	Cd_2O_2	CdOCdO	A244
$C_{12}H^-$	*cum*-$C_{12}H^-$	B380	CeH_2^+	CeH_2^+	B11
$C_{12}H^-$	*acet*-$C_{12}H^-$	B381	CeH_2	CeH_2	B13
$C_{12}H_2$	$HC_{12}H$	B381	CeH_3	CeH_3	B154
$C_{12}H_2^-$	$HC_{12}H^-$	B381	CeH_4	CeH_4	B245
$C_{12}HN^+$	$HC_{11}CN^+$	A363	CeNO	NCeO	B93
$C_{12}H_2^+$	$C_{12}H_2^+$	A355	CeNO	CeNO	B93
$C_{12}N_2^+$	$NC(C{\equiv}C)_5CN^+$	A363	$CeNO^-$	$NCeO^-$	B102
C_{13}	C_{13}	A356,B381	CeN_2	NCeN	B74
C_{13}^-	C_{13}^-	B382	CeN_2	CeNN	B74
$C_{13}H$	$C_{13}H$	B382	CeO_2	OCeO	A179,B109
$C_{13}H^-$	*cum*-$C_{13}H^-$	B382	CeO_2	*cyc*-CeO_2	B109
$C_{13}H^-$	*acet*-$C_{13}H^-$	B382	CeO_2^-	$OCeO^-$	B118
$C_{13}HN^+$	$H(C{\equiv}C)_6CN^+$	A363	Ce_2H_2	*cyc*-$(CeH)_2$	B161
$C_{13}HN^-$	$HC_{12}CN^-$	B390	Ce_2N_2	*cyc*-$(CeN)_2$	B205
$C_{13}H_2^+$	$C_{13}H_2^+$	A356	Ce_2O_2	*cyc*-$(CeO)_2$	B212
$C_{13}H_2$	$HC_{13}H$	A356,B382	$ClFH^-$	$FHCl^-$	53
$C_{13}N$	$C_{13}N$	B389	ClFN	NFCl	108,A201
$C_{13}N^-$	$C_{13}N^-$	B389	ClFO	FClO	116,B152
C_{14}	C_{14}	B382	$ClFO_2S^+$	$FClSO_2^+$	301
C_{14}	*cyc*-C_{14}	B383	$ClFO_3^+$	$FClO_3^+$	300
C_{14}^-	C_{14}^-	A356,B383	ClFS	FSCl	115,A208
$C_{14}H$	$C_{14}H$	A356,B383	ClFSi	SiFCl	B140
$C_{14}H^-$	*cum*-$C_{14}H^-$	B383	ClFXe	XeClF	121
$C_{14}H^-$	*acet*-$C_{14}H^-$	B383	ClF_2	ClF_2	116
$C_{14}H_2^+$	$C_{14}H_2^+$	A356	ClF_2^-	$FClF^-$	117
$C_{14}H_2$	$HC_{14}H$	B384	ClF_2^-	$FFCl^-$	118
$C_{14}H_2^-$	$HC_{14}H^-$	B384	ClF_2P^+	PF_2Cl^+	220
C_{15}	C_{15}	A357,B384	ClF_3^+	ClF_3^+	226
C_{15}^-	C_{15}^-	B384	ClF_3P^-	$PClF_3^-$	304

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
ClF_3S	$SClF_3$	304	ClO_4^-	ClO_4^-	B307
ClF_3Si^+	SiF_3Cl^+	295	ClPS	ClPS	104
ClF_4Si^-	SiF_4Cl^-	357	ClS_2	SSCl	111,A205
ClFeH	HFeCl	35	$ClXe_2$	Xe_2Cl	122
$ClGaH_2$	GaH_2Cl	143	Cl_2Cu	$CuCl_2$	B129
ClGeH	HGeCl	45,B40	Cl_2F	ClClF	116
$ClGeH_2$	H_2GeCl	150	Cl_2F^-	$ClFCl^-$	118
$ClGeH_3^+$	GeH_3Cl^+	241	Cl_2F^-	$FClCl^-$	118
ClHHg	HHgCl	B31	Cl_2F_2	Cl_2F_2	227
$ClHI^-$	$ClHI^-$	55	Cl_2F_2S	SCl_2F_2	304
ClHKr	HKrCl	A158,B47	$Cl_2F_2Si^+$	$SiF_2Cl_2^+$	295
$ClHO^+$	$HOCl^+$	51	$Cl_2F_3Si^-$	$SiF_3Cl_2^-$	357
ClHO	HOCl	52,A155,B45	Cl_2Ga	$GaCl_2$	90
$ClHO_2$	HOClO	A241	Cl_2GaH	$HGaCl_2$	169,B194
$ClHO_2$	$HClO_2$	A241	$Cl_2Ga_2H_4$	$H_2GaCl_2GaH_2$	A339
$ClHO_4$	$HOOClO_2$	B324	Cl_2Ge^+	$GeCl_2^+$	92
ClHP	HPCl	B43	Cl_2Ge	$GeCl_2$	102,A198,B141
ClHSSi	HClSi=S	172	$Cl_2GeH_2^+$	$GeH_2Cl_2^+$	263
ClHSi	HSiCl	44,A150,B39	Cl_2GeS	Cl_2GeS	211
ClHXe	HXeCl	A158,B47	Cl_2H^-	$ClHCl^-$	54,A157,B46
ClH_2^+	H_2Cl^+	26,B21	Cl_2HIn	$HInCl_2$	B194
ClH_2In	InH_2Cl	B172	Cl_2HN^+	$HNCl_2^+$	179
ClH_2InO	HInCl(OH)	B269	$Cl_2H_2^+$	$HClClH^+$	B179
ClH_2N^+	H_2NCl^+	152	$Cl_2H_2Si^+$	$SiH_2Cl_2^+$	262
ClH_2P	H_2PCl	A229	Cl_2Li	ClLiCl	B115
ClH_3Si^+	SiH_3Cl^+	240	Cl_2Mn^+	$MnCl_2^+$	73
ClIO	OICl	116	Cl_2N	NCl_2	108
$ClIO_2$	$ClIO_2$	226	Cl_2Na	ClNaCl	B115
$ClIO_2$	$IClO_2$	A264	Cl_2Ni^+	$NiCl_2^+$	73
$ClIO_2$	IOClO	A264	Cl_2Ni	$NiCl_2$	B128
ClKrNe	NeKrCl	122	Cl_2O^+	Cl_2O^+	111,B148
ClKrXe	KrXeCl	122	Cl_2O	ClClO	116,A208
$ClKr_2$	Kr_2Cl	122	Cl_2OP	$OPCl_2$	220
$ClNO^+$	$ClNO^+$	93	Cl_2OS^+	Cl_2SO^+	223
ClNO	ClON	B143	Cl_2OSi	Cl_2SiO	211,B238
$ClNO_2^+$	$ClNO_2^+$	208	Cl_2O_2	ClOOCl	225,A263,B244
$ClNO_2$	$ClNO_2$	212,A259	Cl_2O_2	$ClClO_2$	225,A263,B244
$ClNO_2$	*c*-ClONO	213,A259	Cl_2O_2	ClOClO	A264
$ClNO_2$	*t*-ClONO	213,A259	$Cl_2O_2S^+$	$Cl_2SO_2^+$	301
$ClNO_3^+$	$ClONO_2^+$	A301	Cl_2O_2Si	*cyc*-Cl_2SiO_2	287
$ClNO_3$	$ClONO_2$	288,A302,B301	Cl_2O_3	Cl_2O_3	302,A307
$ClNO_5$	O_2ClONO_2	371	Cl_2O_4	$ClOClO_3$	355,A322
$ClNS^+$	$NSCl^+$	95	Cl_2O_6	$O_3ClOClO_2$	382
ClN_3^+	ClN_3^+	196	Cl_2P	PCl_2	108,A203,B147
ClOP	ClPO	103,B142	Cl_2S^+	SCl_2^+	112
ClOSi	ClSiO	B135	Cl_2SSi	Cl_2SiS	221
ClO_2^+	$OClO^+$	106,B144	$Cl_2S_2^+$	$S_2Cl_2^+$	224
ClO_2	OClO	113,A205,B149	Cl_2S_2	$SSCl_2$	226
ClO_2	ClOO	110,A204,B147	Cl_2Se^+	$SeCl_2^+$	112
ClO_2^-	$OClO^-$	115,B152	$Cl_2Se_2^+$	$Se_2Cl_2^+$	224
ClO_2P	PO_2Cl	213,B240	Cl_2Si^+	$SiCl_2^+$	92
ClO_2S	$ClSO_2$	B243	Cl_2Si	$SiCl_2$	101,A197
ClO_3	ClO_3	A262	Cl_2Xe	$XeCl_2$	121
ClO_3^-	ClO_3^-	B244	Cl_2Zn^+	$ZnCl_2^+$	72
ClO_4	$OClO_3$	A306	Cl_3^-	Cl_3^-	119,B153

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
Cl_3FS	SCl_3F	304	CrN_2O_2	$Cr(NO)_2$	B293
Cl_3FSi^+	$SiFCl_3^+$	296	$CrN_2O_2^-$	$Cr(NO)_2^-$	B295
$Cl_3F_2Si^-$	$SiF_2Cl_3^-$	357	CrO_2	OCrO	A175,B104
Cl_3Ge	$GeCl_3$	219	CrO_2^-	$OCrO^-$	A182,B117
Cl_3HOSi	$SiCl_3OH$	342	CrO_3	CrO_3	B226
Cl_3HSi^+	$HSiCl_3^+$	276	CrO_3^-	CrO_3^-	B231
Cl_3N^+	NCl_3^+	219	Cr_2H	CrCrH	26
Cl_3NO_3Si	$SiCl_3ONO_2$	382	Cr_2H^-	$CrCrH^-$	26
Cl_3NO_4Si	$SiCl_3OONO_2$	426	Cr_2O	CrOCr	B55
Cl_3OP^+	Cl_3PO^+	298	Cr_2O_2	CrOCrO	B211
Cl_3O_2P	$OPCl_2OCl$	355	Cr_2O_4	Cr_2O_4	B329
Cl_3P^+	PCl_3^+	220,B242	Cr_3	Cr_3	B51
Cl_3PS^+	Cl_3PS^+	299	Cs_3	Cs_3	B51
Cl_3Sb^+	$SbCl_3^+$	222	CuHO	CuOH	31,B27
Cl_3Si^+	$SiCl_3^+$	211	CuH_2N	$CuNH_2$	133
Cl_3Si	$SiCl_3$	218	CuH_2O	HCuOH	137
Cl_4FSi^-	$SiFCl_4^-$	358	CuH_3N	$HCuNH_2$	232
Cl_4Ge^+	$GeCl_4^+$	297,A306,B306	$CuNO^+$	$CuNO^+$	B77
Cl_4Si^+	$SiCl_4^+$	296,A306,B305	CuNO	CuNO	B93
Cl_4SiO	$SiCl_3OCl$	356	CuN_2O_2	$Cu(NO)_2$	B294
Cl_5P^+	PCl_5^+	357	$CuN_2O_2^-$	$Cu(NO)_2^-$	B296
CoH_2	CoH_2	15,A127	CuO_2^+	$CuOO^+$	A172
CoH_2^-	CoH_2^-	17	CuO_2	OCuO	A178,B107
CoH_2O	HCoOH	136	CuO_2	CuOO	A178
$CoNO^+$	$CoNO^+$	B77	CuO_2^-	$OCuO^-$	A182
CoNO	CoNO	B91	CuO_2^-	$CuOO^-$	A182
CoNO	*cyc*-CoNO	B91	CuO_3	CuO_3	A251
$CoNO^-$	$CoNO^-$	B102	CuO_3^-	CuO_3^-	A252
CoN_2	CoNN	B73	CuO_4	O_2CuO_2	A299
CoN_2	*cyc*-CoNN	B73	Cu_2H_2	Cu_2H_2	131
CoN_2O_2	$Co(NO)_2$	B294	Cu_2O	CuOCu	A163
$CoN_2O_2^-$	$Co(NO)_2^-$	B295	Cu_2O^-	$CuOCu^-$	A166
CoN_3O_3	$Co(NO)_3$	B346	Cu_2O_2	Cu_2O_2	A244
CoO_2	OCoO	B106	$Cu_2O_2^-$	$Cu_2O_2^-$	A246
CoO_2	CoOO	B106	Cu_2O_3	Cu_2O_3	A294,B288
CoO_2	*cyc*-CoOO	B106	$Cu_2O_3^-$	$Cu_2O_3^-$	A295
CoO_3	OCoOO	B227	Cu_2O_4	Cu_2O_4	A320
CoO_3	*cyc*-$(O_2Co)O$	B227	$Cu_2O_4^-$	$Cu_2O_4^-$	A320
CoO_4	$OOCoO_2$	B297	Cu_3	Cu_3	59,A161
CoO_4	(*cyc*-$O_2Co)O_2$	B298	Cu_3H_2	Cu_3H_2	244
Co_2N	*cyc*-Co_2N	B53	DyH_2	DyH_2	B14
Co_2N	CoCoN	B53	DyH_4	DyH_4	B246
Co_2N_2	*cyc*-$(CoN)_2$	B205	DyNO	NDyO	B94
Co_2O_2	*cyc*-$(CoO)_2$	B212	DyNO	*cyc*-DyNO	B95
Co_2O_2	CoOCoO	B212	DyN_2	*cyc*-DyNN	B75
Co_2O_3	Co_2O_3	B288	DyO_2	ODyO	B110
CrH_2	CrH_2	15	DyO_2^-	$ODyO^-$	B119
CrH_2O	HCrOH	136	Dy_2N	Dy_2N	B54
CrH_3	CrH_3	123	Dy_2N_2	*cyc*-$(DyN)_2$	B206
CrH_3O_2	$HCr(OH)_2$	316	Dy_2O_2	*cyc*-$(DyO)_2$	B213
CrNO	NCrO	B89	ErH_2	ErH_2	B15
CrNO	CrNO	B89	ErNO	NErO	B95
CrNO	*cyc*-CrNO	B89	ErNO	*cyc*-ErNO	B95
$CrNO^-$	$CrNO^-$	B101	ErN_2	*cyc*-ErNN	B75
CrN_2	NCrN	B71	ErO_2^-	$OErO^-$	B119

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
Er_2N_2	*cyc*-$(ErN)_2$	B207	F_2H^-	FHF^-	53,A156
EuH_2	EuH_2	B13	F_2HN^+	HNF_2^+	178
EuNO	NEuO	B94	F_2HP^+	HPF_2^+	179
EuNO	*cyc*-EuNO	B94	$F_2H_2^+$	$HFFH^+$	B178
EuN_2	*cyc*-EuNN	B74	$F_2H_2Si^+$	$SiH_2F_2^+$	262
EuO_2	OEuO	B109	F_2H_3P	PH_3F_2	324,A315
EuO_2^-	$OEuO^-$	B119	F_2I^-	FIF^-	118
Eu_2N	Eu_2N	B54	F_2I^-	FFI^-	118
Eu_2O_2	*cyc*-$(EuO)_2$	B213	F_2I_2	I_2F_2	227
FFeH	HFeF	35	F_2Kr^+	KrF_2^+	117
FFe_2H	HFe_2F	155	F_2Kr	KrF_2	120,A209
FGaO	OGaF	85	F_2Mg+	MgF_2^+	A181
$FGeH_3^+$	GeH_3F^+	241	F_2Mg	MgF_2	84
FHI^-	FHI^-	54	F_2N^+	NF_2^+	103,A199
FHN	HNF	48,A152	F_2N	NF_2	107,A201
$FHNe^+$	$NeHF^+$	B46	F_2N^-	NF_2^-	A207
FHO^+	HOF^+	51	F_2NO	F_2NO	B241
FHO	HOF	51	$F_2N_2^+$	*t*-$N_2F_2^+$	207
FHSi	HSiF	43,A150,B39	F_2O^+	OF_2^+	111,B148
FH_2^+	H_2F^+	26	F_2OP^+	F_2PO^+	B240
FH_2N^+	NH_2F^+	151	F_2OP^-	F_2PO^-	B244
FH_2N	NH_2F	153	F_2OS^+	F_2SO^+	223,B243
FH_2P	H_2PF	153,A228	F_2OSi	F_2SiO	211
FH_3N_2	NH_2NHF	324	F_2O_2	FOOF	225
FH_3Si^+	SiH_3F^+	240	$F_2O_2S^+$	$F_2SO_2^+$	300
FI_2	IIF	117	F_2O_2Si	*cyc*-F_2SiO_2	287
FKrXe	KrXeF	121,A211	F_2O_2U	UO_2F_2	B299
FKr_2	Kr_2F	121,A210	F_2O_2Xe	XeO_2F_2	304
FNO^+	FNO^+	93	F_2O_3Xe	XeO_3F_2	358
FNO	FON	104	F_2P^+	PF_2^+	104,B143
FNO_2^+	FNO_2^+	208	F_2P	PF_2	108,A202,B146
FNO_2	FONO	212	F_2S^+	SF_2^+	112
FNO_3^+	$FONO_2^+$	A301	F_2S	SF_2	114,A207,B151
FNO_3	$FONO_2$	A302	F_2SSi	F_2SiS	B239
FNS^+	NSF^+	94	$F_2S_2^+$	F_2SS^+	223
FN_2^+	FNN^+	87	$F_2S_2^+$	$FSSF^+$	224
FN_3^+	FN_3^+	196	F_2Se^+	SeF_2^+	112
FN_3	FN_3	199	F_2Se	SeF_2	A208
FNeXe	NeXeF	121	F_2Se_2	FSeSeF	A264
FNe_2	Ne_2F	121	F_2Se_2	$SeSeF_2$	A264
FOP	FPO	103,B142	F_2Si^+	SiF_2^+	91
FOS	FSO	111	F_2Si	SiF_2	100,A197,B140
FO_2	FOO	109	F_2Xe^+	XeF_2^+	117
FO_2S^-	FSO_2^-	225	F_2Xe	XeF_2	120,A209
FO_2U	UO_2F	B231	F_3^-	F_3^-	117
FO_3S^+	FSO_3^+	289	F_3HSi^+	$HSiF_3^+$	276
FO_3S	FSO_3	300	F_3N^+	NF_3^+	219,A262
FPS	FPS	104,B142	F_3NO^+	F_3NO^+	298
FS_2	SSF	A205	F_3NS^+	F_3NS^+	298
FXe_2	Xe_2F	122,A211	F_3OP^+	F_3PO^+	298
F_2Ga	GaF_2	A193	F_3OP^-	F_3PO^-	B307
F_2Ge^+	GeF_2^+	92	F_3OS^-	SOF_3^-	304
F_2Ge	GeF_2	101,A198,B140	$F_3O_2S^-$	$SO_2F_3^-$	358
$F_2GeH_2^+$	$GeH_2F_2^+$	263	F_3P^+	PF_3^+	219,B242
F_2GeO	F_2GeO	212	F_3P^-	PF_3^-	B245

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
F_3PS^+	F_3PS^+	299	Fe_2H_2O	HFeOFeH	247,B261
F_3S^+	SF_3^+	B244	Fe_2H_2O	HFe_2OH	247
F_3S	SF_3	226	Fe_2H_3N	HFe_2NH_2	311
F_3Sb^+	SbF_3^+	222	Fe_2N	*cyc*-Fe_2N	A162
F_3Si^+	SiF_3^+	A258	Fe_2N	FeFeN	A162
F_3Si	SiF_3	218,A262,B241	Fe_2O	FeOFe	A163
F_3Si^-	SiF_3^-	A263	Fe_2O^-	$FeOFe^-$	A166
F_4Ge^+	GeF_4^+	297,B306	Fe_2O_2	*cyc*-$(FeO)_2$	A244,B211
F_4OU	UOF_4	B332	$Fe_2O_2^-$	$Fe_2O_2^-$	A246
F_4OXe^+	$XeOF_4^+$	359	Fe_2O_3	Fe_2O_3	A294
F_4P^+	PF_4^+	B307	$Fe_2O_3^-$	$Fe_2O_3^-$	A295
F_4P	PF_4	B307	Fe_2O_4	Fe_2O_4	A320
F_4P^-	PF_4^-	304,B308	$Fe_2O_4^-$	$Fe_2O_4^-$	A320
$F_4P_2^+$	$P_2F_4^+$	355	Fe_2O_5	Fe_2O_5	B345
F_4P_2	$PF_3{=}PF$	355	$Fe_2O_5^-$	$Fe_2O_5^-$	B345
F_4S^+	SF_4^+	A307,B307	Fe_3	Fe_3	B52
F_4S^-	SF_4^-	B308	GaHO	GaOH	36
F_4Si^+	SiF_4^+	294,A305,B304	GaH_2	GaH_2	18,A129
F_4Xe^+	XeF_4^+	305	GaH_2N	$GaNH_2$	B169
F_5I^+	IF_5^+	358	GaH_2O	HGaOH	139,A223
F_5P^+	PF_5^+	356	GaH_3	GaH_3	A213,B155
F_5P^-	PF_5^-	B333	GaH_3N^+	$GaNH_3^+$	B251
F_5S^+	SF_5^+	B332	GaH_3N	$GaNH_3$	B252
F_5S	SF_5	358,B333	GaH_3N	$HGaNH_2$	B252
F_5S^-	SF_5^-	359,B333	GaH_3P	$GaPH_3$	B254
F_5Si^-	SiF_5^-	357	GaH_3P	$HGaPH_2$	B254
F_6S^+	SF_6^+	A331,B347	GaH_3P	H_2GaPH	B254
F_6S^-	SF_6^-	B348	GaH_4N	H_2GaNH_2	B310
FeHI	HFeI	35	GaInO	InGaO	64
FeH_2	FeH_2	15,A126,B12	GaNO	GaNO	B102
FeH_2^-	FeH_2^-	17	GaN_2	NGaN	B97
FeH_2O	HFeOH	136,B168	GaN_3	GaNNN	B222
FeH_2O_2	$Fe(OH)_2$	251,B265	GaO_2	*cyc*-GaO_2	75
FeH_3	FeH_3	A211	GaO_2	OGaO	75
FeH_3N	$HFeNH_2$	231	GaO_2^-	*cyc*-GaO_2^-	B130
$FeNO^+$	$FeNO^+$	B76	GaO_3	OGaOO	190
FeNO	FeNO	A171,B90	GaP_2	*cyc*-GaP_2	A172,B98
FeNO	*cyc*-FeNO	B91	$GaSb_2$	$GaSb_2$	A172
$FeNO_2$	$NFeO_2$	A249	Ga_2H_2	*cyc*-Ga_2H_2	A220
FeN_2	NFeN	A166	Ga_2H_2	HGaGaH	A220
FeN_2	FeNN	A267	$Ga_2H_6^+$	$Ga_2H_6^+$	A333
FeN_2O	N_2FeO	A248	Ga_2H_6	Ga_2H_6	372,A333
FeN_2O_2	$Fe(NO)_2$	B293	Ga_2N	GaNGa	B63
FeN_2O_2	N_2FeO_2	A296	Ga_2O	Ga_2O	64,B80
FeN_3O_3	$Fe(NO)_3$	B346	Ga_2O_2	GaOGaO	185
FeO_2	OFeO	A176	Ga_2O_2	*cyc*-GaO_2Ga	185
FeO_2	FeOO	A176	Ga_2O_3	Ga_2O_3	283
FeO_2	*cyc*-FeO_2	A177	Ga_2P	Ga_2P	A165,B63
FeO_2^-	$OFeO^-$	A182	Ga_2P^-	Ga_2P^-	B80
FeO_3	FeO_3	A250,B227	Ga_2P_3	Ga_2P_3	B282
FeO_3	(*cyc*-O_2Fe)O	A251	$Ga_2P_3^-$	$Ga_2P_3^-$	B288
FeO_3^-	FeO_3^-	A252	Ga_2Sb	Ga_2Sb	A165
FeO_4	(*cyc*-O_2Fe)O_2	A298,B297	Ga_3H_2	HGa_3H	A275
FeO_4	(*cyc*-O_2Fe)OO	A298	Ga_3N	NGa_3	B208
FeO_4^-	FeO_4^-	B298	GdH_2	GdH_2	B14

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
GdH_3	GdH_3	B155	HNO^-	HNO^-	48
GdNO	NGdO	B94	$HNOS^+$	$HNSO^+$	169
GdNO	*cyc*-GdNO	B94	HNOS	*t*-HONS	174
GdN_2	*cyc*-GdNN	B74	HNOS	*t*-HSNO	174
GdN_2	GdNN	B75	HNOS	*c*-HSNO	174
GdO_2	OGdO	B109	HNOS	*c*-HNSO	175,A240
GdO_2^-	$OGdO^-$	B119	HNOS	*t*-HNSO	175
GdO_3^-	GdO_3^-	B231	HNOS	*c*-HOSN	176
Gd_2H_2	*cyc*-$(GdH)_2$	B161	HNO_2	*t*-HONO	172,B196
Gd_2N	Gd_2N	B54	HNO_2	*c*-HONO	173,B197
Gd_2N_2	*cyc*-$(GdN)_2$	B206	HNO_2	HNOO	B198
GeHI	HGeI	B41	HNO_3^+	HNO_3^+	270
GeH_2	GeH_2	20,A132,B18	HNO_3	$HONO_2$	271,A289,B274
$GeH_2I_2^+$	$GeH_2I_2^+$	263	HNO_3	*c,c*-HOONO	A291
GeH_2O	H_2GeO	146	HNO_3	*t,perp*-HOONO	272,A291,B276
GeH_2O	HGeOH	146	HNO_4	$HOONO_2$	341,A317,B324
GeH_2O_3	H_2GeO_3	338	HNSc	ScNH	A138
GeH_3^+	GeH_3^+	125	HNSi	HNSi	38,A146
GeH_3	GeH_3	128	HNSi	HSiN	A145
GeH_3I^+	GeH_3I^+	242	HNY	YNH	27,B22
GeH_4^+	GeH_4^+	228	HN_2^+	HN_2^+	39
GeH_4O	GeH_4OH	311	HN_2O^+	$HONN^+$	165
GeH_4S^+	GeH_3SH^+	311	HN_2O	*t*-HNNO	B192
GeI_2^+	GeI_2^+	92	HN_2O	*c*-HNNO	B193
GeOS	OGeS	86	HN_3^+	HN_3^+	161
GeO_2	GeO_2	86,B131	$HNaO^+$	$NaOH^+$	27
GeO_2^-	GeO_2^-	A194	HNiO	NiOH	30
GeS_2	GeS_2	86,B132	HOP	HPO	46
Ge_2H_2O	HGe_2OH	256	HOS^+	HSO^+	A152
Ge_2O_2	Ge_2O_2	188,A251,B228	HOS	HSO	50,A154
$Ge_2O_2^-$	$Ge_2O_2^-$	A252	HOSc	HScO	B25
$Ge_2O_3^-$	$Ge_2O_3^-$	A300	HOSc	ScOH	B26
Ge_3	Ge_3	A171	$HOSi^+$	$HOSi^+$	39
Ge_3^-	Ge_3^-	A173	HOSi	HSiO	B36
Ge_3O_3	$(GeO)_3$	346,B329	HOSr	SrOH	29,A140,B23
Ge_4	Ge_4	A246	HOTi	HTiO	B27
Ge_4^-	Ge_4^-	B219	$HOTi^-$	$HTiO^-$	B32
HHfO	HHfO	B27	HOXe	XeOH	53
HIO^+	HIO^+	A155	HOY	YOH	B26
HIO	HOI	52,A156,B46	HOY	HYO	B26
HISi	HSiI	44,B40	HOYb	YbOH	B28
HIXe	HXeI	A158,B48	HOZn	ZnOH	31,A141
HI_2^-	IHI^-	55,A158	HOZr	HZrO	B27
HInO	InOH	37,A144	HO_2^+	HO_2^+	47
HKO^+	KOH^+	27	HO_2	HO_2	49,A153,B43
HKrXe	KrXeH	57	HO_2^-	HO_2^-	51,B44
HKr_2^+	HKr_2^+	56,A159,B48	HO_2P	*c*-HOPO	174,B198
HKr_2	Kr_2H	57,B49	HO_3	HO_3	B199
HLaO	HLaO	B27	HO_3P	$HOPO_2$	273
HLi_2	Li_2H	26,A136	HO_3P	HOOPO	273
HMgO	MgOH	27,A138,B23	HO_3P	$HP(O_2)O$	273
HMgS	MgSH	B23	HO_3S	$HOSO_2$	277
HNO^+	HNO^+	41	HO_3Sb	$HSbO_3$	274
HNO	HNO	45,A151	HO_3Sb	$HOSbO_2$	274
HNO	HON	B42	HO_4S	HSO_4	B324

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
HO_4S^-	HSO_4^-	B324	$H_2N_2^+$	*t*-$N_2H_2^+$	142
HPS_2	HPSS	A241	H_2N_2	*t*-N_2H_2	147,A227,B175
HPS_3	$HSPS_2$	A292	H_2N_2	H_2NN	148
HSSi	HSiS	B36	H_2N_2O	NH_2NO	260
HSSr	SrSH	29,B24	$H_2N_2O_2$	NH_2NO_2	337
HS_2	HS_2	50,A154,B44	H_2Nb	NbH_2	A128
HS_2^-	HS_2^-	53	H_2NbO	HNbOH	B167
HSi_2	*cyc*-HSi_2	B31	H_2NbO	H_2ONb	B167
HSi_2^-	*cyc*-HSi_2^-	B33	H_2NbO	H_2NbO	B167
HSi_3	*cyc*-HSi_3	B184	H_2Nd	NdH_2	B13
HSi_3^-	*cyc*-HSi_3^-	B184	H_2Ni	NiH_2	16,A127
HSi_4	Si_4H	B272	H_2Ni^-	NiH_2^-	17
HSi_4^-	Si_4H^-	B272	H_2NiO	HNiOH	136
HXe_2^+	HXe_2^+	56,B49	H_2NiO_2	$Ni(OH)_2$	252
HXe_2	Xe_2H	57	H_2Ni_2O	HNi_2OH	248
HZn_2	ZnZnH	A136	H_2O^+	H_2O^+	24,A134,B20
H_2Hf	HfH_2	A126	H_2OP	H_2PO	151,A228
H_2HfO	H_2HfO	B166	H_2OP	HPOH	151
H_2Hg	HgH_2	16,A128	H_2OS	HSOH	154
H_2Hg_2	HHgHgH	A218	H_2OSc	HScOH	135,B165
H_2Ho	HoH_2	B14	H_2OSi	HSiOH	146
H_2IP	H_2PI	A229	H_2OSi	H_2SiO	145,A226
$H_2I_2^+$	$HIIH^+$	B179	H_2OSn	HSnOH	146
$H_2I_2Si^+$	$SiH_2I_2^+$	263	H_2OSn_2	HSn_2OH	257
H_2In	InH_2	A129	H_2OSr	HSrOH	134
H_2InN	$InNH_2$	B169	H_2OTa	H_2TaO	B168
H_2InO	HInOH	139	H_2OTi	HTiOH	135,B165
H_2LaO	HLaOH	B165	H_2OTi	H_2TiO	B166
H_2LaO_2	$La(OH)_2$	B265	H_2OV	HVOH	135,B166
H_2LiN	$LiNH_2$	B162	H_2OV	H_2VO	B167
H_2Lu	LuH_2	B15	H_2OXe	HXeOH	B179
H_2Lu_2	*cyc*-$(LuH)_2$	B162	H_2OY^+	$HYOH^+$	B164
H_2Mg	MgH_2	14,A125	H_2OY	HYOH	B165
H_2MgN	$MgNH_2$	B162	H_2OZn	HZnOH	A222
H_2MgO	HMgOH	134	H_2OZr	HZrOH	B166
H_2MgO_2	$Mg(OH)_2$	A282	H_2OZr	H_2ZrO	B166
H_2Mg_2	HMgMgH	A217	$H_2O_2^+$	$HOOH^+$	152,B177
H_2Mg_2	*br*-$(MgH)_2$	A218	H_2O_2	HOOH	153,A229,B177
H_2Mg_2O	HMgOMgH	246	H_2O_2S	HSO_2H	265
H_2Mg_2O	HMg_2OH	246	H_2O_2Si	HSiOOH	260
H_2Mn	MnH_2	15	H_2O_2Y	$Y(OH)_2$	B265
H_2Mn^-	MnH_2^-	17	H_2O_3	H_2O_3	B270
H_2MnO	HMnOH	136,B168	H_2O_3Si	H_2SiO_3	338
H_2MnO_2	$Mn(OH)_2$	B265	H_2P^+	PH_2^+	21,B18
H_2Mn_2O	HMn_2OH	247	H_2P	PH_2	22,A1344,B19
H_2Mn_2O	HMnOMnH	247,B261	H_2PS	HPSH	A228
H_2Mo	MoH_2	16	H_2Pd	*cyc*-PdH_2	B12
H_2N^+	NH_2^+	20,A132	H_2Pd^-	PdH_2^-	B15
H_2N	NH_2	21,A133,B18	H_2Pd_2	*cyc*-Pd_2H_2	B161
H_2N^-	NH_2^-	26	H_2Pr	PrH_2	B13
H_2NNa	$NaNH_2$	B162	H_2Pr_2	*cyc*-$(PrH)_2$	B161
H_2NO^+	H_2NO^+	148	H_2Pt	PtH_2	A127,B12
H_2NO	H_2NO	151	H_2S^+	H_2S^+	24,A135
H_2NS	H_2NS	B177	H_2SXe	HXeSH	B179
H_2NSr	$SrNH_2$	133,B163	$H_2S_2^+$	$HSSH^+$	153

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
H_2S_2	HSSH	155,A230,B178	H_3PS	H_2PSH	A275
H_2S_3	*c*-HSSSH	A285,B270	H_3Pd	$HPd(H_2)$	B153
H_2S_3	*t*-HSSSH	A285,B270	H_3Pt	PtH_3	B154
H_2Sb	SbH_2	23	H_3S^+	H_3S^+	130,A217,B160
H_2Se^+	H_2Se^+	25	H_3Sb^+	SbH_3^+	129
H_2Si^+	SiH_2^+	18,A130	H_3Si^+	SiH_3^+	124,A213
H_2Si	SiH_2	19,A131,B17	H_3Si	SiH_3	126,A215,B158
H_2Si^-	SiH_2^-	21	H_3Si^-	SiH_3^-	129
H_2Si_2	br-Si_2H_2	138,A223,B170	H_3Sm	SmH_3	B154
H_2Si_2	Si(H)SiH	138	H_3Tb	TbH_3	B155
H_2Sm	SmH_2	B13	H_3Th	ThH_3	A212
H_2Tb	TbH_2	B14	H_3Ti	TiH_3	A211
H_2Tb_2	*cyc*-$(TbH)_2$	B161	H_3U	UH_3	A212
H_2Te^+	H_2Te^+	25	H_3Zr	ZrH_3	A211
H_2Th	ThH_2	A128	H_4Hf	HfH_4	A265
H_2Ti	TiH_2	14,A126	H_4HgSi	SiH_3HgH	B309
H_2Tm	TmH_2	B15	H_4InN	H_2InNH_2	B311
H_2U	UH_2	A128	H_4Mg_2	$HMgH_2MgH$	A308
H_2U_2	*cyc*-U_2H_2	A128	H_4N^+	NH_4^+	229,A266
H_2V	VH_2	14	H_4N	NH_4	229,A266,B246
H_2Xe	HXeH	A136,B21	$H_4N_2^+$	$N_2H_4^+$	311
H_2Yb	YbH_2	B15	H_4N_2O	NH_2NHOH	364
H_2Zn	ZnH_2	16,A127	H_4Nd	NdH_4	B245
H_2Zn_2	HZnZnH	130,A218	H_4OSi	SiH_3OH	311
H_2Zr	ZrH_2	A126	$H_4P_2^+$	$P_2H_4^+$	311
H_3^+	H_3^+	11,A123,B9	H_4Pd	$Pd(H_2)_2$	B245
H_3	H_3	12,A123,B9	H_4SSi^+	SiH_3SH^+	310
H_3Hf	HfH_3	A211	H_4Si^+	SiH_4^+	228
H_3ISi^+	SiH_3I^+	241	H_4Sm	SmH_4	B245
H_3In	InH_3	A213	H_4Th	ThH_4	A265
H_3InN^+	$InNH_3^+$	B251	H_4Ti	TiH_4	227,A265
H_3InN	$InNH_3$	B253	H_4U	UH_4	A265
H_3InN	$HInNH_2$	B253	H_4U_2	U_2H_4	A308
H_3InP	$InPH_3$	B255	H_4Zr	ZrH_4	A265
H_3InP	$HInPH_2$	B255	H_5^+	H_5^+	227
H_3InP	H_2InPH	B255	H_5NSi	SiH_3NH_2	360
H_3LaO_2	$HLa(OH)_2$	B319	$H_5O_2^+$	$H_5O_2^+$	360,A323
H_3Lu	LuH_3	B155	H_5Si^+	SiH_5^+	A307
H_3Mo	MoH_3	124	H_6OSi_2	SiH_3SiH_2OH	417
H_3N^+	NH_3^+	128,A217,B159	H_6Pd	$Pd(H_2)_3$	B333
H_3NNi	$HNiNH_2$	231	$H_7O_3^+$	$H_7O_3^+$	414
H_3NO^+	NH_2OH^+	242	$H_9O_4^+$	$H_9O_4^+$	414,A364
H_3NSi	$HSiNH_2$	235	HfNO	NHfO	B88
H_3NSi	SiH_2NH	A270	HfN_2	HfNN	B70
$H_3N_2^+$	$N_2H_3^+$	236	HfN_2	NHfN	B70
H_3Nd	NdH_3	B154	HfO_2	OHfO	A176
H_3O^+	H_3O^+	129,B160	HfO_2^-	$OHfO^-$	A182
H_3OP	PH_3O	242,B261	HfO_3	OHfOO	A250
H_3OP	*c*-H_2POH	243	Hf_2N_2	*cyc*-$(HfN)_2$	B205
H_3OSb	H_3SbO	243	Hf_2O_2	*cyc*-$(HfO)_2$	A244
H_3OSb	H_2SbOH	244	Hf_3	Hf_3	B51
H_3O_2Sc	$HSc(OH)_2$	B318	Hg_3	Hg_3	B53
H_3O_2Y	$HY(OH)_2$	B319	HoNO	NHoO	B95
H_3O_3P	$(HO)_2HPO$	368	HoNO	*cyc*-HoNO	B95
H_3P^+	PH_3^+	129	HoN_2	*cyc*-HoNN	B75

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
HoO_2	OHoO	B110	LaO_2	OLaO	B103
HoO_2^-	$OHoO^-$	B119	LaO_2^-	$OLaO^-$	B116
Ho_2N	Ho_2N	B55	La_2N_2	*cyc*-$(LaN)_2$	B204
Ho_2N_2	*cyc*-$(HoN)_2$	B206	$LiNO_3$	*c*-LiOONO	A295
IKrXe	KrXeI	123	$LiNO_3$	*t*-LiOONO	A295
INO	INO	102	$LiNa_3$	$LiNa_3$	180
INO_2	INO_2	213	LiOSi	LiOSi	B58
INO_3	$IONO_2$	289	Li_2Na_2	Li_2Na_2	180
INS^+	NSI^+	95	Li_2O	LiOLi	B53
INS	NSI	105	Li_3	Li_3	58,A159,B49
IOP	IPO	B142	Li_4	Li_4	180
IO_2	OIO	114,A207	Li_6	Li_6	342
IO_2	IOO	A204	Li_7	Li_7	369
IO_2^-	OIO^-	115	Li_8	Li_8	381
IXe_2	Xe_2I	123	LuNO	NLuO	B95
I_2Li	ILiI	B116	LuN_2	*cyc*-LuNN	B75
I_2Na	INaI	B116	LuO_2^-	$OLuO^-$	B120
I_2S	SI_2	115	Lu_2N	Lu_2N	B55
I_2Si^+	SiI_2^+	92	Lu_2N_2	*cyc*-$(LuN)_2$	B207
I_3	I_3	B153	Lu_2O_2	*cyc*-$(LuO)_2$	B213
I_3^-	I_3^-	119,B153	MgNO	MgNO	B87
InNO	InNO	B102	MgO_2	OMgO	A174
InN_2	NInN	B97	MgO_2	*cyc*-MgO_2	A174
InN_3	InNNN	B222	MgO_4	O_2MgO_2	A298
InO_2	*cyc*-InO_2	75	Mg_2O_2	MgOMgO	A243
InO_2	OInO	75	MnNO	NMnO	B90
InO_2^-	*cyc*-InO_2^-	B130	MnNO	MnNO	B90
InP_2	*cyc*-InP_2	B98	MnNO	*cyc*-MnNO	B90
InP_2^-	*cyc*-InP_2^-	B111	MnN_2	NMnN	B72
In_2N	InNIn	B63	MnN_2	*cyc*-MnNN	B72
In_2O	In_2O	64,B81	MnN_2O_2	$Mn(NO)_2$	B293
In_2O_2	InOInO	185	MnN_3O_3	$Mn(NO)_3$	B346
In_2O_2	*cyc*-InO_2In	185	MnO_2	OMnO	B105
In_2O_3	In_2O_3	283	MnO_2	*cyc*-MnO_2	B105
In_2P	In_2P	A165,B64	MnO_2	MnOO	B105
In_2P^-	In_2P^-	B80	MnO_2^-	$OMnO^-$	B118
In_2Sb	In_2Sb	A165	MnO_3	(*cyc*-O_2Mn)O	B226
In_3N	NIn_3	B208	MnO_4	(*cyc*-O_2Mn)O_2	B297
$IrNO^+$	$IrNO^+$	B77	Mn_2O	MnOMn	B55
IrNO	IrNO	B92	Mn_2O_2	*cyc*-$(MnO)_2$	B211
IrNO	NIrO	B92	Mn_2O_2	MnOMnO	B211
IrN_2O_2	$Ir(NO)_2$	B294	Mn_3	Mn_3	61
IrN_3O_3	$Ir(NO)_3$	B346	MoNO	NMoO	B89
IrO_2	OIrO	B106	MoNO	MoNO	B89
IrO_2	*cyc*-IrOO	B106	MoN_2	NMoN	B71
Ir_2O	*cyc*-Ir_2O	B55	MoN_2	MoNN	B71
KNO_2	*cyc*-KNO_2	A247	MoN_2O_2	$Mo(NO)_2$	B293
KNO_2	*t*-KNO_2	A247	MoO_2	OMoO	A175,B104
KNO_3	*c*-KOONO	A296	MoO_2^-	$OMoO^-$	B117
KNO_3	*t*-KOONO	A296	MoO_3	MoO_3	A250,B226
K_3	K_3	B51	$NNaO_2$	*cyc*-$NaNO_2$	A247
K_4	K_4	B200	$NNaO_2$	*t*-NaONO	A247
LaN_2	*cyc*-LaNN	B69	$NNaO_3$	*c*-NaOONO	A295
LaO_2^+	*cyc*-LaO_2^+	B96	$NNaO_3$	*t*-NaOONO	A296
LaO_2^+	$OLaO^+$	B96	NNbO	NNbO	B89

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
NNdO	NNdO	B93	NOV	NVO	B88
NNd_2	Nd_2N	B54	NOV	VNO	B88
$NNiO^+$	$NiNO^+$	B77	NOV	*cyc*-VNO	B88
NNiO	NiNO	B92	NOW	NWO	B90
NNiO	*cyc*-NiNO	B92	NOYb	NYbO	B95
$NNiO^-$	$NiNO^-$	B102	NOZr	NZrO	B88
NNi_2	NiNiN	B54	NO_2^+	NO_2^+	87,A190,B132
$NOOs^+$	$OsNO^+$	B77	NO_2^-	NO_2^-	102
NOOs	OsNO	B91	NO_2S	*c*-OSNO	B237
NOOs	NOsO	B91	NO_2S	*t*-OSNO	B237
NOOs	*cyc*-OsNO	B91	NO_2U	NUO_2	A249
NOP	PNO	88,B133	NO_3^+	NO_3^+	A255
$NOPd^+$	$PdNO^+$	B77	NO_3	NO_3	207,A257,B237
NOPd	PdNO	B92	NO_3^-	NO_3^-	A259
$NOPd^-$	$PdNO^-$	B102	NO_3^-	*c*-$OONO^-$	B239
NOPr	NPrO	B93	NO_3^-	*t*-$OONO^-$	B239
NOPr	PrNO	B93	NP_2	PNP	A187
$NOPr^-$	$NPrO^-$	B102	NPr_2	Pr_2N	B54
$NOPt^+$	$PtNO^+$	B77	NPt_2	Pt_2N	B54
NOPt	PtNO	B93	NPt_2	PtPtN	B54
$NOPt^-$	$PtNO^-$	B102	NRh_2	*cyc*-RhRhN	B53
NORe	NReO	B90	NRh_2	RhRhN	B53
NORe	*cyc*-ReNO	B90	NS_2^+	SNS^+	A191
$NORe^-$	$NReO^-$	B101	NS_2	NS_2	94,A195
$NORh^+$	$RhNO^+$	B77	NS_2	NSS	94
NORh	RhNO	B92	NS_2^-	NS_2^-	102
NORh	NRhO	B92	NS_3	NSSS	208
$NORu^+$	$RuNO^+$	B77	NSe_2^+	$SeNSe^+$	A191
NORu	RuNO	B91	NSe_2	NSe_2	A195
NORu	NRuO	B91	NSe_2	SeSeN	A195
NOS^+	SNO^+	A191	NSe_3	SeSeNSe	A258
NOS	SNO	93,A194,B136	NSe_3	SeSeSeN	A258
NOS	NSO	94	NSi_2	SiNSi	A174,B101
NOS_2	SSNO	A258	NTb_2	Tb_2N	B54
$NOSc^+$	*cyc*-$ScNO^+$	B76	NTl_3	NTl_3	B208
NOSc	NScO	B87	N_2Nb	NbNN	B70
NOSc	ScNO	B87	N_2Nb	*cyc*-NbN_2	B71
NOSc	*cyc*-ScNO	B88	N_2Nb	NNbN	B71
NOSe	SeNO	A195	N_2NbO_2	$Nb(NO)_2$	B292
NOSm	NSmO	B94	$N_2Nb_3^+$	$Nb_3N_2^+$	B277
NOTa	NTaO	B89	N_2Nd	NNdN	B74
$NOTa^-$	$NTaO^-$	B101	N_2Nd_2	*cyc*-$(NdN)_2$	B206
NOTb	NTbO	B94	N_2Ni	NiNN	B73
NOTb	*cyc*-TbNO	B94	N_2Ni	*cyc*-NiNN	B73
NOTh	NThO	B96	$N_2NiO_2^+$	$Ni(NO)_2^+$	B292
NOTi	NTiO	B88	N_2NiO_2	$Ni(NO)_2$	B294
NOTi	TiNO	B88	$N_2NiO_2^-$	$Ni(NO)_2^-$	B296
$NOTi^-$	$NTiO^-$	B101	N_2Ni_2	*cyc*-$(NiN)_2$	B205
NOTl	TlNO	B103	N_2O^+	N_2O^+	83,A187,B127
NOTm	NTmO	B95	N_2OS	SNNO	A254
NOU^+	NUO^+	B78	$N_2O_2^+$	$ONNO^+$	195,A252,B232
NOU	NUO	A172,B96	N_2O_2	*c*-$(NO)_2$	200,A254,B233
NOU	UNO	A172	N_2O_2	*t*-$(NO)_2$	200,A254,B234
NOV^+	*cyc*-VNO^+	B76	N_2O_2	NNO_2	A254
NOV^+	NVO^+	B76	$N_2O_2^-$	NNO_2^-	207,A256,B236

Formula	*Structure/Name*	*References*
$N_2O_2^-$	*t*-$(NO)_2^-$	207,A257,B236
$N_2O_2^-$	*c*-$(NO)_2^-$	B236
N_2O_2Os	$Os(NO)_2$	B294
N_2O_2Pd	$Pd(NO)_2$	B294
N_2O_2Pt	$Pt(NO)_2$	B294
N_2O_2Re	$Re(NO)_2$	B293
N_2O_2Rh	$Rh(NO)_2$	B294
N_2O_2Ru	$Ru(NO)_2$	B293
N_2O_2S	ON-NSO	286
N_2O_2S	ONSNO	286
N_2O_2Ta	$Ta(NO)_2$	B293
N_2O_2Ti	O_2TiN_2	A296
$N_2O_2U_2$	$(NUO)_2$	A320
N_2O_2V	$V(NO)_2$	B292
N_2O_2W	$W(NO)_2$	B293
N_2O_3	O_2N-NO	286,A300,B299
N_2O_3	O=N-O-N=O	286,A300,B299
N_2O_3	*t*,*c*-ONONO	B300
$N_2O_4^+$	$N_2O_4^+$	349
N_2O_4	N_2O_4	350,A321,B330
N_2O_4	$N_2O_4(V_d)$	350
N_2O_4	ONO-NO_2(D)	351
N_2O_4	ONO-NO_2(D′)	351
N_2O_5	O_2N-O-NO_2	370,A331,B347
N_2Os	NOsN	B72
N_2Pd	PdNN	B73
N_2Pr	NPrN	B74
N_2Pr_2	*cyc*-$(PrN)_2$	B206
N_2Pt	PtNN	B73
N_2Pt^-	$PtNN^-$	B87
N_2Pt_2	Pt_2NN	B205
N_2Pt_2	PtNNPt	B205
N_2Pu	NPuN	A168
N_2Re	ReNN	B72
N_2Re	*cyc*-ReN_2	B72
N_2Rh	RhNN	B73
N_2Rh	NRhN	B73
N_2Rh_2	*cyc*-$(RhN)_2$	B205
N_2Ru	NRuN	B72
N_2S^+	NNS^+	83
N_2S	NNS	88
$N_2S_2^+$	$N_2S_2^+$	196
N_2S_2	NS-SN	200
$N_2S_4^+$	$N_2S_4^+$	349
N_2S_4	*cyc*-N_2S_4	351
N_2Sc	ScNN	B69
N_2Sc	*cyc*-ScNN	B69
$N_2Sc_2^+$	*cyc*-$(ScN)_2^+$	B201
N_2Sc_2	*cyc*-$(ScN)_2$	B204
N_2Se_2	NSeNSe	A255
N_2Si	SiNN	72,B114
N_2Si	*cyc*-SiN_2	B115
N_2Si_2	SiNNSi	B223
N_2Si_2	*cyc*-$(SiN)_2$	B223
N_2Si_2	SiNSiN	B223
N_2Sm	NSmN	B74
N_2Sm	SmNN	B74
N_2Sm	*cyc*-SmNN	B74
N_2Sm_2	*cyc*-$(SmN)_2$	B206
N_2Ta	TaNN	B71
N_2Ta	*cyc*-TaN_2	B71
N_2Ta	NTaN	B71
N_2Tb	*cyc*-TbNN	B75
N_2Tb_2	*cyc*-$(TbN)_2$	B206
N_2Th	NThN	B76
N_2Th	ThNN	B76
N_2Th_2	*cyc*-$(ThN)_2$	B207
N_2Ti	TiNN	A166,B69
N_2Ti	*cyc*-TiNN	B69
N_2Ti	NTiN	B69
N_2Ti_2	*cyc*-$(TiN)_2$	B204
N_2Tm	*cyc*-TmNN	B75
N_2Tm_2	*cyc*-$(TmN)_2$	B207
N_2U	NUN	63,B76
N_2V	NVN	B70
N_2V	VNN	B70
N_2V	*cyc*-VNN	B70
N_2W	NWN	B72
N_2W	WNN	B72
N_2Y	*cyc*-YNN	B69
$N_2Y_2^+$	*cyc*-$(YN)_2^+$	B201
N_2Y_2	*cyc*-$(YN)_2$	B204
N_2Yb	*cyc*-YbNN	B75
N_2Zr	ZrNN	B69
N_2Zr	*cyc*-ZrNN	B70
N_2Zr	NZrN	B70
N_2Zr_2	*cyc*-$(ZrN)_2$	B205
N_3^+	N_3^+	72,A181
N_3	N_3	82,B127
N_3^-	N_3^-	87,B132
N_3NbO_3	$Nb(NO)_3$	B345
$N_3O_3^+$	$(NO)_3^+$	B330
$N_3O_3^-$	*c*-$(NO)_3^-$	B330
N_3O_3Os	$Os(NO)_3$	B346
N_3O_3Rh	$Rh(NO)_3$	B346
N_3O_3Ru	$Ru(NO)_3$	B346
N_3O_3Ta	$Ta(NO)_3$	B346
N_3O_3V	$V(NO)_3$	B345
N_3P_3	$(PN)_3$	346
N_3Pt	PtNNN	B215
N_3Pt	NNPtN	B216
$N_3S_3^+$	$S_3N_3^+$	347
N_3Sr	SrN_3	183
N_3Tl	TlNNN	B222
N_4^+	N_4^+	187,A250,B225
N_4	N_4	B230
N_4Pt	NNPtNN	B287
N_4Pt^-	$Pt(NN)_2^-$	B291
N_4Si	$Si(N_2)_2$	B296
N_4Si_2	$(SiNN)_2$	B329

Formula	*Structure/Name*	*References*
N_4Th	NNThNN	B287
Na_3	Na_3	58,A160,B49
Na_4	Na_4	180
Na_5	Na_5	277
Na_6	Na_6	342
Na_7	Na_7	369
Na_8	Na_8	381
NbO_2^+	$ONbO^+$	B96
NbO_2	ONbO	B104
NbO_2^-	$ONbO^-$	B117
NbO_3^-	NbO_3^-	B231
NbO_4	(*cyc*-$O_2Nb)O_2$	B296
Nb_2O_2	NbONbO	B211
Nb_3	Nb_3	A162
Nb_3O^+	Nb_3O^+	B200
Nb_3O	Nb_3O	B200
Nb_3O^-	Nb_3O^-	B201
Nb_8	Nb_8	B360
Nb_8^-	Nb_8^-	B360
NdO_2^+	$ONdO^+$	B97
NdO_2	ONdO	B109
NdO_2^-	$ONdO^-$	B118
Nd_2O_2	*cyc*-$(NdO)_2$	B212
NiO_2	ONiO	A177,B106
NiO_2	*cyc*-NiO_2	A177,B107
NiO_2	NiOO	A177
NiO_2^-	$ONiO^-$	A182
NiO_2^-	*cyc*-NiO_2	A182
NiO_3	ONiOO	A251
NiO_3	*cyc*-$(O_2Ni)O$	A251
NiO_4	O_2NiO_2	A298
Ni_2O	NiNiO	A163
Ni_2O_2	*cyc*-$(NiO)_2$	A244
Ni_2O_2	NiONiO	A244
Ni_2O_3	Ni_2O_3	B288
Ni_3	Ni_3	61
OP_2	P_2O	88,A191,B133
OP_4	P_4O	284
OP_4	br-P_4O	284
OPb_2	PbOPb	A181
OSSi	OSiS	86
OS_2^+	SSO^+	97
OS_2	SSO	105,A199,B143
OS_2^-	SSO^-	110
OSc2	ScOSc	B55
OSeSi	OSiSe	A189
OSe_2	SeSeO	A201
OTa_3	Ta_3O	B200
OTa_3^-	Ta_3O^-	B201
OTi_2	TiOTi	A163
OTl_2	Tl_2O	65,B81
OV_3	V_3O	B200
OV_3^-	V_3O^-	B201
O_2Os	OOsO	B105
O_2Os^-	$OOsO^-$	B118
O_2P	PO_2	93,A194,B135
O_2P^-	PO_2^-	103,A199,B141
O_2P_2	$(PO)_2$	200
O_2Pb	OPbO	A190
O_2Pb	*cyc*-PbO_2	A190
O_2Pb_2	Pb_2O_2	A252
O_2Pb_2	$PbPb(O_2)$	A252
O_2Pd	*cyc*-PdO_2	A177,B107
O_2Pr^+	$OPrO^+$	B97
O_2Pr	OPrO	A179,B109
O_2Pr	*cyc*-PrO_2	B109
O_2Pr^-	$OPrO^-$	B118
O_2Pr_2	*cyc*-$(PrO)_2$	B212
O_2Pt	OPtO	B107
O_2Pt	*cyc*-PtO_2	A177,B107
O_2Pt_2	*cyc*-$(PtO)_2$	B212
O_2Pu	OPuO	A179
O_2Re	OReO	B105
O_2Re^-	$OReO^-$	B118
O_2Rh	ORhO	B106
O_2Rh_2	*cyc*-$(RhO)_2$	B212
O_2Ru	ORuO	B105
O_2Ru^-	$ORuO^-$	B118
O_2S^+	SO_2^+	96,A195,B136
O_2S	SOO	A199
O_2S^-	SO_2^-	110,B148
O_2Sc^+	*cyc*-ScO_2^+	B96
O_2Sc	OScO	B103
O_2Sc^-	$OScO^-$	B116
O_2Sc_2	ScOScO	B210
O_2Sc_2	*cyc*-$(ScO)_2$	B210
O_2Se	SeO_2	A200,B144
O_2Se	SeOO	A201
O_2Se^-	SeO_2^-	A204
O_2Se_2	*cyc*-(SeOSe)=O	A261
O_2Si	SiO_2	86
O_2Si^-	SiO_2^-	A194
O_2Si_2	Si_2O_2	188
O_2Sm	OSmO	B109
O_2Sm^-	$OSmO^-$	B119
O_2Sm_2	*cyc*-$(SmO)_2$	B212
O_2Sn	OSnO	A189
O_2Sn_2	Sn_2O_2	A251
O_2Sr	OSrO	A174
O_2Sr	*cyc*-SrO_2	A175
O_2Sr_2	*cyc*-$(SrO)_2$	A243
O_2Ta^+	$OTaO^+$	B97
O_2Ta	OTaO	A176,B104
O_2Ta^-	$OTaO^-$	B117
O_2Ta_2	*cyc*-$(TaO)_2$	B211
O_2Tb	OTbO	A179,B110
O_2Tb^-	$OTbO^-$	B119
O_2Tb_2	*cyc*-$(TbO)_2$	B213
O_2Te	TeO_2	B144
O_2Th	OThO	A179,B110

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
O_2Ti	OTiO	A176,B103	O_3Tb^-	TbO_3^-	B231
O_2Ti^-	$OTiO^-$	A181	O_3Ti	OTiOO	A250
O_2Ti_2	*cyc*-$(TiO)_2$	A243	O_3U	UO_3	A251,B228
O_2Tl	*cyc*-TlO_2	B121	O_3V	VO_3	B226
O_2Tl	OTlO	B121	O_3V^-	VO_3^-	B230
O_2Tl^-	*cyc*-TlO_2^-	B131	O_3V_2	OVOVO	B287
O_2Tl_2	TlOTlO	B222	O_3W	WO_3	A250,B226
O_2Tl_2	*cyc*-TlO_2Tl	B223	O_3Y^-	YO_3^-	B230
O_2Tm	OTmO	B110	O_3Zr	OZrOO	A250
O_2Tm_2	*cyc*-$(TmO)_2$	B213	O_4^+	*t*-O_4^+	209,A258,B238
O_2U^+	OUO^+	B97	O_4^+	*cyc*-O_4^+	209,A258,B238
O_2U	OUO	A179,B110	O_4^-	*cyc*-O_4^-	222,B243
O_2U^-	OUO^-	B120	O_4Os	(*cyc*-$O_2Os)O_2$	B297
O_2V	OVO	B104	O_4P_2	O_2PPO_2	B331
O_2V^-	OVO^-	B117	O_4Pd	O_2PdO_2	A298,B298
O_2V_2	VOVO	B210	O_4Pt	O_2PtO_2	A298,B298
O_2V_2	*cyc*-$(VO)_2$	B211	O_4Re	(*cyc*-$O_2Re)O_2$	B297
O_2W	OWO	A175,B105	O_4Re^-	ReO_4^-	B298
O_2W^-	OWO^-	B117	O_4Rh	O_2RhO_2	A298,B298
O_2Y^+	*cyc*-YO_2^+	B96	O_4Ru	(*cyc*-$O_2Ru)O_2$	B297
O_2Y	OYO	B103	O_4Ru	RuO_4	B297
O_2Y^-	OYO^-	B116	O_4S	SO_4	289,B302
O_2Yb	OYbO	B110	O_4S^-	SO_4^-	B306
O_2Yb^-	$OYbO^-$	B119	$O_4S_2^-$	$(SO_2)_2^-$	B332
O_2Yb_2	*cyc*-$(YbO)_2$	B213	O_4Si_2	Si_2O_4	A321
O_2Zn	OZnO	A178	$O_4Si_2^-$	$Si_2O_4^-$	A321
O_2Zn_2	ZnOZnO	A244	O_4Ta	(*cyc*-$O_2Ta)O_2$	B296
O_2Zr	OZrO	A176,B103	O_4V	(*cyc*-$O_2V)O_2$	B296
O_2Zr^-	$OZrO^-$	A182,B117	PS_2	PS_2	95
O_2Zr_2	*cyc*-$(ZrO)_2$	A243	PS_2^-	PS_2^-	104
O_3^+	O_3^+	95	P_2S	P_2S	88
O_3^-	O_3^-	109,A203	P_2S_4	P_2S_4	351
O_3Os	OsO_3	B227	P_3	P_3	82
O_3P	PO_3	209,B238	P_4^+	P_4^+	187
O_3P^-	PO_3^-	B240	P_4	P_4	B230
O_3P_2	OPOPO	B300	P_4S	*cyc*-P_4S	284
O_3Pb	$OPb(O_2)$	A253	Pd_3	Pd_3	61
O_3Pr^-	PrO_3^-	B231	Pt_3	Pt_3	61
O_3Pt	PtO_3	B227	Rb_3	Rb_3	B51
O_3Pt	*cyc*-(O2Pt)O	B227	Rh_3	Rh_3	B52
O_3Pt	OOPtO	B228	Ru_3	Ru_3	B52
O_3Re	ReO_3	B226	S_2Si	SiS_2	86,B131
O_3Re^-	ReO_3^-	B231	S_3	S_3	105,A200
O_3Rh	ORhOO	B227	S_3^-	S_3^-	110,B148
O_3Ru	RuO_3	B227	S_4	S_4	214,A260
O_3S^+	SO_3^+	209	S_4	SS_3	214
O_3S	OSOO	A260	Sb_3	Sb_3	82
O_3S^-	SO_3^-	223	Sb_3^-	Sb_3^-	88
O_3Sc	*cyc*-$(O_2Sc)O$	B225	Sb_4	Sb_4	189
O_3Se	SeO_3	214,A260	Sb_4^-	Sb_4^-	197
O_3Se	OSeOO	A261	Sc_3	Sc_3	61
O_3Si	SiO_3	A253	Se_2Si	$SiSe_2$	A189
$O_3Si_2^-$	$Si_2O_3^-$	A300	Se_3	Se_3	106
O_3Si_3	$(SiO)_3$	346	Se_4	Se_4	214
O_3Ta^-	TaO_3^-	B231	Se_4	$SeSe_3$	215

Formula	*Structure/Name*	*References*	*Formula*	*Structure/Name*	*References*
Si_3	Si_3	67,A170,B83	Sn_3	Sn_3	B84
Si_3^-	Si_3^-	68,A173	Sn_3^-	Sn_3^-	B99
Si_4	Si_4	182,A245,B215	Sn_4^-	Sn_4^-	B219
Si_4^-	Si_4^-	183,A247,B218	Ta_3	Ta_3	B51
Si_5	Si_5	B281	Ta_4	Ta_4	A241
Si_5^-	Si_5^-	B283	Te_3	Te_3	106
Si_6	Si_6	A318,B326	Te_4	Te_4	215
Si_7	Si_7	A329,B344	Te_4	$TeTe_3$	215
Si_7^-	Si_7^-	B344			