

Vibrational and electronic energy levels of polyatomic transient molecules: Supplement 1

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

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New information on the experimentally determined vibrational and electronic energy levels of approximately 500 neutral and ionic transient molecules possessing from 3 to 16 atoms has been evaluated and added to the previously established database for these species. There has been selective extension of the compilation to somewhat less reactive species such as HNCN, HCNO, H₂O₂, and *cis*- and *trans*-HONO, as well as to many transient molecules which include atoms beyond the third row of the Periodic Table. Electronic spectral data are also given for a number of transient molecules which possess more than six atoms. Radiative lifetimes and the principal rotational constants are included. Observations in the gas phase, in molecular beams, and in rare-gas and nitrogen matrices are evaluated. The types of measurement surveyed include conventional and laser-based absorption and emission techniques, laser absorption with mass analysis, and photoelectron spectroscopy.

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

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1. Introduction

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

For some years, the compilation of spectroscopic data for small polyatomic molecules (3–12 atoms) given by Herzberg¹ stood alone as an information source on the vibrational and electronic energy levels of these species. To meet the need for an updated, critically evaluated compilation of the ground-state vibrational energy levels of small polyatomic reaction intermediates, the first publication in this series,² which provided data for approximately 480 transient molecules possessing from 3 to 16 atoms, appeared in 1984. A second compilation,³ concerned with the electronic energy levels of approximately 500 transient molecules possessing from 3 to 6 atoms, was published in 1988. Vibrational fundamentals of the ground and excited electronic states and radiative lifetimes were included. To aid in spectral identification, the principal rotational constants were also given to three decimal places. For many of the approximately 150 molecules common to these two sets of tables, there were significant revisions to the ground-state vibrational energy levels in the four-year period between the two compilations. These two sets of tables have provided the basis for a recently released software database for personal computers,⁴ designed to supplement the published compilations by providing a capability for rapid searches by molecule or wavenumber.

The rapid growth in the scientific literature concerned with the spectroscopic study of transient molecules and with their detection in chemical reaction systems continues. In addition, there has been great progress in the spectroscopic characterization of small metal clusters and of the transient species produced by the reaction of metal atoms with small molecules. With the need for a scientific base to support new technologies such as those of plasma processing and chemical vapor deposition, studies of reaction intermediates which contain the heavier elements have also multiplied rapidly. This compilation revises and extends the evaluated spectral database for transient molecules, in order to support further research.

2. Scope of Review

New and revised data for approximately 500 molecules are included in this compilation. There has been selective inclusion of data for somewhat less reactive molecules, including HNCO, HCNO, H₂O₂, and *cis*- and *trans*-HONO. These species are important in many chemical reaction mechanisms but are difficult to study in conventional systems because of the ease with which they decompose, rearrange, or polymerize. Reaction intermediates containing the heavier elements are also included. The subject matter of the two published databases has been merged; in this and future supplements all of the properties given in the published electronic spectral tables plus the approximate relative infrared absorption intensities given in the first vibrational data compilation will appear together. The evaluation of electronic energy levels has also been selectively

extended to transient species which possess from 7 to 16 atoms.

3. Types of Measurement

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

As in the two earlier compilations, spectral data obtained in rare gas and small covalent molecule matrices are included. The application of matrix isolation sampling for the stabilization and spectroscopic study of reaction intermediates has recently been reviewed.⁵ Because nitrogen and the rare gases are transparent through the entire infrared spectral region, matrix isolation measurements provide a potentially valuable survey tool. In these matrices, infrared absorptions are typically sharp, with half band widths between 0.1 and 1 cm⁻¹. Rotational structure is, with few exceptions, quenched. Multiple trapping sites occur, often resulting in the appearance of several absorption maxima—usually one or two of these predominate—over a range of a few cm⁻¹. A comparison⁶ of the positions of the ground-state vibrational fundamentals of over two hundred diatomic molecules observed in the gas phase and in nitrogen and rare-gas matrices has shown that, typically, the smallest matrix shift occurs for neon matrix observations, with successively greater matrix shifts for the heavier rare gases and for nitrogen. Except for very weakly bonded molecules and for the alkali metal and Group IIIa halides, matrix shifts of most diatomic molecules isolated in solid argon are smaller than 2%. A similar comparison is shown in Fig. 1 for the ground-state vibrational fundamentals of both neutral and charged transient molecules in the gas phase and in neon and argon matrices. Many of the available neon-matrix data are for molecular cations, with a heavy representation of halogen-substituted benzene cations. For these species, as well as for uncharged molecules, the maximum in the distribution lies near 0.0%, and most of the matrix deviations from the gas-phase values amount to less than 1%. Many more data are available for the argon-matrix comparison. Again, there is almost an equal probability of a negative or positive shift from the gas-phase band origin, and matrix shifts greater than 1% occur for only about 10% of the frequencies available for the comparison.

Many other matrix materials have been employed for spectroscopic studies. However, complications due to reaction or to relatively strong interaction (e.g., hydrogen bonding) of the transient molecule with the matrix frequently occur. Therefore, observations in such media as solid hydrocarbons and aqueous solution and studies

of condensed reaction products without an inert carrier have been excluded.

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

The range of tunability of visible and ultraviolet lasers, like that of infrared lasers, is limited. Therefore, a preliminary survey using conventional gas-phase and/or matrix isolation spectroscopic studies is often desirable. A comparison of the positions of the electronic band origins of diatomic molecules in the gas phase and in rare-gas and nitrogen matrices has been published.⁷ As for the determination of ground-state vibrational energy levels, neon is the matrix material of choice, with a sharp maximum at 0.0% in the distribution of matrix deviations for valence transitions of covalently bonded molecules. In argon-matrix observations, most such band origins are shifted by less than 2% from the gas-phase values. At the somewhat higher temperatures often used for electronic spectral observations in matrices of the heavier rare gases or of nitrogen, relatively broad phonon bands become prominent. The blue shift of the phonon maximum from the zero-phonon line in absorption measurements, and the red shift in emission measurements, typically amount to approximately 1 to 1.5%. Rydberg transitions of molecules in matrices often are greatly broadened and experience much larger shifts. Further details of the behavior of electronic transitions of matrix-isolated molecules have previously been discussed.^{3,5,7}

Contrary to earlier expectation, it has been found that the radiative lifetime of a relatively large molecule isolated in a rare-gas matrix is frequently related to the radiative lifetime in the gas phase by a simple refractive index correction.⁸ In a neon matrix, such a correction typically decreases the radiative lifetime by about 15%. For relatively large molecules, often intramolecular

mechanisms for nonradiative energy transfer are available both in the gas phase and in the matrix. On the other hand, the density of excited states is much lower for small molecules, and matrix shifts may alter perturbation interactions between two strongly coupled electronic states, providing a path for nonradiative deactivation. In this circumstance, fluorescence which is prominent in the gas phase may even be completely quenched in the matrix.

The earlier electronic spectral data compilation³ contained spectral data for many molecular cations derived from observations of the photoelectron spectrum of the corresponding neutral molecule. Most of these studies were conducted at low to moderate resolution, and uncertainties amounting to more than 100 cm⁻¹ are common. There have been comparatively few more recent ultraviolet photoelectron studies of small molecules; most of the photoelectron data given in this supplement have been carried over from the earlier compilation, in which a more detailed discussion is given.

4. Guide to the Compilation

The goals of this compilation are to bring up to date the earlier evaluations of spectroscopic data for small polyatomic transient molecules and to provide a selective extension of these evaluations to other important, comparatively unstable simple molecules and to transient species which contain heavier atoms. The literature has been surveyed through February 1990; only limited addition of more recent data has been possible. Unfortunately, it is not possible to include data for stable molecules. However, the spectra of many of these species are relatively well established, and sources of data such as the tables of Herzberg¹ remain extremely useful. In using the present compilation and its two earlier companions^{2,3} for spectral identifications, it is crucial that the literature on the spectra of stable molecules also be consulted.

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

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

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

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

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

<i>br</i>	—	bridged
<i>cyc</i>	—	cyclic. If parentheses follow, only the atoms enclosed in them are included in the ring.
<i>c</i>	—	<i>cis</i>
<i>t</i>	—	<i>trans</i>

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

As in the earlier compilations, the tables are grouped by the number of atoms in the molecule and, secondarily, by the number of hydrogen atoms present. As in *V* and *E*, molecules within a given section of the tables are arranged in the order of increasing number of valence electrons. For species with the same number of valence electrons, molecules with a simple chain of three heavy atoms are listed in the order, first, of the number of valence electrons in the central atom of the chain and, second, of the row which this atom occupies in the Periodic Table. For larger molecules, the sequence is somewhat arbitrary, but criteria of increasing molecular size and grouping in the Periodic Table (e.g., N before O) are used. Halogen-substituted species are placed immediately after related hydrides. Data for substituted acetylene and benzene cations, which were placed in special groupings in the earlier vibrational tables, are merged with data for other species of similar size (e.g., eight-atom molecules, large molecules) in this compilation. As before, data are given for both the normal and the fully deuterium-substituted molecule. However, only the hydrogen-containing species is listed in the Master Index.

The heading for each electronic state gives its symmetry, the point group to which the molecule belongs in that electronic state, and, where available, references to a quantitative molecular structure. For *C*_{2v} molecules, there is potential ambiguity in the definition of the molecular symmetry axes. The convention in which the *x* axis is chosen perpendicular to the plane of the molecule, recommended by the Joint Commission for Spectroscopy of IAU and IUPAP,⁹ has been adopted. Often this has required the interchange of published assignments of energy levels with *B*₁ and *B*₂ symmetry.

The energy of the electronic transition follows the state designation and symmetry information. Where possible, *T*₀, the energy separation between the electronic energy level of interest and the ground electronic, vibrational, and rotational states of the molecule, is given. However, where only low resolution data or photoelectron data are available, often only band maxima have been given in the literature. With photoelectron data, *T*₀ is derived by subtracting the value of the first ionization potential from that of the higher ionization potential which corresponds to the state of interest. When data for the first adiabatic ionization potential are available either from the photoelectron studies or from other photoionization measurements, the footnote phrase "from vertical ionization potential" implies that the first adiabatic ionization potential is known but that the higher ionization potential is measured to the peak maximum; the phrase "from vertical ionization potentials" implies that the energy difference between the higher and the first absorption maximum was used. Because of inherent uncertainties in the determination of higher ionization potentials in many photoelectron measurements, photoelectron data above about 18 eV are often omitted. Except where otherwise indicated, the units of all quantities in these tables are cm⁻¹. Error estimates are those

of the authors of the original literature. The numbers in parentheses give these estimated errors in relation to the last digits of the vibrational frequency (e.g., 1234.56(78) $\equiv 1234.56 \pm 0.78$). Where the error includes a decimal point, the decimal point has been included. As in the tables of Herzberg,¹ T_0 values are given to the center of multiplet structure. For doublet states the two components differ by $\pm A$ (the spin-orbit splitting constant) and the energy difference is measured from the average of the two bands, whereas for triplet states the three components fall at 0, $\pm A$ with respect to the position from which the band energy is measured. This convention is also followed here unless specific states are given. However, in matrix isolation absorption and laser excitation studies only the lowest component is accessible. Except for transitions with relatively small values of A , this is also likely to be true of studies using cooled molecular beams. Often these latter studies give T_0 values with a precision better than that to which A is known.

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

The format of the vibrational tables is similar to that used in the two earlier compilations. The vibrational numbering convention is that used by Herzberg.¹ Within a given symmetry species, vibrations are numbered starting with the highest frequency. The same convention is followed for deuterated species. Therefore, a given type of vibration may be numbered differently for the deuterated than for the unsubstituted molecule. For triatomic molecules, the bending vibration is always designated as ν_2 . For aromatic molecules, an alternate vibrational numbering scheme developed by Wilson¹⁰ has often been used in the literature. Where both the Herzberg and the Wilson numbering schemes have been used for the published data, the Herzberg numbering is adopted, and the Wilson numbering is shown in parentheses. For a few species, only the Wilson numbering has been used. To avoid confusion, this is retained in the present tables, and the use of the Wilson numbering is indicated in a footnote. Where possible, the values of $\Delta G(\frac{1}{2})$, the separation between the $\nu = 0$ and $\nu = 1$ levels for the vibration of interest, have been used. For some systems, vibrational frequencies have been determined with a precision greater than two decimal places, and the tabulated values have been rounded off. If a bending fundamental is split by Renner-Teller interaction, the position of the unperturbed fundamental is given. Where specific components of such a split fundamental have been studied, they may also be listed, with the transition designated in a footnote. For a more complete treatment of the Renner effect and definitions of the parameters included in many

of these footnotes, see the discussion by Herzberg¹ and the references cited for the molecule of interest. A few of the species in these tables possess out-of-plane vibrations which have resolved inversion splitting structure. For these, the specific component for which the vibrational frequency is reported is designated in a footnote. Relative intensities of vibrational bands are dependent on the technique used for the measurement. It is not feasible to give these intensities for various techniques. However, the relative intensities of *ground-state infrared absorptions*, omitted from the electronic data tables, have been restored in this supplement. Abbreviations used for these include:

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

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

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

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

5. Abbreviations

Many sophisticated laser techniques—frequently employing two or more laser beams—have been used for studies of transient molecules. Often the developers of these techniques have designated them by complicated acronyms. In these tables, an attempt has been made to avoid relatively lengthy and unfamiliar acronyms by designating only the generic type of detection, using the symbols defined below. (Velocity modulation, designated as a separate detection technique in the first of this series of data evaluations,² is widely used and is considered to be a measurement tool rather than a type of ob-

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

AB	—	near infrared-visible-ultraviolet absorption
CC	—	color-center laser absorption
CL	—	chemiluminescence
DL	—	diode laser absorption
ED	—	electron diffraction
EF	—	electron-excited fluorescence
EM	—	near infrared-visible-ultraviolet emission
ESR	—	electron spin resonance
HFD	—	high frequency deflection
IB	—	ion beam
ID	—	ion drift
IR	—	infrared absorption (conventional or Fourier transform)
LD	—	laser difference frequency absorption
LF	—	laser-excited fluorescence (excitation and resolved emission)
LMR	—	laser magnetic resonance

LS	—	laser Stark spectroscopy
MO	—	molecular orbital calculations
MODR	—	microwave-optical double resonance
MPI	—	multiphoton ionization
MW	—	microwave and millimeter wave absorption
ND	—	neutron diffraction
PD	—	electron photodetachment
PE	—	photoelectron spectroscopy
PEFCO	—	photoelectron-photon coincidence
T-PEFCO	—	threshold photoelectron-photon coincidence
PEPICO	—	photoelectron-photoion coincidence
PF	—	photofragment spectroscopy
PI	—	photoionization
PIFCO	—	photoion-photon coincidence
PIR	—	photoionization resonance
Ra	—	Raman scattering
SEP	—	stimulated emission pumping
TPE	—	threshold photoelectron spectroscopy
UV	—	near infrared-visible-ultraviolet absorption and emission

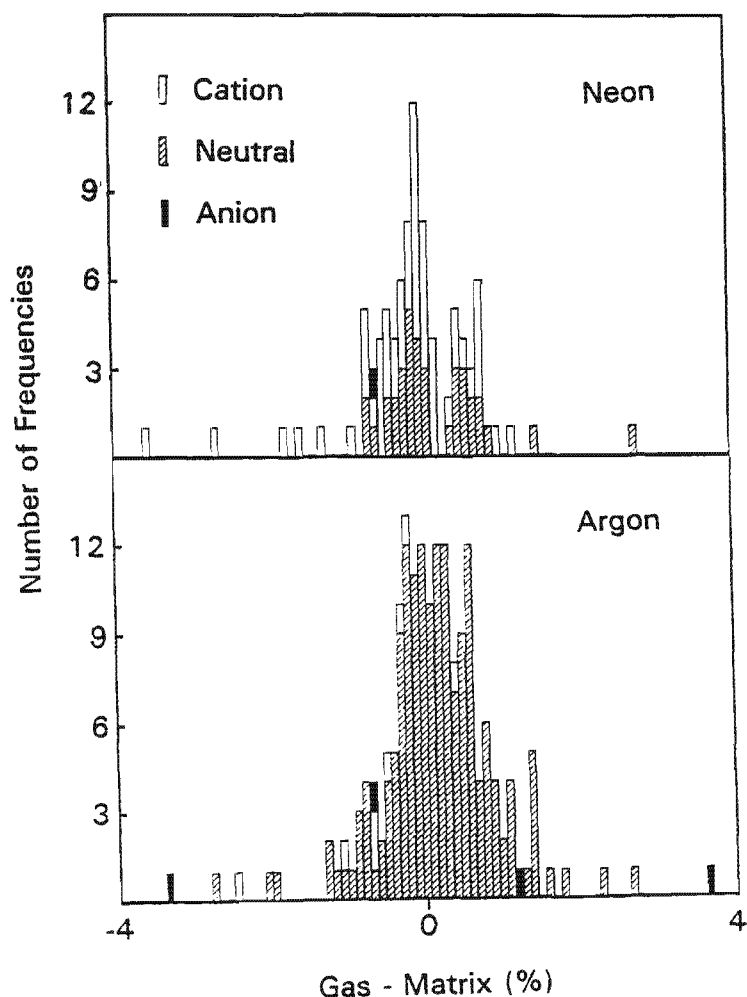


FIG. 1. Comparison of ground-state vibrational frequencies reported for transient molecules (2-16 atoms) in neon and argon matrices with corresponding values obtained from gas-phase measurements.

Beyond scale of neon-matrix plot: XeF—7.8%

Beyond scale of argon-matrix plot: $C_6H_6^+(\nu_{17})$ —9.4%; (ν_{18}) —5.6%

6. Tables

6.1. H_3^+ , H_3 , and Triatomic Dihydrides H_3^+

$\bar{X}$ D_{3h}						
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Ring breathing	3178.3	gas	IR,PI	11,13,14
e'	2	Deformation	2521.31	gas	LD,IR	1,4,16
$B_0 = 43.571(5); C_0 = 20.62 \text{ LD}^{1,4}\text{DL}^4\text{IR}^{11}$						

 H_2D^+

$\bar{X}$						
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Ring breathing	2992.51	gas	LD	3,6,12
	2	Deformation	2205.87	gas	LD,DL	7
b_2	3	Deformation	2335.45	gas	LD,DL	7
$A_0 = 43.438(2); B_0 = 29.134; C_0 = 16.601 \text{ LD,MW}^{6,7,12}$						

 D_2H^+

$\bar{X}$						
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Ring breathing	2736.98	gas	LD	5,12,15
	2	Deformation	1968.17	gas	DL	9,15
b_2	3	Deformation	2078.43	gas	DL	9,15
$A_0 = 36.199; B_0 = 21.869; C_0 = 13.070 \text{ LD}^{5,12,15}\text{DL}^{9,15}$						

 D_3^+

$\bar{X}$						
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Ring breathing	2303 ^a	gas	MO	8
e'	2	Deformation	1834.67	gas	IB,DL	2,10
$B_0 = 21.824; C_0 = 10.510 \text{ DL}^{10}$						

^a*Ab initio* calculation⁸ of gas-phase band center. All other calculated band centers for the fundamentals of H_3^+ and its deuterium-substituted counterparts agree within 5 cm^{-1} with the observed band centers.

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 H_3

Higher Rydberg states have been detected using photoionization and field ionization. The ionization limit observed for vibrationally and rotationally unexcited H_3 from its $2p^2A_1'$ state is $29562.6(5)$.^{12,15,16} Ion depletion studies have also yielded frequencies for the ring breathing vibration of a number of these higher Rydberg states.²³

$3d^2A_1'$ D_{3h} Structure: EM^8						
$T_0^a = 18511$	gas	EM^8	$3d-2p^2A_1'$	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	$\text{EM}^8\text{PF}^{14}$	$3d-2p^2A_1'$	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
$B_0 = 42.99; C_0 = 22.735 \text{ EM}^8$						
$3d^2E'$ D_{3h} Structure: EM^8						
$T_0^a = 18037$	gas	EM^8	$3d-2p^2A_1'$	568–615 nm		
		EM^8	$3d-3p^2E'$	3891–4456 cm^{-1}		
$B_0 = 42.99;$	$C_0 = 22.735$	EM^8				
$3p^2A_1'$ D_{3h} Structure: EM^3						
$T_0^a = 17789$	gas	$\text{EM}^{2,3,8}$	$3p^2A_1'-2s^2A_1'$	556–574 nm		
$\tau = 37(4) \text{ ns}$	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	$\text{EM}^3\text{PF}^{13,14}$	$3s^2A_1'-2p^2A_1'$	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
$B_0 = 44.19; C_0 = 22.676 \text{ EM}^6$						

$3p\ ^2E'$	D_{3h}	Structure: EM^6			
$T_0^a = 13961$	gas	$EM^{2,4}$	$3p\ ^2E' - 2s\ ^2A_1$	708–736 nm	
		EM^6	$3s\ ^2A_1 - 3\ ^2E'$	3178–3847 cm^{-1}	
		EM^8	$3d - 3\ ^2E'$	3891–4456 cm^{-1}	
$\tau = 1.1(+0.2, -1.0)$ 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

$$B_0 = 44.58; C_0 = 22.288 \quad EM^6$$

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

H₂D

$3s\ ^2A_1$	C_{2v}				
$\tau \sim 4$ ns	gas	EM^{20}			
$3p\ ^2B_1$	C_{2v}				
$\tau = 29(3)$ ns	gas	EM^{20}			
$3p\ ^2A_1, ^2B_2$					
$\tau = 2.5(+0.3, -0.7)$ ns	gas	EM^{21}			

D₂H

$3s\ ^2A_1$	C_{2v}				
$\tau \sim 5$ ns	gas	EM^{20}			
$3p\ ^2B_1$	C_{2v}	Structure: EM^9			
$T_0^a = 17834.4$ gas	EM^9	$3p\ ^2B_1 - 2s\ ^2A_1$	560 nm		
$\tau_1 = 31.5(3.2)$ ns; $\tau_2 \sim 8.9$ ns	gas	EM^{20}			
$3p\ ^2A_1, ^2B_2$	C_{2v}				
$\tau = 5.0(7)$ ns	gas	EM^{21}			
$2s\ ^2A_1$	C_{2v}	Structure: EM^9			

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

D₃

The ionization limit of D₃ with respect to the vibrationless level of its $2p\ ^2A_2'$ state has found to be 29602.²¹

$3d\ ^2A_1$	D_{3h}	Structure: EM^8			
$T_0^a = 18530$	gas	EM^8	$3d - 2p\ ^2A_2'$	569–601 nm	
		EM^8	$3d - 3p\ ^2E'$	3772–4517 cm^{-1}	
$\tau = 12(1)$ 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	$3d - 3p\ ^2E'$	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			
$T_0^a = 18098$	gas	EM^8	$3d - 2p\ ^2A_2'$	569–601 nm	
		EM^8	$3d - 3p\ ^2E'$	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	$EM^{2,3,8}LF^7$	$3p\ ^2A_2' - 2s\ ^2A_1$	553–569 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	$3s\ ^2A_1 - 3p\ ^2E'$	3382–3768 cm^{-1}	
$\tau \sim 10$ ns	gas	EM^{20}			
$B_0 = 21.98$; $C_0 = 12.41$		EM^6			

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Ring breathing	$\sim 2145^d$	gas	EM	21
e'	2	Deformation	$\sim 1750^d$	gas	EM	4,21

$$\tau = 17.5(2.0)$$
 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	
$B_0 = 22.112$; $C_0 = 11.056$		EM^6			

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Ring breathing	2457(10)	gas	EM	4,20,21
e'	2	Deformation	~ 1890	gas	EM	21

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

^aMeasured with respect to lowest bound state, $2s\ ^2A_1$. Structure observed¹ in the dissociation spectrum of H₂ has been reinterpreted⁵ as arising from the predissociation of H₃ ($2s\ ^2A_1$) into H + H₂. Unstructured emission observed¹¹ between 190 and 280 nm, with a maximum near 230 nm, upon charge transfer between K and H₃⁺ or D₃⁺ has been attributed to transitions originating in bound Rydberg states of H₃ or D₃ and terminating in the dissociative ground state continuum. Photofragment spectroscopy¹⁴ has placed the $2p\ ^2A_2'$ state 5.563(20) eV above the ground-state H + H₂ dissociation limit.

^bObserved for N = 1 rotational level.

^cPredissociated by vibronic interaction with the $2p\ ^2E'$ repulsive ground state; linewidth is approximately 15 cm^{-1} for H₃ and 6 cm^{-1} for D₃.²

^dTentative assignment.

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MgH₂

$\tilde{X}$	$D_{\infty h}$					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Π	2	Bend	430	Kr	IR	1
			417	Xe	IR	1
Σ_u^+	3	Asym. stretch	1558	Kr	IR	1
			1569	Xe	IR	1
			1544			

MgD₂

$\tilde{X}$	$D_{\infty h}$					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Π	2	Bend	309	Kr	IR	1
			300	Xe	IR	1
Σ_u^+	Asym. stretch		1153	Kr	IR	1
			1160	Xe	IR	1
			1144			

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CrH₂

$\tilde{X}$	C_{2v}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
b_2	3	CrH a-stretch	1591	Ar	IR	1

CrD₂

$\tilde{X}$	C_{2v}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
b_2	3	CrD a-stretch	1145	Ar	IR	1

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AlH₂

$\tilde{A}^2B_1(\Pi)$	$D_{\infty h}$	Structure:	AB^1
$T_0 < 15200$	gas	$\tilde{A}-\tilde{X}$	658.4 nm

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

$$B_0 = 3.57 \quad AB^1$$

$\tilde{X}^2A_1$	C_{2v}	Structure:	AB^1
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Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	AlH s-stretch	1766vw	Kr	IR	2
	2	Bend	760m	Kr	IR	2
b_2	3	AlH a-stretch	1799w	Kr	IR	2

$$A_0 = 13.6; \quad B_0 = 4.4; \quad C_0 = 3.3 \quad AB^1$$

AlD₂

$\tilde{X}^2A_1$	C_{2v}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	AlD s-stretch	1275vw	Kr	IR	2
	2	Bend	560m	Kr	IR	2
b_2	3	AlD a-stretch	1320w	Kr	IR	2

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CH₂

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

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

$$\tau = 1.90(15) \mu s \quad LF^8$$

$$\tau(0,14,0) = 4.2(2) \mu s \quad LF^9$$

$$\tau(0,16,0) = 1.3(3) \mu s \quad LF^{11}$$

$$B_0 = 7.74 \quad AB^1$$

$$\text{Barrier to linearity} = 1617^{29}$$

$\tilde{a}^1A_1^b$ C_{2v} Structure: $AB^{3,29,31}$
 $T_0 = 3147(5)$ gas $AB^{1,3,27,28}$ LMR^{21,26,30} PE^{23,24} LF³² SEP³²
 $\tilde{b}-\tilde{a}$ 490–920 nm

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

$\tau \sim 18$ s^c

$A_0 = 20.118(2)$; $B_0 = 11.205(2)$; $C_0 = 7.069(2)$ $AB^{3,27,28}$
 Barrier to linearity = 9750²⁹

$\tilde{X}^3B_1$ C_{2v} Structure: ESR⁴⁻⁶ AB⁷ LMR^{15,17} IR^{17,26}

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

$A_0 = 73.811$; $B_0 = 8.450$; $C_0 = 7.184$ IR²⁵

Barrier to linearity = 1931(30)²⁶

^aValue given for ¹³CH₂.

^bThe $\tilde{a}^1A_1$ and $\tilde{b}^1B_1$ states are perturbed by strong Renner-Teller interaction.^{13,14,29} They are also strongly perturbed by interaction with the $\tilde{X}^3B_1$ state.^{27,28}

^cCalculated value.²¹

^dFrom analysis of perturbations involving combination bands.³¹

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SiH₂

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

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

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

^cIn Fermi resonance with $2\nu_2$, observed for SiH₂ at 1993 cm⁻¹ and for SiD₂ at 1445 cm⁻¹.

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NH $\frac{1}{2}$

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	2	Bend	840(50)	gas	PE	1
b_2	3	Asym. stretch	3359.93	gas	LD	3

$B_0 = 8.273$; $C_0 = 7.644$ LD³

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PH $\frac{1}{2}$

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

$T_0 \sim 5650$ gas PI^{1,2}

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

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NH₂

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

$T_0 = 11122.6$ gas $AB^{1,8,22}$ LF^{6,21} $\tilde{A}-\tilde{X}$ 430–2700 nm
 Ar, Kr, Xe^b $AB^{2,3,5}$ $\tilde{A}-\tilde{X}$ 344–790 nm
 N₂^b AB^5 $\tilde{A}-\tilde{X}$ 480–620 nm

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

$\tau_{090\Sigma} = 10.0(1.7)$ μ s gas LF⁷

$\tau_{080\Pi} = 10(3)$ μ s gas LF¹⁷

Approximate ν^3 dependence.^{7,17} In another LF study,¹² τ varied from 25 to 46 μ s for relatively unperturbed rotational sublevels, and there was a weaker ~ 100 μ s component associated with levels which are substantially perturbed.

$B_0 = 8.78$ AB¹

Barrier to linearity = 730¹⁴

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

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

$A_0 = 23.693$; $B_0 = 12.952$; $C_0 = 8.173$ $AB^{1,8}$ LMR¹³ IR²⁰

Barrier to linearity = 12024¹⁴

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

^bOrigin not observed. A detailed comparison of the argon-matrix data of Ref. 2 with gas-phase data has been given in Ref. 22. Rotational structure is resolved in the rare-gas matrices. In nitrogen,⁵ bands are very broad and red-shifted by approximately 400 cm⁻¹, with no evidence for rotational structure.

^cAssigned⁵ in matrix studies to ν_3 . Gas-phase observation of ν_1 at 3219.37 cm⁻¹ and demonstration¹⁶ that ν_1 is more intense than ν_3 dictate reassignment to ν_1 .

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PH₂

$\tilde{A}^2A_1$, ^a	C _{2v}	Structure: AB ⁴
$T_0 = 18276.59(3)$ gas 18215(4) Ar		AB ^{1,4,6} EM ^{2,3,5} AB ^{13,19} $\tilde{A}-\tilde{X}$ 360–880 nm $\tilde{A}-\tilde{X}$ 405–550 nm

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

$\tau = 4(1) \mu\text{s}$ gas LF^{11,20}EM¹²

$A_0 = 20.41$; $B_0 = 5.60$; $C_0 = 4.295(3)$ AB^{4,6}EM⁵

Barrier to linearity = 6840⁷

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SbH₂

$\tilde{X}$	C _{2v}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
b_2	3	SbH ₂ a-stretch	1840.5	Ar	IR	3

SbD₂

$\tilde{X}$	C_{2v}					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	SbD ₂ a-stretch	1320.2	Ar	IR	3

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H₂O⁺

$\tilde{X}^2B_1^b$	C _{2v}	Structure: EM ^{5,7} LMR ⁸ LD ¹¹				
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	3213.0	gas	PE,LD	9,11,13
	2	Bend	1408.42	gas	EM,PE	1,5,9
b_2	3	Asym. stretch	3259.03	gas	DL	12
					LD	11

$A_0 = 29.037(3)$; $B_0 = 12.417(2)$; $C_0 = 8.468$ LMR⁸LD¹¹DL¹²

Barrier to linearity = 9187⁷

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NH₂⁻

Threshold for electron detachment from ground-state NH₂⁻ is 6220(40).^{1-3,7}

$\tilde{X}^1A_1$		C _{2v}	Structure: CC ⁵			
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	3121.93	gas	CC	4,5
	2	Bend	1523	Ar	IR	6
b_2	3	Asym. stretch	3190.29	gas	CC	5
			3152	Ar	IR	6

$A_0 = 23.051(2)$; $B_0 = 13.068(2)$; $C_0 = 8.115$ CC^{4,5}

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H₂F⁺

$\tilde{X}$	C _{2v}	Structure: CC ^{1,2}				
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	3348.71	gas	CC	1,2
b_2	3	Asym. stretch	3334.69	gas	CC	1,2

$A_0 = 34.511$; $B_0 = 12.885$; $C_0 = 9.080$ CC^{1,2}

References

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 I_2Cl^+

$\bar{X}$ C_{2v} Structure: $\text{DL}^1\text{MW}^2\text{LD}^3$						
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
ν_1	1	Sym. stretch	2643.22	gas	LD	3
	2	Bend	1184.13	gas	DL	1
ν_2	3	Asym. stretch	2630.14	gas	LD	3

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

References

- ¹K. Kawaguchi and E. Hirota, *J. Chem. Phys.* **85**, 6910 (1986).
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6.2. Triatomic Monohydrides

BeOH

gas EM¹ 300–332 nm

A complicated pattern of red-degraded emission bands observed in this spectral region in discharges through a controlled pressure of H_2O or D_2O using beryllium electrodes has been attributed¹ to BeOH and BeOD, respectively.

References

- ¹A. Antic-Jovanovic, V. Bojovic, and D. Pesic, *Spectrosc. Lett.* **21**, 757 (1988).

ScOD

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

References

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

NiOH

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

NiOD

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

References

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

ZnOH

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

ZnOD

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

References

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

HCC

$A^2\Pi$ $C_{\infty v}$
 $T_0 < 3800$ Ar AB²¹

In an argon matrix, a complicated absorption band system of HC_2 extends from approximately 3600 to 7800.²¹ This band system is extensively perturbed by high vibrational levels of the ground state. A few of the individual bands have been observed in the gas phase by color-center laser absorption^{10,14,29}, by high resolution emission spectroscopy,²⁴ or by time-resolved emission spectroscopy.³⁰ Because of the extensive perturbations and because of the high energy input in the gas-phase studies, high ground state vibrational levels are prominent both in the gas phase^{10,14,19,26,27} and in an argon matrix.^{20,21}

Quasicontinuous 400–900 nm emission results on 136–110 nm photolysis of C_2H_2 or HCCBr in the gas phase.^{5,11,13,17} The fluorescence lifetimes vary from 6 to 20 μs .^{11,13,17} Unstructured emission from 1 to 5 μm has been detected¹⁸ upon 193-nm photolysis of gas-phase C_2H_2 , with maximum intensity between 3600 and 5000. The HCC fluorescence resulting from the 193-nm photolysis of HCCBr extends from 500 nm to 5 μm ,¹⁸ with lifetime increasing from ~ 5 μs near 500 nm to ~ 60 μs near 4000. Unstructured HCC emission between 400 and 500 nm has also been observed¹⁵ on vacuum UV irradiation of C_2H_2 isolated in the solid rare gases.

$\bar{X} \ ^2\Sigma^+$ $C_{\infty v}$ Structure: MW³¹

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

 $A = \sim 10$ IR¹⁴ $B_{000} = 1.457$ MW^{4,6,7,9} LMR¹² $B_{020} = 1.451$ LMR²⁸

DCC

 $\bar{A} \ ^2\Pi$ $T_0 < 3800$ Ar AB²¹

A complicated absorption band system extends to approximately 7500 in argon-matrix studies of DC₂.²¹ As for HC₂, the band system is extensively perturbed by high vibrational levels of the ground state. A few of the bands, some of which arise from excited ground-state vibrational energy levels, have been studied in the gas phase using color-center laser absorption.^{22,29}

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

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

 $B_0 = 1.203$ MW¹⁶

^cDerived from $(\nu_2 + \nu_3) - [(\nu_2 + \nu_3) - \nu_2]$. The detailed assignment of $(\nu_2 + \nu_3)$ is given in Ref. 27 and that of $(\nu_2 + \nu_3) - \nu_2$ in Ref. 26.

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HFeF

 $\bar{X}$

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

References

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

HFeCl

 $\bar{X}$

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

References

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

HFeBr

 $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		FeH stretch	1738	Kr	IR	1

References

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

HFeI

 $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		FeH stretch	1754	Ar	IR	1

References

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

HBO

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Π	2	Bend	754.42	gas	DL	6
			754m	Ar	IR	1
Σ^+	3	BO stretch	1825.56	gas	DL	2
			1817s	Ar	IR	1

 $B_0 = 1.308$ DL²MW^{3,4}

DBO

$\tilde{\nu}$	$C_{\infty v}$					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BD stretch	2253.53	gas	DL	5
			2259w	Ar	IR	1
Π	2	Bend	606m	Ar	IR	1
Σ^+	3	BO stretch	1647.69	gas	DL	5
			1648m	Ar	IR	1

$$B_0 = 1.049 \text{ gas MW}^4$$

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⁶J. E. Butler, unpublished data.

HBF⁺

$\tilde{\nu}$	$C_{\infty v}$	Structure: MW ^{2,3}				
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	BF stretch	1633.22	gas	DL	1

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

DBF⁺

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

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- ¹K. Kawaguchi and E. Hirota, *Chem. Phys. Lett.* **123**, 1 (1986).
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HCC⁻

Threshold for electron detachment from ground-state
 $HCC^- = 23950(50) \text{ gas PE}^1$

$\tilde{\nu}$	$C_{\infty v}$					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	505(20)	gas	PE	1
Σ^+	3	CC stretch	1800(20)	gas	PE	1

References

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

HCO⁺

$\tilde{\nu}$	$C_{\infty v}$	Structure: MW ²⁻⁴				
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3088.74	gas	LD,IB	5,6,15
Π	2	Bend	829.72	gas	DL	10,11
Σ^+	3	CO stretch	2183.95	gas	DL	7,8,14

$$B_0 = 1.488 \text{ MW}^{2-4}$$

DCO⁺

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

$$B_0 = 1.201 \text{ MW}^{2-4}$$

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HCS⁺

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

$$B_0 = 0.712 \text{ MW}^{1,2} \text{DL}^3 \text{CC}^{4,5}$$

References

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HN $\frac{1}{2}$

$\tilde{X}$	$C_{\infty v}$	Structure: MW ⁴ IR ¹⁰				
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ^+	1	NH stretch	3233.96	gas	CC,IB IR	5,11,12
Π	2	Bend	686.80	gas	DL	8,10
Σ^+	3	NN stretch	2257.87	gas	DL	6

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

DN $\frac{1}{2}$

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

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

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HOC⁺

$\tilde{X}$	$C_{\infty v}$	Structure: MW ¹⁻³				
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ^+	1	OH stretch	3268.03	gas	LD	4

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

DOC⁺

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

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HOSi⁺

$\tilde{X}$	$C_{\infty v}$	Structure: LD,DL ¹				
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ^+	1	OH stretch	3662.36	gas	LD	1
	3	SiO stretch	1127.01	gas	DL	2

$$B_0 = 0.609 \text{ LD}^1\text{DL}^2$$

DOSi⁺

$\tilde{X}$	$C_{\infty v}$					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ^+	1	OD stretch	2716.56	gas	LD	1
	3	SiO stretch	1103.11	gas	DL	2

$$B_0 = 0.541 \text{ LD}^1\text{DL}^2$$

References

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HCO

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

$T_0 =$	38695.5	gas	EM ⁶ LF ^{25,26}	$\tilde{B}-\tilde{X}$ 235–410 nm
	38595(35)	Ar	AB ^{5,11}	$\tilde{B}-\tilde{X}$ 210–260 nm
	38567(35)	CO	AB ⁵	$\tilde{B}-\tilde{X}$ 210–260 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	CH stretch	2589 ^a	gas	EM,LF	6,25,26
			2570(30)	Ar	AB	5,11
			2570(30)	CO	AB	5
2		~1375	gas	LF		25,26
		1375(35)	Ar	AB		5,11
		1375(35)	CO	AB		5
3		1058	gas	LF		25,26
		1035(35)	Ar	AB		5,11
		1035(35)	CO	AB		5

 $A_0 = 15.87$; $B_0 = 1.192$; $C_0 = 1.107$ LF²⁶ $\tau_0 \sim 50$ ns gas LF²⁶ $\tilde{A}^2A''(\Pi)$ $C_{\infty v}$

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

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

 $\tau_{090} = 46(4)$ ns LF¹⁵ $B_0 = 1.34$ UV^{1,3,8} $\tilde{X}^2A'$ C_s Structure: MW⁷UV⁸

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

 $A_0 = 24.329$; $B_0 = 1.494$; $C_0 = 1.399$ UV^{1,3,8}MW¹⁶

DCO

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

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

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

 $B_0 = 1.10$ UV^{1,3,8}

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

References

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HCF

 $\tilde{A}^1A''$ C_s Structure: AB¹LF^{5,6}

$T_0 =$	17277.47	gas	AB ¹ CL ³ LF ^{5,10}	$\tilde{A}-\tilde{X}$ 430–635 nm
	17320(15)	Ar	AB ²	$\tilde{A}-\tilde{X}$ 469–546 nm

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

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

 $A_0 = 25.69$; $B_0 = 1.162$; $C_0 = 1.107$ AB¹LF⁵ $\tau_0 = 2.45(10)$ μ s gas LF⁴ $\tau_1 = 2.57(16)$ μ s; $\tau_2 = 12.5(8)$ μ s gas EM¹³ $\tilde{a}^3A''$ C_s $T_0 < 5140(700)$ gas PE¹²

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

 $\tilde{X}^1A'$ C_s Structure: AB¹LF^{5,6}SEP¹¹

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
3	CF stretch		1406vw	Ar	SEP	11
			1180(30)	gas	PE	12
			1181.5m	Ar	IR	2

 $A_0 = 15.563$; $B_0 = 1.223$; $C_0 = 1.130$ AB¹LF⁵SEP¹¹

DCF

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

$T_0 =$	17293.426(3)	gas	CL ³ LF ⁶	$\tilde{A}-\tilde{X}$ 460–585 nm
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Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	2	Bend	780(5)	gas	CL	3

 $A_0 = 15.10$; $B_0 = 1.014$; $C_0 = 0.945$ LF⁶

$\tilde{a}^3A'$ C_s $T_0 < 5140(700)$ gas PE¹²

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	2	Bend	820(50)	gas	PE	12
	3	CF stretch	1170(50)	gas	PE	12

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	2	Bend	1046m	Ar	IR	2
	3	CF stretch	1190(30)	gas	PE	12
			1183m	Ar	IR	2

 $A_0 = 8.828$; $B_0 = 1.120$; $C_0 = 0.990$ LF⁶

References

- ¹¹T. Suzuki and E. Hirota, J. Chem. Phys. **88**, 6778 (1988).
¹²K. K. Murray, D. G. Leopold, T. M. Miller, and W. C. Lineberger, J. Chem. Phys. **89**, 5442 (1988).
¹³T. Ibuki, A. Hiraya, K. Shobatake, Y. Matsumi, and M. Kawasaki, J. Chem. Phys. **92**, 4277 (1990).

HCCI

 $\tilde{a}^3A''$ C_s $T_0 < 3990(1050)$ gas PE⁵

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

 $\tilde{X}^1A'$ C_s Structure: AB¹LF³

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	2	Bend	1201wm	Ar	IR	2
	3	CCl stretch	810(30)	gas	PE	5
			815s	Ar	IR	2

 $A_0 = 15.759$; $B_0 = 0.605$; $C_0 = 0.581$ AB¹LF³

References

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

HCB^r $\tilde{a}^3A''$ C_s $T_0 < 3150(700)$ gas PE¹ $\tilde{X}^1A'$ C_s

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

References

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

HCl

 $\tilde{a}$ C_s $T_0 < 3150(700)$ gas PE¹ $\tilde{X}$ C_s

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

References

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

HNO

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

$T_0 = 13154.4$ gas AB^{1,4}LF^{13,20} $\tilde{A}-\tilde{X}$ 550–770 nm
 13118(2) Ar AB^{2,3} $\tilde{A}-\tilde{X}$ 590–762 nm
 Onset of predissociation at 16450(10) LF¹³

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

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

DNO

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

$T_0 = 13180.3$ gas AB¹ $\tilde{A}-\tilde{X}$ 550–770 nm
 Onset of predissociation at 17010(10) LF^{18,19}

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

 $\tau_{011} = 32.4(1.6)$ μ s gas LF²² $A_0 = 12.630$; $B_0 = 1.199$; $C_0 = 1.088$ AB^{1,4}

References

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

HCF⁻

Threshold for electron detachment from ground-state HCF⁻ = 4490(40) gas PE¹

$\tilde{X}^2A''$	C_s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	3	CF stretch	745(30)	gas	PE	1

DCF⁻

$\tilde{X}^2A''$	C_s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	3	CF stretch	730(30)	gas	PE	1

References

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

HCCI⁻

Threshold for electron detachment from ground-state HCCI⁻ = 9790(40) gas PE¹

$\tilde{X}^2A''$	C_s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	3	CCl stretch	470(30)	gas	PE	1

References

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

HCB⁻

Threshold for electron detachment from ground-state HCB⁻ = 12550(65) gas PE¹

$\tilde{X}^2A''$	C_s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	3	CBr stretch	430(40)	gas	PE	1

References

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

HCl⁻

Threshold for electron detachment from ground-state HCl⁻ = 13580(100) gas PE¹

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	3	CI stretch	350(40)	gas	PE	1

References

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

HNO⁻

Threshold for electron detachment from ground-state HNO⁻ = 2730(120) gas PE¹

$\tilde{X}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	1	NH stretch	2750.78	gas	PD	2
	3	NO stretch	1153(170)	gas	PE	1

$A_0 = 15.233$; $(B_0 + C_0)/2 = 1.097$; $(B_0 - C_0)/2 = 0.034$ PD²

DNO⁻

Threshold for electron detachment from ground-state DNO⁻ = 2660(120) gas PE¹

$\tilde{X}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	3	NO stretch	1113(170)	gas	PE	1

References

¹H. B. Ellis, Jr., and G. B. Ellison, J. Chem. Phys. **78**, 6541 (1983).

²H. C. Miller, J. L. Hardwick, and J. W. Farley, J. Mol. Spectrosc. **134**, 329 (1989).

HO₂

$\tilde{X}^2A''$ C_s Structure: MW¹⁴UV²¹LMR²³ESR²³ IR^{31,33}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	1	OH stretch	3436.20	gas	LD	26
			3415.1	Ne	IR	36
			3412.5s ^a	Ar	IR	1,4,7
			3400	O ₂	IR	32
	2	Bend	1391.75	gas	DL	24
			1397.8	Ne	IR	36
			1388.5vs ^a	Ar	IR	1,4,7
			1392	O ₂	IR	32
	3	OO stretch	1097.63	gas	LMR	18
					DL	29,30
			1100.3	Ne	IR	36
			1101.1s ^a	Ar	IR	1,4,7
			1109	O ₂	IR	32

$A_0 = 20.356$; $B_0 = 1.118$; $C_0 = 1.056$ LMR^{5,11,12,18}MW^{13,17,25}EM¹⁶

DO₂

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

$A_0 = 11.194$; $B_0 = 1.056$; $C_0 = 0.961$ MW^{14,27,34}EM²¹LMR^{22,23,34}ESR²³

^aRefined value from unpublished Fourier transform spectra.

References

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

DSO

$\tilde{A}^2A'$ C_s
 $T_0 = 14371$ gas CL¹LF^a $\tilde{A}-\tilde{X}$ 520-960 nm

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

$\tau^a = 76 \mu s$ gas LF⁶

$A_0^b = 4.969(7)$; $B_0^b = 0.566$; $C_0^b = 0.507$ LF^{7,8}

^aMeasured at 606.0 nm.

^bExtrapolated from values for 021 and 022.

References

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

HOI

$\tilde{X}$		C_s				
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	OH stretch	3597m	N ₂	IR	1
	2	Bend	1075	Ar	IR	1
3	OI stretch		1103m	N ₂	IR	1
			577	Ar	IR	1
			575m	N ₂	IR	1

DOI

$\tilde{X}$		C_s				
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	OD stretch	2653	N ₂	IR	1
	2	Bend	808	N ₂	IR	1
	3	OI stretch	571	N ₂	IR	1

References

¹N. Walker, D. E. Tevault, and R. R. Smardzewski, J. Chem. Phys. **69**, 564 (1978).

HS₂⁻

Threshold for electron detachment from ground-state HS₂⁻ = 15390(185) gas PE¹

$\tilde{X}$		C_s				
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	3	SS stretch	610(80)	gas	PE	1

DS₂⁻

Threshold for electron detachment from ground-state DS₂⁻ = 15430(120) gas PE¹

$\tilde{X}$		C_s				
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	3	SS stretch	580(90)	gas	PE	1

References

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

FHF⁻

$\tilde{X}$		$D_{\infty h}$ Structure: DL ⁵				
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	583.05	gas	DL	5
Π_u	2	Bend	1286.03	gas	DL	5
			1217m	Ar ^a	IR	1,2
Σ_u^+	3	Asym. stretch	1331.15	gas	DL	5
			1379	Ne	IR	4
			1377.0s	Ar	IR	3,4
			1364vs	Ar ^a	IR	1,2

$B_0 = 0.334$ DL⁵

FDF⁻

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

^aCs⁺ in adjacent site.

References

- ¹B. S. Ault, J. Phys. Chem. **82**, 844 (1978).
²B. S. Ault, J. Phys. Chem. **83**, 837 (1979).
³S. A. McDonald and L. Andrews, J. Chem. Phys. **70**, 3134 (1979).
⁴R. D. Hunt and L. Andrews, J. Chem. Phys. **87**, 6819 (1987).
⁵K. Kawaguchi and E. Hirota, J. Chem. Phys. **87**, 6838 (1987).

ClHCl⁻

An absorption maximum which appeared at 287 nm in argon-matrix studies² of the 122-nm photolysis of Ar:HCl or Ar:H₂O:Cl₂ samples and in argon-matrix studies⁶ of the electron bombardment of Ar:HCl samples has been assigned to an electronic transition of ClHCl⁻.

$\tilde{X}$	$D_{\infty h}$	Structure:	DL ⁵			
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	260 ^{ab}	Ar	IR	1-3
Σ_u^+	3	Asym. stretch	722.90 696s ^a	gas Ar	DL IR	5 1-3

$B_0 = 0.0974$ DL⁵

ClDCI⁻

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

^aAttributed 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 ³⁷Cl + H³⁵Cl reaction for vibrationally excited HCl⁴ indicates that there is a potential barrier, rather than a minimum, for the ClHCl neutral species.

^bAssignment deduced from weak to moderately intense combination with 696 cm⁻¹ fundamental that appears at 956 cm⁻¹.

^cAssignment deduced from weak to moderately intense combination with 463 cm⁻¹ fundamental that appears at 730 cm⁻¹.

References

- ¹P. N. Noble and G. C. Pimentel, J. Chem. Phys. **49**, 3165 (1968).
²D. E. Milligan and M. E. Jacox, J. Chem. Phys. **53**, 2034 (1970).
³C. A. Wight, B. S. Ault, and L. Andrews, J. Chem. Phys. **65**, 1244 (1976).
⁴M. Kneba and J. Wolfrum, J. Phys. Chem. **83**, 69 (1979).
⁵K. Kawaguchi, J. Chem. Phys. **88**, 4186 (1988).
⁶J. Hacaloglu and L. Andrews, Chem. Phys. Lett. **160**, 274 (1989).

6.3. Triatomic Nonhydrides

Li₃

$2^2E'$	D_{3h}^a					
$T_0 = 14583$	gas	MPI ²				$2^2E'-\tilde{X}$ 660-690 nm
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	326	gas	MPI	2

$\tilde{X}$	D_{3h}^a					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	303	Xe	Ra	1

^aSubject to dynamic Jahn-Teller distortion. Structure in the $2^2E'$ state is characterized by a radial frequency $\omega_0 = 191$ and linear and quadratic Jahn-Teller parameters $k = 0.77$ and $g = 0.15$. In the $\tilde{X}$ state, as well, a complicated pattern of absorptions accompanies the absorption attributed to ν_1 .

References

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

Na₃

Evidence for a predissociated state near 420 nm was obtained from the depletion of the single-photon ionization signal of Na₃⁺, with a corresponding increase in the Na₃⁺ signal, as this region was scanned by a second laser.^{4,5}

$\tilde{C}^2E''$	D_{3h}^a					
$T_0 = 20813$	gas	MPI ^{2,4,6,8} PF ⁸				$\tilde{C}-\tilde{X}$ 467-481 nm
Higher vibrational bands are predissociated. ⁷						

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

Extensive vibronic structure has been tentatively assigned⁸ to energy levels derived from excitation of ν_2 (e'), perturbed by dynamic Jahn-Teller interaction.

$\tau_0 = 7(3)$ ns gas MPI⁷

$\tilde{B}, \tilde{B}'^2E'$	D_{3h}^a					
$T_0 = 15996$	gas	MPI ¹⁻⁶				$\tilde{B}, \tilde{B}'-\tilde{X}$ 550-625 nm
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	127	gas	MPI	1,3

$\tau(\tilde{B}, 16255) = 14(5)$ ns gas MPI⁷
 $\tau(\tilde{B}', 17418) = 7(3)$ ns gas MPI⁷

Vibronic pseudorotation accompanied by fractional quantization occurs.³

$\bar{A}^2E''$ D_{3h}^a $T_0 = 14896.5$ gas MPI^{1,2,4-6} $\bar{A}-\bar{X}$ 660–675 nm

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

 $\tau_0 = 60(10)$ ns gas MPI⁷ **$\bar{X}^2E'$** D_{3h}^a

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

^aDistorted by Jahn-Teller interaction.

References

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

Ag₃In argon, krypton, and xenon matrices, absorption bands near 40660, 43130, and 45020 have been attributed^{2,3} to Ag₃. **$^2E''$** D_{3h}^a $T_0 = 26971(10)$ gas MPI⁴

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'_1	1	Sym. stretch	158.2(1.9)	gas	MPI	4

Extensive vibronic structure has been assigned⁴ to energy levels derived from excitation of ν_2 (e'), perturbed by dynamic Jahn-Teller interaction.In argon, krypton, and xenon matrices, an absorption maximum near 23700 has been attributed^{2,3} to Ag₃. **$\bar{X}^b$**

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

^aDistorted by Jahn-Teller interaction.^bPossibly the ground state of a linear isomer.

References

- ¹W. Schulze, H. U. Becker, R. Minkwitz, and K. Manzel, Chem. Phys. Lett. **55**, 59 (1978).
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⁴K. LaiHing, P. Y. Cheng, and M. A. Duncan, Z. Phys. D **13**, 161 (1989).

Sc₃ **$\bar{X}^2E'$?** D_{3h}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'_1	1	Sym. stretch	248	Ar	Ra	1
e'	2	Bend	~150	Ar	Ra	1

References

- ¹M. Moskovits, D. P. DiLella, and W. Limm, J. Chem. Phys. **80**, 626 (1984).

Mn₃A broad absorption with maximum near 14750 (678 nm) has been assigned¹ to Mn₃ isolated in an argon matrix. **$\bar{X}$** D_{3h}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'_1	1		196	Ar	Ra	1
e'	2		124 ^a	Ar	Ra	1

^aStructure due to Jahn-Teller interaction observed.

References

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

Ni₃In an argon matrix, an absorption maximum at 420 nm has been attributed¹ to Ni₃. **$\bar{A}$**

gas LF³ $\bar{A}-\bar{X}$ 455–470 nm
 $T_0 = 20820$ Ar AB¹ $\bar{A}-\bar{X}$ 449–481 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
1		Sym. stretch	205(5)	gas	LF	3
			202	Ar	AB	1
2		Bend	90(5) ^a	gas	LF	3

$\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
	1	Sym. stretch	230(5)	gas	LF,PE	3,4
			232	Ar	Ra	2
	2	Bend	100(5) ^a	gas	LF	3

^aTentative assignment.

References

- ¹M. Moskovits and J. E. Hulse, *J. Chem. Phys.* **66**, 3988 (1977).
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³J. R. Woodward, S. H. Cobb, and J. L. Gole, *J. Phys. Chem.* **92**, 1404 (1988).
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 Pd_3

Structure in the photoelectron spectrum¹ of Pd_3 can be interpreted in terms of an electronic state with origin < 720(30) and with vibrational spacings of approximately 230. There may also be an electronic state near 1900, as well as one near 2570. A series of bands with a spacing of approximately 210 appears above the band at 2570.

References

- ¹K. M. Ervin, J. Ho, and W. C. Lineberger, *J. Chem. Phys.* **89**, 4514 (1988).

 Pt_3

The photoelectron spectrum of Pt_3 suggests¹ that Pt_3 may possess an electronic state 1225(30) above the ground-state. Structure may be contributed by a short vibrational progression with spacings of approximately 180 or by other low-lying electronic states.

 $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		Sym. stretch	225(30) ^a	gas	PE	1
		Bend	105(30)	gas	PE	1

^aIn an alternate assignment, this band is contributed by a low-lying electronic state.

References

- ¹K. M. Ervin, J. Ho, and W. C. Lineberger, *J. Chem. Phys.* **89**, 4514 (1988).

 Al_3

$T_0^a = 16610$ gas MPI¹ 516–602 nm

Overlapping continuum with high-frequency edge at 19378(10). This continuum may be associated with unresolved high vibrational levels of another electronic state.

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
1			270.6	gas	MPI	1
2			205	gas	MPI	1

Lifetimes (possibly radiative) vary¹ from 98 to 21 μs .

 $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			132.6(8)	gas	MPI	1

^aPossibly a 1 $\bar{g}$ band.

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

BBO

A

 $C_{\infty v}$

$T_0 = 16301$ gas CL¹ $\bar{A}-\bar{X}$ 590–695 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ^+	3	BB stretch	437	gas	CL	1

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ^+	3	BB stretch	583	gas	CL	1

References

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 C_3 $^1\Sigma_g^+$ $D_{\infty h}$

$T_0 = 52826(30)$ Ar AB¹⁵ 170–190 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1080(30)	Ar	AB	15
Π_u	2	Bend	300(30) ^a	Ar	AB	15
Σ_u^+	3	Asym. stretch	780(30) ^{ab}	Ar	AB	15

 $\bar{B}$

In 2-photon ionization studies of jet-cooled C_3 , a complicated group of bands, all with rotational structure appropriate for a $\Sigma_u^+ - \Sigma_g^+$ vibronic transition arising from the $\bar{X}$ state, has been observed between 266 and 302 nm.²⁰ Lifetimes of these bands range from 0.4 to 2.5 μs , and the B' value for the first intense band, at 33153(5), is 0.396(3). These same bands, as well as bands at somewhat lower energies (possibly below the ionization threshold) and some bands arising from a $\Sigma_u^+ - \Pi_g$ vibronic transition, have also been studied using LF measurements on cooled beams.²³

$\tilde{A}^1\Pi_u$	$D_{\infty h}$	Structure: UV ⁶
$T_0 = 24675.5$	gas	EM ^{1,2,6} AB ^{3,6,9} LF ^{17,23} $\tilde{A}-\tilde{X}$ 340–640 nm
24640	Ne	AB ^{4,5,8} EM ⁵ LF ¹¹ $\tilde{A}-\tilde{X}$ 347–488 nm
24370 ^c	Ar	AB ^{4,5,7} LF ¹¹ $\tilde{A}-\tilde{X}$ 352–411 nm
24350	Kr	AB ⁷
23610	Xe	AB ^{4,7}
24635	N ₂	AB ⁷

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1085.9	gas	AB	6
			1094(6)	Ne	AB	5
			1093(6)	Ar	AB	5,7
			1090	Kr	AB	7
			1120	Xe	AB	7
			1050	N ₂	AB	7
Π_u	2	Bend	307.9 ^d	gas	AB	6
Σ_u^+	3	Asym. stretch	~840 ^a	Ne	AB	8

$\tau_0 = 200(10)$ ns gas LF^{12,13}

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

$B_0 = 0.430$ UV⁶

$\tilde{a}^3\Pi_u$	$D_{\infty h}$	Structure: UV ⁶
$T_0 = 17080$	Ne	EM ⁵ LF ¹¹ $\tilde{a}-\tilde{X}$ 585–631 nm
16930	Ar	EM ⁵
$\tau \sim 0.02$ s	Ne	EM ⁵

$\tilde{X}^1\Sigma_g^+$ $D_{\infty h}$ Structure: UV⁶

This state of C₃ is highly anharmonic. The term values of 144 excited vibrational energy levels have been determined in SEP²¹ and LF²³ studies.

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1224.5	gas	AB,LF	9,17,23
			1226	Ne	EM	5
			1207 ^e	Ar	IR	19
			1234 ^c	N ₂	IR	19
Π_u	2	Bend	63.7 ^f	gas	UV,DL	6,22,23
			~70 ⁸	Ne,Ar	SEP	24
					AB	5
Σ_u^+	3	Asym. stretch	2040.02	gas	IR,DL	16,18
					LF	23
			2042	Ne	IR	4
			2038s	Ar	IR	4,10
			2031	N ₂	IR	19

$B_0 = 0.430$ UV⁶IR¹⁶DL¹⁸

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

^bAlternate assignment gives 1320.

^cIn the LF studies,¹¹ a second site was observed with $T_0 = 24408$.

^d 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. Ref. 14 also gives a more detailed analysis of electronic orbital angular momentum effects in the gas-phase molecule.

^e $(\nu_1 + \nu_3) - \nu_3$.

^f~45 in X(011).²²

^gGreatly broadened in a rare-gas matrix by interaction with lattice modes.¹¹

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SiCC

$\tilde{A}^1B_2$	C_{2v}	Structure: PI ⁵ AB ¹¹
$T_0 = 20085.505$	gas	EM ¹ AB ^{3,11} LF ⁴ $\tilde{A}-\tilde{X}$ 402–507 nm
20142	Ne	AB ² LF ⁴ $\tilde{A}-\tilde{X}$ 409–611 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	CC stretch	1464	gas	EM,AB	1,3,4
					LF	11
				Ne	AB,LF	2,4
				Ar	AB	9
	2	CSi s-stretch	1462	gas	AB,LF	3,4
			1011	Ne	AB,LF	2,4
			1021	Ar	AB	9
b_2	3	CSi a-stretch	228 ^a	gas	EM,AB	1,3,4
					LF	11
			231 ^a	Ne	AB,LF	2,4
			224 ^a	Ar	AB	9

$\tau_0 = 370$ ns gas LF⁴

310 ns Ne LF⁴

$A_0 = 1.589$; $B_0 = 0.411$; $C_0 = 0.324$ AB¹¹

$\tilde{X}^1A_1$	C_{2v}	Structure: $PI^5MW^{6,7}AB^{11}$				
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CC stretch	1742	gas	EM	1
			1746s	Ne	IR,LF	2,4
			1741.3	Ar	IR	8,14
	2	CSi s-stretch	837	gas	EM	1,10
b_2	3	CSi a-stretch	836m	Ne	IR,LF	2,4
			824.3	Ar	IR	8,14
			177 ^a	gas	LF	4
			186(11)	gas	MW	13
			172 ^a	Ne	LF	4
			160.4	Ar	IR	14

$A_0 = 1.750$; $B_0 = 0.439$; $C_0 = 0.348$ $MW^{6,7,12,13}AB^{11}$

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

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Si₂C

$\tilde{X}$	C_{2v}	Structure: IR^1				
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	658wm	Ar	IR	1
b_2	3	Asym. stretch	1189s	Ar	IR	1

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AICO

$\tilde{X}$	C_{2v}	Structure: IR^1				
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1872s	Ar	IR	1

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CCN

$\tilde{A}^2\Delta$	$C_{\infty v}$	Structure: $AB^1LF^4EM^9$				
$T_0 =$	21259.203	gas	AB ¹ LF ⁴ EM ⁹	$\tilde{A}-\tilde{X}$ 376–471 nm		
	21377	Ar	LF ² AB ³	$\tilde{A}-\tilde{X}$ 373–550 nm		
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Stretch	1770.77	gas	AB	1
			1732(2)	Ar	LF	2
Π	2	Bend	~ 475	gas	AB	1
Σ^+	3	Stretch	1241.64	gas	AB	1
			1225(2)	Ar	LF	2

$\tau = 170$ ns Ar LF²

$A_{eff} = -0.807$ gas AB¹LF^{4,6}

$B_0 = 0.414$ AB¹LF^{4,6}MODR⁷

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Stretch	1923.25	gas	LF,EM	5,8,9
			1717	Ar	LF	2
Π	2	Bend	324	gas	AB,LF	1,8
Σ^+	3	Stretch	1050.76	gas	LF,EM	5,8,9
			1066	Ar	LF	2

$A = 41.76$; $\epsilon\omega_2 = 132.8$ gas LF⁸

$B_0 = 0.398$ AB¹LF^{4,6}

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NCN

$\tilde{A}^2\Pi_u$	$D_{\infty h}$	Structure: AB^1				
$T_0 =$	30383.74	gas	AB ¹	$\tilde{A}-\tilde{X}$ 326–329 nm		

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1254(5)	gas	LF	8
Π_u	2	Bend	460(50)	gas	AB	1

$A = -37.56$; $\epsilon\omega_2 = -85.7^b$ gas AB¹

$\tau_0 = 183(6)$ ns gas LF⁸

$B_0 = 0.396$ AB¹

References

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CNN

An absorption which appears in a nitrogen matrix at 51070 when a high concentration of CNN is present has been tentatively attributed to this species.¹⁰

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

$T_0 =$	48540(50)	Ar	AB ¹⁰	$\tilde{C}-\tilde{X}$ 206 nm
	49100(50)	N ₂	AB ¹⁰	$\tilde{C}-\tilde{X}$ 203.7 nm

$B^2\Sigma^- ?$ $C_{\infty v}$						
$T_0 <$	39950	Ar	AB ¹⁰		$\tilde{B}-\tilde{X}$ 210-251 nm	
	39850	N ₂	AB ¹⁰		$\tilde{B}-\tilde{X}$ 210-251 nm	
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ^+		Stretch	1450(40) ^a	Ar, N ₂	AB	10
		Stretch	990(40)	Ar, N ₂	AB	10
$A^2\Pi$ $C_{\infty v}$						
$T_0 =$	23850 ^b	gas	AB ⁶ LF ¹¹		$\tilde{A}-\tilde{X}$ 395-420 nm	
	23750	Ne	AB ⁵		$\tilde{A}-\tilde{X}$ 397-420 nm	
	23830					
	23597	Ar	AB ^{2,3} LF ^{8,9}		$\tilde{A}-\tilde{X}$ 401-424 nm	
	23865	N ₂	AB ^{2,3}		$\tilde{A}-\tilde{X}$ 396-419 nm	
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ^+	1	"Sym." stretch	1325(10)	Ne	AB	5
			1322(2)	Ar	AB, LF	2,3,8,9
			1335(10)	N ₂	AB	2,3
Π	2	Bend	525(2)	Ar	LF	8
Σ^+	3	"Asym." stretch	1807(2)	Ar	LF	8
$\tau_0 = 250(30)$ ns						
$A = -26.5^b$		Ar	LF ^{8,9}			
$A = 9; \epsilon = -0.07$		gas	LF ¹¹			
$B_0 = 0.425(10)^b$		Ar	LF ⁸			
			LF ¹¹			
$X^2\Sigma^- ?$ $C_{\infty v}$ Structure: ESR ¹						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ^+	1	CN stretch	2824	Ar	LF	8
			2847m	Ar ^c	IR	3
			2856m	N ₂	IR	3,4,7,12
Π	2	Bend	394	Ar	LF	8
			393	Ar ^c	IR	3
			394	N ₂	IR	4,7
Σ^+	3	NN stretch	1235	Ne	EM	5
			1235	Ar	LF	8
			1241	Ar ^c	IR	3
			1252	N ₂	IR	3,4,7
$B_0 = 0.414(10)^b$ LF ¹¹						

$B_0 = 0.414(10)^b$ LF¹¹

^aPossibly 2440(40).¹⁰

^bApproximate value, used in simulation.

^cN₂ trapped in adjacent site.

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BO₂

$A^1\Pi_u$			$D_{\infty h}$	Structure: UV ¹		
$T_0 =$	18291.597	gas	UV ¹ LF ^{3-5,14}		$\tilde{A}-\tilde{X}$ 396-700 nm	
	17915 ^c	Ar	AB ²		$\tilde{A}-\tilde{X}$ 423-558 nm	
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	994	gas	UV	1
Π_u	2	Bend	477.29	gas	UV,LF	1,14
Σ_u^+	3	Asym. stretch	2357 ^b	gas	UV	1
$\tau_0 = 91(4)$ 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}				
$X^2\Pi_g$			$D_{\infty h}$	Structure: UV ¹		
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1056.4	gas	UV,LF	1,3-5
Π_u	2	Bend	448.18 ^d	gas	UV,LF	1,3-5
Σ_u^+	3	Asym. stretch	1278.26	gas	DL,IR	8,12
			1276	Ar	IR	2
$A = -148.6$; $\epsilon\omega_2 = -86.91$						
$B_0 = 0.329$		UV ¹ LF ^{3,7,13,14}	DL ⁸ IR ¹²	UV ¹ LF ^{3,7,14}		

^aEstimated from isotopic shifts.

^b $\frac{1}{2}(2\nu_2)$.

^cIndependent 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 R₁ branch band head.

^dBand origin of (010)κ²Σ[−] — (000)²Π_{3/2} vibration rotation transition observed¹¹ at 633.8049(9) using diode laser spectroscopy.

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NCO

$\tilde{A}^2\Sigma^+$	$C_{\infty v}$	Structure: UV ²⁰				
$T_0 = 22754.0$		gas	AB ¹	$\tilde{A}-\tilde{X}$	360–450 nm	
22800(10)		Ne	AB ³	$\tilde{A}-\tilde{X}$	398–440 nm	
22712(2)		Ar	LF ⁸	$\tilde{A}-\tilde{X}$	390–530 nm	
22956(10)		N ₂	AB ³	$\tilde{A}-\tilde{X}$	395–440 nm	

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ^+	1	Stretch	2338.0	gas	UV	1
			2325(20)	Ne	UV	3
			2332(4)	Ar	UV,LF	3,8
			2321(20)	N ₂	UV	3
Π	2	Bend	680.8	gas	UV	1
			673(20)	Ne	UV	3
Σ^+	3	Stretch	1289.3 ^a	gas	UV	1
			1270(20)	Ne	UV	3
			1291(4)	Ar	UV,LF	3,8

$\tau_0 = 435(10)$ 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	1272.97 ^b	gas	LF,LMR	14,15
						17,19
			1275vw	Ar	IR,LF	3,8
Π	2	Bend	535.4	gas	UV,LF	1,7,15
			529.5 ^c	Ar	LF	8
Σ^+	3	Asym. stretch	1921.30	gas	LMR	10,14
					LF,DL	15,21
			1923m	Ar	IR,LF	3,8
			1935	N ₂	IR	3

$A_{010} = -94.19$; $\epsilon\omega_2 = -76.9$ gas UV⁷

$B_0 = 0.390$ UV¹MW¹⁶LMR²²

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NCS

$\tilde{B}^2\Sigma^+$	$C_{\infty v}$					
$T_0 = 26971.01$	gas	EM ¹ AB ² LF ⁴		$\tilde{B}-\tilde{X}$	353–485 nm	
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Π	2	Bend	343(10)	gas	AB	2
Σ^+	3	CS stretch	921.5	gas	LF	4
$\tau_{001} = 225(5)$ 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		$\tilde{A}-\tilde{X}$	337–417 nm	

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ^+	1	CN stretch	1916.18(3)	gas	AB	2
Π	2	Bend	378(10)	gas	AB	2
Σ^+	3	CS stretch	755.28(3)	gas	AB	2

$\tau_0 = 160(5)$ ns	gas	LF ^{3,4} EF ⁶				
$A = -91.58(1)$; $ \epsilon\omega_2 = 103(5)$	gas	AB ² LF ⁴				
$B_0 = 0.193$ AB ² LF ⁴						

$\tilde{X}^2\Pi$	$C_{\infty v}$	Structure: AB ²				
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ^+	1	CN stretch	1942.2	gas	LF	4
Π	2	Bend	387(10)	gas	AB,LF	2,4
Σ^+	3	CS Stretch	765.8	gas	SEP	5

$A = -323.4$; $|\epsilon\omega_2| = 55(15)$ gas AB²LF⁴
 $B_0 = 0.206$ AB²LF⁴

References

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CO₂

$\tilde{C}^2\Sigma_g^+$	$D_{\infty h}$	Structure: MP ²³				
$T_0 = 45157(3)$	gas	TPE ²⁰ PE ²² MP ²³		$\tilde{C}-\tilde{A}$	585–640 nm	

The band origin is perturbed by another state of $^2\Sigma_g^+$ symmetry at 45188 which has a rotational constant of 0.353.²³ This state may be an excited vibrational level of the $\tilde{A}$ or $\tilde{B}$ state.

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1352(4) ^a	gas	PE	22
Π_u	2	Bend	614(4)	gas	TPE,PE	20,22
Σ_u^+	3	Asym. stretch	1567(4)	gas	PE	22

$B_0 = 0.395$ MP²³

$\tilde{B}^2\Sigma_g^+$	$D_{\infty h}$	Structure: EM ⁹				
$T_0 = 34597.9$	gas	EM ^{1,9}		$\tilde{B}-\tilde{X}$	287–291 nm	
Perturbations by the $\tilde{A}$ state are considered in Refs. 14–16.						

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1275(1)	gas	TPE,PE	20,22
Π_u	2	Bend	557(4)	gas	EM,PE	9,22
Σ_u^+	3	Asym. stretch	1840(5)	gas	TPE,PE	20,22

$\tau_0 = 140(7)$ ns gas T-PEFCO¹⁰PEFCO¹³LF¹⁶
 $B_0 = 0.378$ EM¹

$\bar{A}^2\Pi_u$ $D_{\infty h}$ Structure: EM^{11}
 $T_0 = 28500.5$ gas $EM^{2,11}$ $\bar{A}-\bar{X}$ 290–490 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1126	gas	EM	2,5,11
Π	2	Bend	461	gas	EM, PE	11,22
Σ_u^+	3	Asym. stretch	2731	gas	EM	6

$\tau_0 = 102(8)$ ns gas EF^7T -PEFCO¹⁰
 $124(6)$ ns gas $PEFCO^{13}HFD^{17}$
 $A = -95.86$; $\epsilon\omega_2 = -42.6$ gas EM^{11}
 $B_0 = 0.350$ $EM^{2,11}$

$\bar{X}^2\Pi_g$ $D_{\infty h}$ Structure: $EM^{2-5,9,11}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1244.3(3)	gas	EM, DL	4,5,8, 12,21
Π_u	2	Bend	511.4(3)	gas	EM, DL	11,19, 21
Σ_u^+	3	Asym. stretch	1423.08	gas	DL	18
			1421.7	Ne	IR	24

$A = -161.02(6)^b$ $\epsilon\omega_2 = -98.8(3)^b$ gas $EM^{1,9,11}DL^{19,21}$
 $B_0 = 0.380$ $EM^{1,3,9,11}$

^aCorrected for Fermi resonance.

^bReanalysis by Ref. 25 gives $A = -161.48(5)$ and $\epsilon\omega_2 = -100.4$.

References

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²⁴M. E. Jacox and W. E. Thompson, *J. Chem. Phys.* **91**, 1410 (1989).
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OCS⁺

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

$T_0 = 54640(30)$ 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

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

$T_0 = 39180(20)$ 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

$\bar{A}^2\Pi_{3/2}$ $C_{\infty v}$

$T_0 = 31404.099(7)$ gas $EF^1LF^8PF^9$ $\bar{A}-\bar{X}$ 318–432 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	2036(6)	gas	PE	10
Π	2	Bend	336(20) ^b	gas	PE	10
Σ^+	3	CS stretch	803.8 ^c	gas	PF	9

$\tau_0 = 93(9)$ ns^d gas $PEFCO^5$
 $\tau_0(\Omega = 3/2) = 105(3)$ ns; $\tau_0(\Omega = 1/2) = 77(3)$ ns gas HFD^6EF^7
 $A = -111.8$ gas EF^1PF^9
 $B_0 = 0.187$ LF^8

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CS stretch	695.7 ^c	gas	PF	9
Π	2	Bend	476(16)	gas	PE	10
Σ^+	3	CO stretch	2038.98 ^f	gas	DL	11

$A = -367.2$ gas EF^1PF^9

$B_0^f = 0.201$ DL^{11}

^aRef. 10 gives value of 742(7).

^b $\frac{1}{2}(2\nu_2)$.

^c816.9 for $\Omega = 1/2$.⁹

^dAbsence of emission from states above the $\bar{A}^2\Pi$ band origin in photoionization experiments² suggested that the molecule is predissociated into $CO + S^+$ ($^4S^o$), as was later confirmed.³ PEFCO studies⁵ have yielded the branching ratio for photoexcitation vs. predissociation for the transition origin, permitting an estimate of 550(50) ns for the radiative lifetime.

^e699.7 for $\Omega = 1/2$.⁹

^fMeasured for $\Omega = 1/2$.

References

- ¹⁰L.-S. Wang, J. E. Reutt, Y. T. Lee, and D. A. Shirley, *J. Electron Spectrosc. Relat. Phenom.* **47**, 167 (1988).
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CS $\frac{1}{2}$

$\bar{C}^2\Sigma_g^+$ $D_{\infty h}$ Structure: MP^{15}

$T_0 = 49064$ gas $PI^4PF^{13}MP^{15}$ $\bar{C}-\bar{B}$ 658–724 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	652(2)	gas	PI, PE	5,9,11
Π_u	2	Bend	348(9)	gas	PF, MP	13–15
Σ_u^+	3	Asym. stretch	1024(6)	gas	PE	14

$\tau_0 = 11(2)$ ps gas MP^{15}
 $B_0 = 0.111$ $PF^{13}MP^{15}$

$\tilde{B}^2\Sigma^+_g$	$D_{\infty h}$	Structure: EM^1
$T_0 = 35238.01$	gas	$EM^1 \quad \tilde{B}-\tilde{X} \text{ 277-307 nm}$
35270	Ne	LF^7
35226		

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+_g	1	Sym. stretch	602 ^b	gas	EM	3
Π_u	2	Bend	351(5)	gas	PE	14
Σ^+_u	3	Asym. stretch	1320(5) ^c	gas	PE	14

$\tau_0 = 290(10) \text{ ns}$ gas $EF^2PIFCO^4PEFCO^8UV^{12}$

There is also a long-lifetime component, with $\tau = 1.44(22) \mu s$.^{8,12}

$B_0 = 0.108 \text{ EM}^1$

$\tilde{A}^2\Pi_u$	$D_{\infty h}$	Structure: EM^3
$T_0 = 20975$	gas	$EM^3 \quad \tilde{A}-\tilde{X} \text{ 426-512 nm}$
21017	Ne	$LF^{6,7} \quad \tilde{A}-\tilde{X} \text{ 400-638 nm}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+_g	1	Sym. stretch	$\sim 610^a$	gas	EM	3
			621	Ne	LF	6,7
Π_u	2	Bend	$\sim 275^c$	gas	EM	3
			280 ^c	Ne	LF	6,7
Σ^+_u	3	Asym. stretch	1644 ^c	Ne	LF	7

$\tau = 4.09(19) \mu s$ gas $PIFCO^4ID^{10}UV^{12}$
 $2.3(1) \mu s$ Ne $LF^{6,7}$

$A = -176$ gas EM^3PE^{14}

$B_0 = 0.101 \text{ EM}^3$

$X^2\Pi_g$	$D_{\infty h}$	Structure: EM^1
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Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+_g	1	Sym. stretch	617 ^a	gas	EM	3
			618 ^a	Ne	LF	6,7
Π_u	2	Bend	348 ^c	gas	EM	3
			349 ^c	Ne	LF	6,7
Σ^+_u	3	Asym. stretch	1203 ^c	gas	EM,PE	3,14
			1224 ^c	Ne	LF	6,7

$A = -440.39(3)$ gas $EM^{1,2}$

$B_0 = 0.109 \text{ EM}^1$

^aStrong Fermi resonance with $2\nu_2$; Ref. 7 has suggested a reversed assignment for ν_1 and $2\nu_2$ of the $\tilde{A}$ state.

^bHigh resolution PE value 633(2).¹⁴

^c $\frac{1}{2}(2\nu_i)$.

References

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¹⁴L.-S. Wang, J. E. Reutt, Y. T. Lee, and D. A. Shirley, *J. Electron Spectrosc. Relat. Phenom.* **47**, 167 (1988).

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CICN⁺

$\tilde{B}^2\Pi_{3/2}$	$C_{\infty v}$	
$T_0 = 22515.54$	gas	$EF^8LF^{10,12} \quad \tilde{B}-\tilde{X} \text{ 365-569 nm}$
22598(5)	Ne	$AB^6 \quad \tilde{B}-\tilde{X} \text{ 380-442 nm}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CN stretch	2128.5(7)	gas	LF	10
Π	2	Bend	303.1(7)	gas	LF	10
Σ^+	3	CCl stretch	531.90	gas	LF	10,11
			539(4)	Ne	AB	6

$\tau_1 = 205(40) \text{ ns}$ gas EF^3
 $280(56) \text{ ns}$ gas $PEFCO^5$
 $170(20) \text{ ns}$ gas $PIFCO^{4,7}$
 $\tau_2 = 900(100) \text{ ns}$ gas EF^3
 $970(80) \text{ ns}$ gas $PIFCO^7$

Both lifetimes are dependent on extent of vibrational excitation⁵.

$A = -368(2)$ gas $EF^{8,9}LF^{10}$

$B_0 = 0.177 \text{ LF}^{11}$

$\tilde{X}^2\Pi_{3/2}$	$C_{\infty v}$	Structure: UV, PE^3LF^{12}
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Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡N stretch	1915(2)	gas	EF,LF	8-10
Π	2	Bend	376 ^a	gas	LF	10
Σ^+	3	CCl stretch	827(2)	gas	EF,LF	8-10

$B_0 = 0.205 \text{ LF}^{11}$

^aTentative assignment.

References

¹²M. Rösslein and J. P. Maier, *J. Phys. Chem.* **93**, 7342 (1989).

BrCN⁺

$\tilde{B}^2\Pi_{3/2}$	$C_{\infty v}$	
$T_0 = 18759.78(4)$	gas	$EF^7LF^{10,11} \quad \tilde{B}-\tilde{X} \text{ 445-620 nm}$
18586(14)	Ne	$AB^5 \quad \tilde{B}-\tilde{X} \text{ 418-538 nm}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡N stretch	1958(2)	gas	EF,LF	7,10
			1830(10)	Ne	AB	5
Π	2	Bend	395.7(2) ^a	gas	EF,LF	7,10
			377(10)	Ne	AB	5
Σ^+	3	CBr stretch	473.1(2)	gas	EF,LF	7,10
			478(10)	Ne	AB	5

$\tau_1 = 197(10) \text{ ns}$ gas $EF^3PIFCO^6T-PEFCO^8$
 $\tau_2 = 713(40) \text{ ns}$ gas $PIFCO^6T-PEFCO^8$
 $A = -880(40)$ gas EF^7PE^9
 $B_0 = 0.127$ gas $LF^{10,11}$

$X^2\Pi_{3/2}$		$C_{\infty v}$	Structure: LF^{11}			
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	$C\equiv N$ stretch	1906(2)	gas	EF,LF	7,10
Π	2	Bend	287.2(2) ^a	gas	EF,LF	7,10
Σ^+	3	CBr stretch	649.4(5)	gas	EF,LF	7,10

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

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

References

- ¹⁰M. A. Hanratty, M. Rösslein, F. G. Celii, T. Wyttenbach, and J. P. Maier, *Mol. Phys.* **64**, 865 (1988).
¹¹M. Rösslein, M. A. Hanratty, and J. P. Maier, *Mol. Phys.* **68**, 823 (1989).

N₃

$B^2\Sigma_g^+$		$D_{\infty h}$	Structure: AB^2			
$T_0^a = 36738.750(2)$	gas	$AB^{1,2}LF^3$	$\tilde{B}-\tilde{X}$ 260–273 nm			

All bands above 37000 are diffuse.

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

$\tau < 20$ ns gas LF^3
 $B_0 = 0.432$ gas AB^2

$X^2\Pi_g$		$D_{\infty h}$	Structure: AB^2IR^6			
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	~ 1320 1287 ^b	gas N_2^c	LF IR	3 4
Π_u	2	Bend	~ 457 472.7	gas N_2^c	LF IR	3 4
Σ_u^+	3	Asym. stretch	1644.68 1657.5	gas N_2^c	LMR,IR IR	5,6 4

$A_{eff} = -71.3$; $\epsilon\omega_2 = -94.38$ gas AB^2IR^6
 $B_0 = 0.431$ $AB^2LMR^3IR^6$

^aRevised value resulting from reanalysis by Ref. 6.

^b $(\nu_1 + \nu_3) - \nu_3$.

^cMixed with argon.

References

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⁶C. R. Brazier, P. F. Bernath, J. B. Burkholder, and C. J. Howard, *J. Chem. Phys.* **89**, 1762 (1988).

P₃

$T_0 = 23420(10)$		Ar	AB^1	418–427 nm		
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	480(20)	Ar	AB	1

References

- ¹L. Andrews and Z. Mielke, *J. Phys. Chem.* **94**, 2348 (1990).

Sb₃

$\tilde{X}$		$C_{\infty v}$	Structure: EM^3			
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	Sym. stretch	217.5(3) 217.0(5)	Ar Kr	Ra Ra	1 1

References

- ¹H. Sontag and R. Weber, *Chem. Phys.* **70**, 23 (1982).

N₂O⁺

$B^2\Pi$		$C_{\infty v}$	Structure: EM^3PF^{16}			
$T_0 = 38440(100)^a$	gas	PE^1PF^{15}	$\tilde{B}-\tilde{A}$ 538–866 nm			
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Sym. stretch	$\sim 900^b$	gas	PE	1

$\tilde{A}^2\Sigma^+$		$C_{\infty v}$	Structure: EM^3PF^{16}			
$T_0 = 28162.33$	gas	$EM^{3,14}PF^{6,10,11,16}$	$\tilde{A}-\tilde{X}$ 317–421 nm			
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Sym. stretch	1345.52	gas	EM,PF	3,10
Π	2	Bend	614.45	gas	EM	3,14
Σ^+	3	Asym. stretch	2451.7	gas	EM	3

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

$\tilde{X}^2\Pi$		$C_{\infty v}$	Structure: EM^3			
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Sym. stretch	1126.51	gas	EM	3
Π	2	Bend	452.42	gas	EM,PF	3,11,14
Σ^+	3	Asym. stretch	1737.6	gas	EM	3

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

- ^aCalculated using first ionization potential of 12.886(2) eV, from Ref. 5.
^bSomewhat irregular band spacings.

References

- ¹⁵P. O. Danis, T. Wyttenbach, and J. P. Maier, *J. Chem. Phys.* **88**, 3451 (1988).
¹⁶M. Larzillière and Ch. Jungen, *Mol. Phys.* **67**, 807 (1989).

NNS⁺ $\tilde{X} \ ^2\Pi^*$ $C_{\infty v}$ $T_0 \sim 41500$ gas PE¹ $\tilde{A} \ ^2\Sigma$ $C_{\infty v}$ $T_0 = 38810(160)$ gas PE¹

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ^+		NS stretch	820(50)	gas	PE	1

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ^+		N-S stretch	~ 500	gas	PE	1

 $A \sim 400$ gas PE¹¹Tentative assignment.

References

- ¹H. Bender, F. Carnovale, J. B. Peel, and C. Wentrup, *J. Am. Chem. Soc.* **110**, 3458 (1988).

FBO

 $\tilde{X}$ $C_{\infty v}$ Structure: MW,DL²

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ^+	1	B=O stretch	2078.87	gas	DL	2
			2081	Ne	IR	1
			2071	Ar	IR	1
Π	2	Bend	502	Ne	IR	1
			493	Ar	IR	1

 $B_0 = 0.312$ DL,MW²

References

- ¹A. Snelson, *High Temp. Sci.* **4**, 141 (1972).
²Y. Kawashima, K. Kawaguchi, Y. Endo, and E. Hirota, *J. Chem. Phys.* **87**, 2006 (1987).

NCO⁻ $\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ^+	3	Asym. stretch	2124.31	gas	DL	1

 $B_0 = 0.384$ DL¹

References

- ¹M. Gruebele, M. Polak, and R. J. Saykally, *J. Chem. Phys.* **86**, 6631 (1987).

NCS⁻ $\tilde{X}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ^+	3	CN stretch	2065.93	gas	DL	1

 $B_0 = 0.197$ DL¹

References

- ¹M. Polak, M. Gruebele, and R. J. Saykally, *J. Chem. Phys.* **87**, 3352 (1987).

OSiS

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ^+	1	SiO stretch	1265.4	Ar	IR	1
	3	SiS stretch	643.0	Ar	IR	1

References

- ¹H. Schnöckel, *Angew. Chem.* **92**, 310 (1980); *Angew. Chem. Int. Ed. Engl.* **19**, 323 (1980).

SiS₂ $\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ_g^+	3	SiS a-stretch	918.0	Ar	IR	1

References

- ¹H. Schnöckel and R. Köppe, *J. Am. Chem. Soc.* **111**, 4583 (1989).

N₃⁻

Threshold for electron detachment from ground-state N₃⁻ is 22270(350).¹

 $\tilde{X} \ ^1\Sigma_g^+$ $D_{\infty h}$ Structure: DL^{2,3}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ_g^+	3	Asym. stretch	1986.47 2003.5	gas N ₂ ^a	DL IR	2,3 4

 $B_0 = 0.426$ DL^{2,3}^aMixed with argon.

References

- ¹E. Ilenberger, P. B. Comita, J. I. Brauman, H. P. Fenzlatt, M. Heni, N. Heinrich, W. Koch, and G. Frenking, *Ber. Bunsenges. Phys. Chem.* **89**, 1026 (1985).
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PNO

$\tilde{X}$	$C_{\infty v}$					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med. meas.	Type meas.	Refs.
Σ^+	1	NO stretch	1754.7	Ar	IR	1
	3	PN stretch	865.2	Ar	IR	1

References

- ¹R. Ahlrichs, S. Schunck, and H. Schnöckel, *Angew. Chem.* **100**, 418 (1988); *Angew. Chem. Int. Ed. Engl.* **27**, 421 (1988).

P₂O

$\tilde{X}$	$C_{\infty v}$					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		P=O stretch	1270.4	Ar	IR	1

References

- ¹Z. Mielke, M. McCluskey, and L. Andrews, *Chem. Phys. Lett.* **165**, 146 (1990).

NNS

$\tilde{X}$	$C_{\infty v}$		Structure: IR ²			
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ^+	1	NN stretch	2047.59	gas	IR	2
			2030	Ar	IR	1
$B_0 = 0.216$ gas IR ²						

References

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BCl₂

Emission which is observed between 200 and 260 nm on excitation of BCl₃ by radiation of wavelength shorter than 91 nm has been attributed⁵ to BCl₂.

Emission which is observed between 240 and 380 nm on excitation of BCl₃ by radiation of wavelength shorter than 118 nm has been attributed^{4,5} to BCl₂, as has been a similar chemiluminescence emission observed^{1,2} on reaction of H atoms with BCl₃.

Emission which is observed between 280 and 380 nm on excitation of BCl₃ by radiation of wavelength shorter than 124 nm has been attributed^{4,5} to BCl₂.

Emission which is observed between 380 and 500 nm on excitation of BCl₃ by radiation of wavelength shorter than 138 nm has been attributed^{4,5} to BCl₂.

$\tilde{X}$	C_{2v}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	731w	Ar	IR	3
b_2	3	Asym. stretch	966vs	Ar	IR	3

References

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AlCl₂

$\tilde{X}$	C_{2v}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	460.0	Ar	IR	2
b_2	3	Asym. stretch	563.6	Ar	IR	1,2

References

- ¹G. A. Olah, O. Farooq, S. M. F. Farnia, M. R. Bruce, F. L. Clouet, P. R. Morton, G. K. S. Prakash, R. C. Stevens, R. Bau, K. Lammertsma, S. Suzer, and L. Andrews, *J. Am. Chem. Soc.* **110**, 3231 (1988).
²E. D. Samsonova, S. B. Osin, and V. F. Pevel'kov, *Zh. Neorgan. Khim.* **33**, 2779 (1988); *Russ. J. Inorg. Chem.* **33**, 1598 (1988).

GaCl₂

$\tilde{X}$	C_{2v}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	373.0	Ar	IR	1
b_2	3	Asym. stretch	415.1	Ar	IR	1

References

- ¹E. D. Samsonova, S. B. Osin, and V. F. Pevel'kov, *Zh. Neorgan. Khim.* **33**, 2779 (1988); *Russ. J. Inorg. Chem.* **33**, 1598 (1988).

CO₂⁻**X** C_{2v}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
b ₂	3	Asym. stretch	1658.3	Ne	IR	1

References¹M. E. Jacox and W. E. Thompson, J. Chem. Phys. **91**, 1410 (1989).**PO₂****²B₁**, ? C_{2v}

T₀ = 30378(3) gas AB¹LF³ ²B₁-²X̃ 268-600 nm
 Ar AB⁶ ²B₁-²X̃ 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 NO₂ suggests that the quascontinuum may be contributed by high vibrational levels of the ground state.

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a ₁	1	Sym. stretch	933	gas	AB	1
			942	Ar	AB	6
	2	Bend	396	gas	AB	1

τ ~ 500 ns gas LF³
 τ_{cont} ~ 4.5 μs gas LF³

X²A₁ C_{2v} Structure: AB¹MW,LMR²

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a ₁	1	PO s-stretch	1117(20)	gas	MW,LMR 2,3 LF	
	2	Bend	387(20)	gas	MW,LMR 2,3 LF	7
			386.4	Ar	IR	
b ₂	3	PO a-stretch	1278 ^a	gas	MW,LMR 2	
			1319.1	Ar	IR	4,5,7

A₀ = 3.486; B₀ = 0.287; C₀ = 0.264 MW,LMR²^aAverage of values of 1059, 1371, and 1405 cm⁻¹, obtained from centrifugal distortion constants.**References**

- ⁴L. Andrews and R. Withnall, J. Am. Chem. Soc. **110**, 5605 (1988).
⁵R. Withnall and L. Andrews, J. Phys. Chem. **92**, 4610 (1988).
⁶R. Withnall, M. McCluskey, and L. Andrews, J. Phys. Chem. **92**, 126 (1989).
⁷Z. Mielke, M. McCluskey, and L. Andrews, Chem. Phys. Lett. **165**, 146 (1990).

NSBr⁺**D²A'** C_sT^a = 24200(160) gas PE¹**C²A'** C_sT^a = 19520(160) gas PE¹**B²A'** C_sT^a = 5160(160) gas PE¹**A²A''** C_sT^a = 3230(160) gas PE¹^aFrom vertical ionization potentials.**References**¹A. W. Allaf, G. Y. Matti, R. J. Suffolk, and J. D. Watts, J. Electron Spectrosc. Relat. Phenom. **48**, 411 (1989).**NSI⁺****E²A'** C_sT^a = 35820(800) gas PE¹**C,D²A',²A''** C_sT^a = 23720(800) gas PE¹**A,B²A'',²A'** C_sT^a = 5490(800) gas PE¹^aFrom vertical ionization potentials.**References**¹A. W. Allaf, G. Y. Matti, R. J. Suffolk, and J. D. Watts, Chem. Phys. Lett. **155**, 32 (1989).**SSO⁺****F²A'** C_sT^b = 64000(1000) gas PE^{2,3}**E²A'** ^a C_sT^b = 42100(320) gas PE¹⁻³**D²A''** ^a C_sT^b = 34200(320) gas PE¹⁻³**C²A'** ^a C_sT^b = 32600(320) gas PE¹⁻³**B²A''** ^a C_sT^b = 6132(40) gas PE^{1-3,5}PI⁵

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	SO stretch	915(20) ^c	gas	PE,PI	1,5

$\tilde{A}^2A'$, C_s $T_0 = 5665(40)$ gas $PE^{1-3,5}PI^5$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	SO stretch	923(20) ^c	gas	PE,PI	1,5

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	3	SS stretch	480(20)	gas	PE,PI	1,4,5

^aTentative assignment.^bFrom vertical ionization potential. The first ionization potential is taken to be 10.58 eV.^{4,5}^cAn alternate assignment is given by Ref. 3.

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CF₂ $\tilde{A}^1B_1$, C_{2v} Structure: AB¹⁰

$T_0 = 37226$	gas	EM ¹ AB ^{2,3,5,10}	$\tilde{A}-\tilde{X}$ 220–380 nm
37219(2)	Ne	LF ¹⁷	
36878(2)	Ar	AB ^{4,6,16} EM ¹⁶ LF ¹⁷	$\tilde{A}-\tilde{X}$ 210–346 nm
37054(2)	N ₂	LF ¹⁷	

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	2	Bend	496	gas	UV	1–3,5,10
			496(2)	Ne	LF	17
			496(2)	Ar	AB	4,6,16
					LF	17
			496(2)	N ₂	LF	17

$\tau_0 = 61(3)$ ns	gas	LF ^{20,21,28} EM ³²
31 ns	Ne	LF ¹⁷
27 ns	Ar	LF ¹⁷
23 ns	Kr	LF ¹⁷

 $A_0 = 4.577$; $B_0 = 0.334$; $C_0 = 0.311$ AB¹⁰ $\tilde{a}^3B_1$, C_{2v} $T_0 = 19828$ gas CL^{18,19,22,24,29}PE³¹ $\tilde{A}-\tilde{X}$ 430–800 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	2	Bend	517	gas	CL	18,22,24,29

 $\tau \sim 1$ s gas CL¹⁹ $\tilde{X}^1A_1$, C_{2v} Structure: MW⁸AB^{9,10}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1225.08	gas	DL,IR	23,30
			1220	Ne	PE	31
			1222vs	Ar	IR,LF	12,17
	2	Bend	667	gas	IR,LF	6,11,17
			668vw	Ar	UV,PE	1,10,31
b_2	3	Asym. stretch	1114.44	gas	IR,LF	6,11,17
					IR,DL	7,13
						27,30
			1104	Ne	IR	12
			1102vs	Ar	IR	6,11

 $A_0 = 2.947$; $B_0 = 0.417$; $C_0 = 0.365$ MW^{8,15,26}AB^{9,10}^aTentative assignment. This band system was associated with the $\tilde{C}$ transition in Ref. 10. Subsequent studies^{14,25} have dictated the reassignment to CF₂ of almost all of the bands between 136 and 160 nm which had tentatively been attributed¹⁰ to CF₂.

References

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CFCI

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

$T_0 = 25283(5)$	gas	LF ^{6,7}	$\tilde{A}-\tilde{X}$ 359–390 nm
24983	Ar	UV ¹ LF ^{2,3}	$\tilde{A}-\tilde{X}$ 340–667 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	CF stretch	1263	gas	LF	7
	2	Bend	394(3)	gas	LF	6
			392(1)	Ar	LF	3
	3	CCI stretch	726(6)	gas	LF	6,7
			712(2)	Ar	LF	3

 $\tau_0 = 650(40)$ ns gas LF⁴⁻⁶EM⁸
330(20) ns Ar LF³ $\tilde{X}^1A'$, C_s

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

References

⁷T.-X. Xiang, Chem. Phys. Lett. **147**, 183 (1988).

⁸T. Ibuki, A. Hiraya, and K. Shobatake, J. Chem. Phys. **90**, 6290 (1989).

CCl₂

$\tilde{A} \text{ } ^1B_1$	C_{2v}	Structure: LF^{16}				
$T_0 = 16913(3)$ 17092	gas Ar	$CL^8LF^{7,9,10,15,16}EM^{11}$ $AB^{1,3}LF^{4-6}$	$\tilde{A}-\tilde{X}$ 400–800 nm $\tilde{A}-\tilde{X}$ 440–827 nm			
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	644	gas	LF	10,15
			624	Ar	LF	6
	2	Bend	308	gas	LF	9,10,15
			304	Ar	AB,LF	1,3,6

$\tau = 3.81(30) \mu s$ gas LF^7

$\tau_1 = 1.83(2) \mu s$, $\tau_2 = 3.72(6) \mu s$ gas $EM^{11,13}$

$\tau = 3.6 \mu s$ Ar LF^6

$A_{020} = 3.745$; $B_{020} = 0.106$; $C_{020} = 0.103$ LF^{16}

$\tilde{X} \text{ } ^1A_1$	C_{2v}	Structure: $MW^{14}LF^{16}$				
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	730(40)	gas	PE	12
			721wm	Ar	IR,LF	1–3,5,6
	2	Bend	340(40)	gas	PE	12
			333	Ar	LF	4–6
b_2	3	Asym. stretch	748vs	Ar	IR	1–3
$A_0 = 1.675$; $B_0 = 0.123$; $C_0 = 0.115$ $MW^{14}LF^{16}$						

References

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¹⁵J.-I. Choe, S. R. Tanner, and M. D. Harmony, J. Mol. Spectrosc. **138**, 319 (1989); J. Mol. Spectrosc. **140**, 193 (1990).

¹⁶D. J. Clouthier and J. Karolczak, J. Phys. Chem. **93**, 7542 (1989).

CBr₂

$\tilde{A}$	C_{2v}					
$T_0 =$	14885	gas	LF^5	$\tilde{A}-\tilde{X}$ 614–663 nm		
	14962	Ar	$LF^{3,4}$	$\tilde{A}-\tilde{X}$ 600–857 nm		
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	460	gas	LF	5
			468	Ar	LF	4
	2	Bend	189	gas	LF	5
			186	Ar	LF	4
$\tau = 14.5(1.5) \mu s$ Ar LF^4						

References

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SiCl₂

$\tilde{A} \text{ } ^1B_1$	C_{2v}					
$T_0 = 30013.4(1.0)$	gas	$AB^4EM^5-7LF^{8,10}$	$\tilde{A}-\tilde{X}$ 308–430 nm			
In an argon matrix, unstructured absorption attributable to SiCl ₂ has been observed ¹ between 310 and 320 nm, with a maximum at approximately 315 nm.						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	435(5)	gas	LF	8
	2	Bend	149.9(5)	gas	UV,LF	3,7,8
$\tau_{070} = 77(3) ns$ gas LF^8						
$A_{060} = 0.909$; $B_{060} = 0.076$; $C_{060} = 0.069$ LF^{10}						

$\tilde{X} \text{ } ^1A_1$	C_{2v}	Structure: ED^4MW^9				
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	526.5	gas	LF	8
			518.7	Ne	IR	2
			512.5s	Ar	IR	1,2
	2	Bend	201.2	gas	EM,LF	7,8
b_2	3	Asym. stretch	202.2	Ar	IR	2
			509.4	Ne	IR	2
			502vs	Ar	IR	1,2
$A_0 = 0.493$; $B_0 = 0.094$; $C_0 = 0.079$ MW^9LF^{10}						

References

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GeCl₂**B** $T_0 \sim 30969$ gas AB²330–314 nm^a

Structured absorption is superposed on a continuum with maximum near 32280, presumably due to predissociation of GeCl₂ into GeCl + Cl.

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

 $\tau = 89.7(6.8)$ ns gas EM¹⁰**B¹B₁**C_{2v} $T_0 = 22388$ gas CL¹410–490 nm^a

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

 $\tau = 17.4(6)$ gas EM¹⁰**References**¹⁰T. Ibuki, Chem. Phys. Lett. **169**, 64 (1990).**NO₂⁻**

Threshold for electron detachment from ground-state NO₂⁻ = 18340(40) gas PD³PE⁴

$\tilde{X}$	C _{2v}	Structure: PE ⁴				
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	NO stretch	1284(30)	gas	PE	4
	2	Bend	776(30)	gas	PE	4
b_2	3	NO stretch	1244	Ar	IR	1,2

References¹D. E. Milligan, M. E. Jacox, and W. A. Guillory, J. Chem. Phys. **52**, 3864 (1970).²D. E. Milligan and M. E. Jacox, J. Chem. Phys. **55**, 3404 (1971).³S. B. Woo, E. M. Helmy, and A. P. Paszek, Phys. Rev. A **24**, 1380 (1981).⁴K. M. Ervin, J. Ho, and W. C. Lineberger, J. Phys. Chem. **92**, 5405 (1988).**PO₂⁻****X**C_{2v}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
b_2	3	PO a-stretch	1198.8	Ar	IR	1

References¹Z. Mielke, M. McCluskey, and L. Andrews, Chem. Phys. Lett. **165**, 146 (1990).**FPO****X**C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	PO stretch	1292.2	Ar	IR	1
	2	Bend	416.0	Ar	IR	1
	3	PF stretch	811.4	Ar	IR	1

References¹R. Ahlrichs, R. Becherer, M. Binnewies, H. Borrmann, S. Schunck, and H. Schnöckel, J. Am. Chem. Soc. **108**, 7905 (1986).**CIPO****X**C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	PO stretch	1258vs	Ar	IR	1–4
	2	Bend	308wm	Ar	IR	1
	3	PCI stretch	489vs	Ar	IR	1–3

References¹M. Binnewies, M. Lakenbrink, and H. Schnöckel, Z. Anorg. Allg. Chem. **497**, 7 (1983).²M. Binnewies, H. Schnöckel, R. Gereke, and R. Schmutzler, Z. Anorg. Allg. Chem. **534**, 143 (1986).³H. Schnöckel and S. Schunck, Z. Anorg. Allg. Chem. **548**, 161 (1987).⁴B. W. Moores and L. Andrews, J. Phys. Chem. **93**, 1902 (1989).**BrPO****X**C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	PO stretch	1253.0	Ar	IR	1,2
	2	Bend	253.7	Ar	IR	1
	3	PBr stretch	407.1	Ar	IR	1,2

References¹M. Binnewies, M. Lakenbrink, and H. Schnöckel, High Temp. Sci. **22**, 83 (1986).²H. Schnöckel and S. Schunck, Z. Anorg. Allg. Chem. **548**, 161 (1987).

FPS

$\tilde{X}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	PF stretch	791.4	Ar	IR	1
	2	Bend	313.6	Ar	IR	1
	3	PS stretch	720.2	Ar	IR	1

References

¹H. Schnöckel and S. Schunck, Z. Anorg. Allg. Chem. **552**, 163 (1987).

BrPS

$\tilde{X}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	PS stretch	712	Ar	IR	1
	2	Bend	185 ^a	Ar	IR	1
	3	PBr stretch	372	Ar	IR	1

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

References

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

CIAso

$\tilde{X}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	AsO stretch	984.4	Ar	IR	1
	3	AsCl stretch	378.7	Ar	IR	1

References

¹H. Schnöckel, M. Lakenbrink, and Lin Zhengyan, J. Mol. Struct. **102**, 243 (1983).

NSBr

$\tilde{X}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	N=S stretch	1311	gas	IR	2
			1312.9m	Ar	IR	1
	2	Bend	226.2wm	Ar	IR	1
	3	SBr stretch	346.1s	Ar	IR	1

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NSI

$\tilde{X}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NS stretch	1295 ^a	gas	IR	1

^a Tentative assignment.

References

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SSO

$\tilde{A}$	$\tilde{A}'$	C_s	Structure:	AB^{11}
$T_0 =$	29689.6	gas	$AB^{1,7,11}LF^{12,13,16}$	$\tilde{A}-\tilde{X}$ 250–395 nm
	29285(20)	Xe	AB^4	$\tilde{A}-\tilde{X}$ 280–342 nm
Predissociation limit between 31172 and 31307. AB^{11}				

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SO stretch	1032	gas	AB,LF	11,13,16
	2	Bend	253	gas	AB,LF	11,13,16
	3	SS stretch	407	gas	AB,LF	7,11,13
			415(20)	Xe	AB	16
						4

$A_{020} = 1.016$; $B_{020} = 0.148$; $C_{020} = 0.129$ AB^{11}
 $\tau \sim 10$ ns gas LF^{13}

$\tilde{X}$	$\tilde{A}'$	C_s	Structure: MW ^{2,6}			
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	SO stretch	1166.45	gas	IR,DL	1,3,14
			1156.2	Ar	IR,Ra	8,9
	2	Bend	380	gas	LF	16
			382	Ar	IR,Ra	8,9
	3	SS stretch	679.1	gas	IR,LF	1,3,13
			672.2	Ar	IR,Ra	8,9

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

References

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

Se₃

$\tilde{X}$	C_{2v}					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	311	Ar	Ra	1
			311	N ₂	Ra	1

References

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

Te₃

$\bar{X}$	C_{2v}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	203 ^a	N ₂	Ra	1

^a ¹³⁰Te.**References**¹H. Schnöckel, Z. Anorg. Allg. Chem. **510**, 72 (1984).**CF₂⁻**Threshold for electron detachment from ground-state CF₂⁻ = 1440(40) gas PE¹

$\bar{X}$ ² B 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

References¹K. K. Murray, D. G. Leopold, T. M. Miller, and W. C. Lineberger, J. Chem. Phys. **89**, 5442 (1988).**CCl₂⁻**Threshold for electron detachment from ground-state CCl₂⁻ = 12930(65) gas PE¹**References**¹K. K. Murray, D. G. Leopold, T. M. Miller, and W. C. Lineberger, J. Chem. Phys. **89**, 5442 (1988).**PF₂**

$\bar{X}$	C_{2v}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		PF ₂ stretch	852.1ms	Ar	IR	1
		PF ₂ stretch	831.4s	Ar	IR	1

References¹J. K. Burdett, L. Hodges, V. Dunning, and J. H. Current, J. Phys. Chem. **74**, 4053 (1970).**AsF₂**

When gas-phase AsF₃ is subjected to 124 nm radiation, an emission band system, tentatively assigned to AsF₂, is observed between 330 and 610 nm, with a maximum near 450 nm.¹ The radiative lifetime of the species which contributes this band system is 25.5(1.8) μs.²

References¹Y. Ni, X. Wang, M. Suto, and L. C. Lee, J. Phys. B **21**, 1821 (1988).²C. Ye, M. Suto, L. C. Lee, and T. J. Chuang, J. Phys. B **22**, 2527 (1989).**O₃⁻**Threshold for electron detachment from ground-state O₃⁻ = 16970(20) gas PE⁷PD⁹

X^2B_1	C_{2v}	Structure: PD ⁹				
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	975(10)	gas	PD,PF	6-8
			1016 ^a	Ar	Ra	3,5
			1011 ^b	Ar	Ra	3,5
	2	Bend	590(10)	gas	PD,PF	7,8
			600w ^a	Ar	IR	4
b_2	3	Asym. stretch	796.3	Ne	IR	10
			789s ^a	Ar	IR	2,4
			802s			
			802s ^b	Ar	IR	1,2,4

^aCs⁺ present.^bNa⁺ present.**References**⁹L. J. Wang, S. B. Woo, and E. M. Helmy, Phys. Rev. A **35**, 759 (1987).¹⁰W. E. Thompson and M. E. Jacox, J. Chem. Phys. **91**, 3826 (1988)**FOO**

$\bar{X}$	C_s		Structure: DL ⁷			
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	OO stretch	1486.93	gas	IR	8,9
			1490vs	Ar	IR	1,6
			1500vs	N ₂	IR	3
	2	Bend	376	N ₂	IR	3
			3	OF stretch	579.32	gas
	584s	Ar			IR	1,6
	586s	N ₂			IR	3

 $A_0 = 2.616$; $B_0 = 0.334$; $C_0 = 0.295$ DL⁷IR⁹MW¹⁰**References**¹⁰M. Bogey, P. B. Davies, C. Demuynck, and J. L. Destombes, Mol. Phys. **67**, 1033 (1989).**BrOBr**

In a nitrogen matrix, a strong absorption maximum at approximately 47000, a weaker shoulder near 31200, and a much weaker shoulder near 22100 have been attributed³ to electronic transitions of BrOBr.

$\tilde{\chi}$	C_{2v}	Structure: EXAFS ³				
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	526.1s	Ar	IR	1,2
			528	N ₂	IR	3
b_2	3	Asym. stretch	623.4w	Ar	IR	2
			626	N ₂	IR	3

References

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²S. D. Allen, M. Poliakoff, and J. J. Turner, *J. Mol. Struct.* **157**, 1 (1987).
³W. Levason, J. S. Ogden, M. D. Spicer, and N. A. Young, *J. Am. Chem. Soc.* **112**, 1019 (1990).

SF₂ $\tilde{E}$ 4p Rydberg state C_{2v}

$T_0 = 62015(30)$ gas MPI¹⁰

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	931(59)	gas	MPI	10
	2	Bend	383(42)	gas	MPI	10

C

gas MPI

$\tilde{C}-\tilde{\chi}$ 165–175 nm

 $\tilde{B}^1B_1(4s)$ C_{2v}

$T_0 = 54433(30)$ gas MPI¹⁰

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	991(12)	gas	MPI	10
	2	Bend	361(24)	gas	MPI	10

 $\tilde{A}$

$T_0 = 18500(1200)$ gas CL^{7,8} 550–860 nm

Chemiluminescence in the reaction of F₂ with CS₂, originally assigned^{7,8} to FCS, has been reassigned⁹ to SF₂.

$\tilde{\chi}$	C_{2v}	Structure: MW ^{1,2,4}				
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	838.53	gas	IR,CL	5,7–9
			834	Ne	IR	3
			832vs	Ar	IR	3
			825	N ₂	IR	3
	2	Bend	357(2)	gas	MW,CL	2,7–9
			358	Ne	IR	3
			358m	Ar	IR	3
			358	N ₂	IR	3
b_2	3	Asym. stretch	813.04	gas	IR	5
			807.5	Ne	IR	3
			804vs	Ar	IR	3
			795	N ₂	IR	6

$A_0 = 0.898$; $B_0 = 0.307$; $C_0 = 0.228$ MW^{1,2}

References

- ¹D. R. Johnson and F. X. Powell, *Science* **164**, 950 (1969).
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FSCI

$\tilde{\chi}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	SF stretch	781vs	Ne	IR	1
			778vs	Ar	IR	1
			277vw	Ne	IR	1
	2	Bend	274vw	Ar	IR	1
			552s ^a	Ne	IR	1
			543s ^a	Ar	IR	1

^a In Fermi resonance with $2\nu_2$.

References

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

OICI

$\tilde{\chi}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	IO stretch	779.1	Ar	IR	1
			772.2			
			778.2	Kr	IR	1
			775.1			
			778.2	N ₂	IR	1
	3	ICl stretch	325.6	Ar	IR	1
			320.2			
			317.4	Kr	IR	1
			322.6	N ₂	IR	1

References

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

Cl $\bar{3}$

An absorption maximum which appears at 251 nm when CsCl is codeposited with Cl₂ in an argon matrix³ and at 253 nm when an Ar:Cl₂ sample is subjected to electron bombardment during deposition⁵ has been assigned to Cl $\bar{3}$.

$\bar{X}$	$D_{\infty h}$					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	225 ^{ac}	Ar	Ra	2
			253 ^b	Ar	Ra	2
			258 ^c	Ar	Ra	2
			276 ^d	Ar	Ra	2
Σ_u^+	3	Asym. stretch	327 ^a	Ar	IR,Ra	2
			340 ^b	Ar	IR,Ra	2
			345 ^c	Ar	IR,Ra	2
			375 ^d	Ar	IR,Ra	2
			374 ^f	Kr	IR	1

^aCs⁺ present.^bRb⁺ present.^cK⁺ present.^dNa⁺ present.^eTentative assignment.^fAttributed in Ref. 1 to the uncharged species. Reassigned by Ref. 4 to the anion.

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- ⁴C. A. Wight, B. S. Ault, and L. Andrews, *J. Chem. Phys.* **65**, 1244 (1976).
- ⁵J. Hacaloglu and L. Andrews, *Chem. Phys. Lett.* **160**, 274 (1989).

Kr₂F 9^2T C_{2v} gas AB^{6,8,9} 9^2T-4^2T

Broad absorption, with maximum near 315 nm.

 4^2T C_{2v} Unstructured gas-phase emission¹⁻⁴ between 340 and 480 nm, with maximum near 410 nm. $\tau = 200(28)$ ns gas LF⁵EF⁷

References

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- ⁹D. P. Greene and A. W. McKown, *Appl. Phys. Lett.* **54**, 1965 (1989).

6.4. Four-Atomic Trihydrides

BH₃ $\bar{X}^1A_1'$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	1140.88	gas	DL	2
			1125w	Ar	IR	1
e'	3	BH stretch	2808w	Ar	IR	1

BD₃ $\bar{X}^1A_1'$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	845	Ar	IR	1
e'	3	BD stretch	2112?	Ar	IR	1

References

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

SiH₃⁺ $\bar{X}$ D_{3h}

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

References

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

GeH₃⁺ $\bar{X}$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	393(15)	gas	PI	1

References

- ¹B. Ruscic, M. Schwarz, and J. Berkowitz, *J. Chem. Phys.* **92**, 1865 (1990).

BH₃⁻Threshold for electron detachment from ground-state BH₃⁻ = 310(120) gas PE¹

BD₃

Threshold for electron detachment from ground-state BD₃ = 220(113) gas PE¹

References

¹C. T. Wickham-Jones, S. Moran, and G. B. Ellison, *J. Chem. Phys.* **90**, 795 (1989).

CH₃

4p²A₂⁺ D_{3h}

*T*₀ = 69853.44(13) gas MPI¹⁵

*B*₀ = 9.90 gas MPI¹⁵

X²A₂⁺ D_{3h} Structure: AB²IR^{9,18}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₁ ⁺	1	CH stretch	3004.8(2)	gas	CAR,Ra	13,16
<i>a</i> ₂ ⁺	2	OPLA	606.453	gas	IR,DL	5,9
			617vs	Ne	IR	4
			603 ^c	Ar	IR	3,8
			611	N ₂	IR	3
<i>e</i> ⁺	3	CH stretch	3160.821	gas	LD	11
			3162wm	Ne	IR	4
			3150	Ar	IR	6
<i>e</i> ⁺	4	Deformation	1396w	Ne	IR	4
			1398 ^d	Ar	IR	8

*B*₀ = 9.578 AB²DL⁹; *C*₀ = 4.742 DL⁹

CD₃

4p²A₂⁺ D_{3h}

*T*₀ = 69777.40(4) gas MPI¹⁵

*B*₀ = 4.846(2) gas MPI¹⁵

3p²A₂⁺ D_{3h} Structure: MPI¹²

*T*₀ = 59886 gas MPI^{12,17}

Higher members of Rydberg series observed (MPI¹²) at 69789, 73645, and 75557.

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₁ ⁺	1	CD stretch	2031 ^c	gas	MPI	12,17
<i>a</i> ₂ ⁺	2	OPLA	1032	gas	MPI	12,17

*B*₀ = 4.76(2); *C*₀ = 2.38 MPI^{12,17}

X²A₂⁺ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₁ ⁺	1	CD stretch	2157.5(2)	gas	Ra,CAR	19,20
<i>a</i> ₂ ⁺	2	OPLA	457.81	gas	DL	14,18
			463s	Ne	IR	4
			453 ^c	Ar	IR	3,8
			463	N ₂	IR	3
<i>e</i> ⁺	3	CD stretch	2381.09	gas	IR	21
			2381w	Ne	IR	4
			2369	Ar	IR	6
	4	Deformation	1026vw	Ne	IR	4
			1029	Ar	IR	6

*B*₀ = 4.802 AB²DL¹⁴

^aTentative assignment.

^b $\frac{1}{2}(2\nu_2)$.

^cBand center. Rotational structure assigned.⁸

^dR(0₀) transition.

^eApproximate value; perturbed by Fermi resonance.

References

¹⁴J. M. Frye, T. J. Sears, and D. Leitner, *J. Chem. Phys.* **88**, 5300 (1988).

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SiH₃

M²A₂⁺ (6p) D_{3h}

*T*₀ = 60341 gas MPI⁷

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₂ ⁺	2	OPLA	800(30)	gas	MPI	7

J²A₂⁺ (5p) D_{3h}

*T*₀ = 56929 gas MPI⁷

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₂ ⁺	2	OPLA	821(4)	gas	MPI	7

E²A₂⁺ (4p) D_{3h}

*T*₀ = 48438 gas MPI^{5,7}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₂ ⁺	2	OPLA	796(7)	gas	MPI	5,7
<i>e</i> ⁺	4	Deformation	870(5) ^a	gas	MPI	7

X²A₁ C_{3v} Structure: ESR^{1,2}DL³

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₁	2	Umbrella	727.94 ^b 721.05 ^c	gas gas	DL,MPI DL,MPI	3,6,7 3,6,7

Barrier to inversion = 1935 gas PE⁴MPI⁷

*B*₀ = 4.763 DL³

SiD₃**P²A₂⁺ (7p)** D_{3h} $T_0 = 62002$ gas MPI⁷

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_2''	2	OPLA	615(3)	gas	MPI	7

N²E' (4f) D_{3h} $T_0 = 61005$ gas MPI^{7,8}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_2''	2	OPLA	619(7)	gas	MPI	7

M²A₂⁺ (6p) D_{3h} $T_0 = 60267$ gas MPI⁷

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_2''	2	OPLA	615(4)	gas	MPI	7

K²E' (4f) D_{3h} $T_0 = 58417$ gas MPI^{7,8}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_2''	2	OPLA	615(3)	gas	MPI	7

J²A₂⁺ (5p) D_{3h} $T_0 = 56874$ gas MPI⁷

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_2''	2	OPLA	608(3)	gas	MPI	7

H²E' (4p) D_{3h} $T_0 \sim 50000$ gas MPI^{7,8}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_2''	2	OPLA	602(5)	gas	MPI	7

E²A₂⁺ (4p) D_{3h} $T_0 = 48391$ gas MPI⁷

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1'	1	SiD ₃ stretch	1576(3)	gas	MPI	7
a_2''	2	OPLA	589(3)	gas	MPI	7
e'	4	Deformation	635(6) ^a	gas	MPI	7

X²A₁ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	2	Umbrella	545 ^b 542 ^c	gas gas	MPI MPI	7 7

Barrier to inversion = 1925 gas MPI⁷^a $\frac{1}{2}(2\nu_4)$.^b $1^- \rightarrow 0^+$ transition.^c $1^+ \rightarrow 0^-$ transition.**References**

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GeH₃**5p²A₂⁺** D_{3h} $T_0 = 47705(5)$ gas MPI¹

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_2''	2	OPLA	756(5)	gas	MPI	1

X²A₁ C_{3v}^a

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	2	Umbrella	663(10)	gas	MPI	1

^aEstimated inversion barrier is 1530.**References**

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

NH₃

$\tilde{X}^2A_2'$	D_{3h}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1'	1	NH stretch	~2740	gas	PE	3
a_2''	2	OPLA	903.536	gas	PE,DL	3,6
e'	3	NH stretch	3388.65	gas	LD	5

$$B_0 = 10.644; C_0 = 5.246 \text{ LD}^5$$

References

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

AsH₃

$\tilde{X}^2A_1$	C_{3v}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_2	2	OPLA ^a	452(25)	gas	PE,PI	1,2

^aLow inversion barrier. Observed vibrational structure is above this barrier.

References

- ¹A. W. Potts and W. C. Price, *Proc. Roy. Soc. (London)* **A326**, 181 (1972).
²J. Berkowitz, *J. Chem. Phys.* **89**, 7065 (1988).

H₃O⁺

$\tilde{X}$	C_{3v} Structure: CC ^d					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	2	Umbrella	954.40 ^a	gas	DL	2,3,5,7
			525.82 ^b	gas	DL	5-7
e	3	OH stretch	3535.96 ^c	gas	CC	1,4,10
			3519.40 ^d	gas	CC	1,4,10
	4	Deformation	1625.95 ^c	gas	DL	11
			1638.53 ^d	gas	DL	11

$$B(0^+) = 11.254; (C-B)(0^+) = -4.91(6) \text{ IR, MW}^{9,12}$$

D₃O⁺

$\tilde{X}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	2	Umbrella	645.13 ^a	gas	DL	8
			438.39 ^b	gas	DL	8
e	3	OD stretch	2629.65 ^c	gas	LD	13
			2624.24 ^d	gas	LD	13

$$B(0^+) = 5.675 \text{ DL}^8 \text{ LD}^{13}$$

^a1⁻ → 0⁺ transition.

^b1⁺ → 0⁻ transition. For H₃O⁺, 0⁸ → 0⁺ = 55.35 cm^{-1,6,12} and for D₃O⁺, 15.39 cm^{-1,8}

^c1⁺ → 0⁺ transition.

^d1⁻ → 0⁻ transition.

References

- ¹M. H. Begemann, C. S. Gudeman, J. Pfaff, and R. Saykally, *Phys. Rev. Lett.* **51**, 554 (1983).
²N. N. Haese and T. Oka, *J. Chem. Phys.* **80**, 572 (1984).
³B. Lemoine and J. L. Destombes, *Chem. Phys. Lett.* **111**, 284 (1984).
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⁵P. B. Davies, P. A. Hamilton, and S. A. Johnson, *J. Opt. Soc. Am. B* **2**, 794 (1985).
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¹¹M. Grubele, M. Polak, and R. J. Saykally, *J. Chem. Phys.* **87**, 3347 (1987).
¹²P. Verhoeve, M. Versluis, J. J. Ter Meulen, W. L. Meerts, and A. Dymanus, *Chem. Phys. Lett.* **161**, 195 (1989).
¹³H. Petek, D. J. Nesbitt, J. C. Owrrutsky, C. S. Gudeman, X. Yang, D. O. Harris, C. B. Moore, and R. J. Saykally, *J. Chem. Phys.* **92**, 3257 (1990).

H₃S⁺

$\tilde{X}$	C_{3v}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	SH stretch	2521.05	gas	LD	3
	2	Umbrella	1033.31	gas	DL	2
e	3	SH stretch	2525.74	gas	D	1,3

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

References

- ¹T. Nakanaga and T. Amano, *Chem. Phys. Lett.* **134**, 195 (1987).
²T. Amano, K. Kawaguchi, and E. Hirota, *J. Mol. Spectrosc.* **126**, 177 (1987).
³T. Nakanaga and T. Amano, *J. Mol. Spectrosc.* **133**, 201 (1989).

6.5. Four-Atomic Dihydrides**Cu₂H₂**

$\tilde{X}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			1341.7	Ar	IR	1
			938.7	Ar	IR	1
			528.0	Ar	IR	1

Cu₂D₂ $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			975.3	Ar	IR	1
			687.7	Ar	IR	1

References

¹R. H. Hauge, Z. H. Kafafi, and J. L. Margrave, in "Physics and Chemistry of Small Clusters," P. Jena, B. K. Rao, and S. N. Khanna, Eds., p. 787 (Plenum, New York, 1987).

ZnCH₂

Photolysis threshold near 360 nm. In an argon matrix,¹ rearranges to HZnCH.

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a ₁	1	CH ₂ s-stretch	2958.5 2956.1	Ar	IR	1
	2	CH ₂ scissors	1341.5 1339.1	Ar	IR	1
	3	ZnC stretch	513.7 512.0	Ar	IR	1
b ₁	4	OPLA	524.8	Ar	IR	1
b ₂	5	CH ₂ a-stretch	3047.2	Ar	IR	1
	6	CH ₂ rock	543.8	Ar	IR	1

ZnCD₂ $\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a ₁	1	CD ₂ s-stretch	2165.7	Ar	IR	1
	2	CD ₂ scissors	1009.8	Ar	IR	1
	3	ZnC stretch	472.2	Ar	IR	1
b ₁	4	OPLA	419.0	Ar	IR	1
b ₂	6	CD ₂ rock	412.2	Ar	IR	1

References

¹S.-C. Chang, R. H. Hauge, Z. H. Kafafi, J. L. Margrave, and W. E. Billups, J. Chem. Soc., Chem. Commun. 1682 (1987).

HZnCH $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		ZnH stretch	1924.4ms	Ar	IR	1
		ZnC stretch	647.5wm	Ar	IR	1
		HZnC bend	469.3s	Ar	IR	1

DZnCD $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		ZnD stretch	1386.8m	Ar	IR	1
		ZnC stretch	627.2wm	Ar	IR	1
		DZnC bend	344.7s	Ar	IR	1

References

¹S.-C. Chang, R. H. Hauge, Z. H. Kafafi, J. L. Margrave, and W. E. Billups, J. Chem. Soc., Chem. Commun. 1682 (1987).

FeCH₂

Photolysis threshold near 360 nm. In an argon matrix,² rearranges to HFeCH.

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a ₁	1	CH ₂ s-stretch	2941.6m	Ar	IR	1,2
	3	FeC stretch	623.9vs	Ar	IR	1,2
b ₁	4	OPLA	700.3s 697.4	Ar	IR	1,2
b ₂	5	CH ₂ a-stretch	3011.5	Ar	IR	2
	6	CH ₂ rock	452.0	Ar	IR	2

FeCD₂ $\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a ₁	1	CD ₂ s-stretch	2134.3	Ar	IR	2
	3	FeC stretch	575.2	Ar	IR	2
b ₁	4	OPLA	552.7 550.9	Ar	IR	2
b ₂	5	CD ₂ a-stretch	2201.0	Ar	IR	2
	6	CD ₂ rock	347.6	Ar	IR	2

References

¹S.-C. Chang, Z. H. Kafafi, R. H. Hauge, W. E. Billups, and J. L. Margrave, J. Am. Chem. Soc. **107**, 1447 (1985).

²S.-C. Chang, R. H. Hauge, Z. H. Kafafi, J. L. Margrave, and W. E. Billups, J. Am. Chem. Soc. **110**, 7975 (1988).

HFeCH

Photolysis threshold near 400 nm. In an argon matrix,¹ rearranges to FeCH₂.

 $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		FeH stretch	1681.6	Ar	IR	1
		FeC stretch	674.2	Ar	IR	1
		FeCH bend	632.1	Ar	IR	1

DFeCD $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		FeD stretch	1209.2	Ar	IR	1
		FeC stretch	648.3	Ar	IR	1
		FeCD bend	503.7	Ar	IR	1

References

- ¹S.-C. Chang, R. H. Hauge, Z. H. Kafafi, J. L. Margrave, and W. E. Billups, *J. Am. Chem. Soc.* **110**, 7975 (1988).

CuCH₂ $\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	CH ₂ s-stretch	2960.7	Ar	IR	1
	2	CH ₂ scissors	1344.9	Ar	IR	1
	3	CuC stretch	614.0	Ar	IR	1
b_1	4	OPLA	526.0	Ar	IR	1
b_2	5	CH ₂ a-stretch	3034.7	Ar	IR	1

CuCD₂ $\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	2	CD ₂ scissors	1013.7	Ar	IR	1
	3	CuC stretch	570.4	Ar	IR	1
b_1	4	OPLA	409.1	Ar	IR	1

References

- ¹S.-C. Chang, Z. H. Kafafi, R. H. Hauge, W. E. Billups, and J. L. Margrave, *J. Am. Chem. Soc.* **109**, 4508 (1987).

CaNH₂ $\tilde{C}^2A_1$ C_{2v} Structure: LF²

$T_0^a = 17375.129(5)$ gas CL¹LF²
 $B^a = 0.306$; $C^a = 0.298$ LF²

 $\tilde{C}-\tilde{X}$ 575 nm $\tilde{B}^2B_1$ C_{2v}

$T_0 = 15886$ gas CL¹LF^{3,4}
 $A = 14.6(2)$; $\frac{1}{2}(B + C) = 0.304$ LF⁴

 $\tilde{B}-\tilde{X}$ 620–650 nm $\tilde{A}^2B_2$ C_{2v} $T_0 = 15464$ gas CL¹LF^{3,4} $\tilde{A}-\tilde{X}$ 620–650 nm

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

 $A = 11.4$; $\frac{1}{2}(B + C) = 0.304$ LF⁷ $\tilde{X}^2A_1$ C_{2v} Structure: LF²

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	3	CaN stretch	524(10)	gas	F	3

 $A = 13.0$; $B^a = 0.301$; $C^a = 0.293$ LF^{2,4}*From analysis of $K_{-1} = 1$ subband of $\tilde{C}-\tilde{X}$ transition.**References**

- ¹R. F. Wormsbecher, M. Trkula, C. Martner, R. E. Penn, and D. O. Harris, *J. Mol. Spectrosc.* **97**, 29 (1983).
²R. F. Wormsbecher, R. E. Penn, and D. O. Harris, *J. Mol. Spectrosc.* **97**, 65 (1983).
³A. M. R. P. Bopegedera, C. R. Brazier, and P. F. Bernath, *J. Phys. Chem.* **91**, 2779 (1987).
⁴C. J. Whitham and Ch. Jungen, *J. Chem. Phys.* **93**, 1001 (1990).

CuNH₂ $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		NH stretch	3369.3	Ar	IR	1
		NH ₂ deform.	1528.0	Ar	IR	1
		CuN stretch	748.2	Ar	IR	1

CuND₂ $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		ND stretch	2471.7	Ar	IR	1
		ND ₂ deform.	1147.9	Ar	IR	1

References

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

HBNH

$\tilde{\chi}$	$C_{\infty v}$	Structure: $MO^{1,2}$				
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NH stretch	3700m	Ar	IR	3
Σ^+	3	BN stretch	1786.19 1785m	gas Ar	L IR	4 3
Π	4	Bend	460m	Ar	IR	3

$$B_0 = 1.099 \text{ DL}^4$$

DBND

$\tilde{\chi}$	$C_{\infty v}$					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	ND stretch	2836	Ar	IR	3
Σ^+	2	BD stretch	2730	Ar	IR	3
Σ^+	3	BN stretch	1734	Ar	IR	3
Π	4	Bend	360	Ar	IR	3

References

¹N. C. Baird and R. K. Datta, *Inorg. Chem.* **11**, 17 (1972).

²D. R. Armstrong and D. T. Clark, *Theor. Chim. Acta* **24**, 307 (1972).

³E. R. Lory and R. F. Porter, *J. Am. Chem. Soc.* **95**, 1766 (1973).

⁴Y. Kawashima, K. Kawaguchi, and E. Hirota, *J. Chem. Phys.* **87**, 6331 (1987).

HMgOH

$\tilde{\chi}$	$C_{\infty v}$					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	MgH stretch MgO stretch	1591.8 742.3	Ar Ar	IR IR	1 1

DMgOD

$\tilde{\chi}$	$C_{\infty v}$					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	MgD stretch MgO stretch	1162.8 715.3	Ar Ar	IR IR	1 1

References

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

HCaOH

$\tilde{\chi}$	$C_{\infty v}$					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	OH stretch	3697	Ar	IR	1
	2	CaH stretch CaO stretch	1232.8 574.8	Ar Ar	IR IR	1 1

DCaOD

$\tilde{\chi}$	$C_{\infty v}$					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	CaD stretch CaO stretch	887.3 576.5	Ar Ar	IR IR	1 1

References

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

HSrOH

$\tilde{\chi}$	$C_{\infty v}$					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	SrH stretch SrO stretch	1143.2 498.2	Ar Ar	IR IR	1 1

DSrOD

$\tilde{\chi}$	$C_{\infty v}$					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	SrD stretch SrO stretch	818.0 487.4	Ar Ar	IR IR	1 1

References

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

HBaOH

$\tilde{\chi}$	$C_{\infty v}$					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	BaH stretch BaO stretch	1059.4 458.9	Ar Ar	IR IR	1 1

DBaOD

$\bar{\chi}$	$C_{\infty v}$					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	BaD stretch	757.2	Ar	IR	1
		BaO stretch	447.7	Ar	IR	1

References

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

HCrOH

$\bar{\chi}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CrH stretch	1639.9	Ar	IR	1
		CrO stretch	674.1	Ar	IR	1
		Bend	433.8	Ar	IR	1

DCrOD

$\bar{\chi}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CrD stretch	1184.5	Ar	IR	1
		CrO stretch	654.0	Ar	IR	1

References

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

HMnOH

$\bar{\chi}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	MnH stretch	1663.4	Ar	IR	1
		MnO stretch	648.1	Ar	IR	1

DMnOD

$\bar{\chi}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	MnD stretch	1197.1	Ar	IR	1
		MnO stretch	628.5	Ar	IR	1

References

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

HFeOH

$\bar{\chi}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	FeH stretch	1731.9	Ar	IR	1
		FeO stretch	682.4	Ar	IR	1
		Bend	457.6	Ar	IR	1

DFeOD

$\bar{\chi}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	FeD stretch	1245.3	Ar	IR	1
		FeO stretch	660.5	Ar	IR	1

References

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

HCoOH

$\bar{\chi}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CoH stretch	1790.4	Ar	IR	1
		CoO stretch	667.4	Ar	IR	1

DCoOD

$\bar{\chi}$						
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CoD stretch	1291.2	Ar	IR	1
		CoO stretch	641.9	Ar	IR	1

References

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

HNiOHPhotodissociates, losing H, on 280–360 nm irradiation.¹ $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OH stretch	3698.6	Ar	IR	1
			3688.4	Kr	IR	1
		NiH stretch	1901.0	Ar	IR	1
			1837.3			
			1893.0	Kr	IR	1
			1830.8			
		NiO stretch	707.0	Ar	IR	1
			690.6			
			699.1	Kr	IR	1
			685.8			

DNiOD $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OD stretch	2726.4	Ar	IR	1
		NiD stretch	1336.2	Ar	IR	1
			1323.9			
		NiO stretch	681.2	Ar	IR	1
			664.8			

References¹M. Park, R. H. Hauge, and J. L. Margrave, High Temp. Sci. **25**, 1 (1988).**HCuOH** $\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	2	CuH stretch	1910.8	Ar	IR	1
		⁶³ CuO stretch	615.6	Ar	IR	1
		CuOH bend	668.6	Ar	IR	1

DCuOD $\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	2	CuD stretch	1380.8	Ar	IR	1
		⁶³ CuO stretch	613.8	Ar	IR	1
		CuOD bend	496.0	Ar	IR	1

References¹J. W. Kauffman, R. H. Hauge, and J. L. Margrave, J. Phys. Chem. **89**, 3541 (1985).**H₂C=C** $\tilde{b}^3A_2$ C_{2v} $T_0 = 22200(160)$ gas PE⁶ $\tilde{a}^3B_2$ C_{2v} $T_0 = 16660(50)$ gas PE⁶

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	CH ₂ s-stretch	2930(10)	gas	PE	6
	2	C=C stretch	1530(70)	gas	PE	6
	3	CH ₂ scissors	1375(10)	gas	PE	6

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	CH ₂ s-stretch	3025(30)	gas	PE	6
	2	C=C stretch	1635(10)	gas	PE	3,6
	3	CH ₂ scissors	1165(10)	gas	PE	3,6

D₂C=C $\tilde{a}^3B_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	CD ₂ s-stretch	2160(10)	gas	PE	6
	2	C=C stretch	1495(10)	gas	PE	6
	3	CD ₂ scissors	1010(10)	gas	PE	6

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	CD ₂ s-stretch	2190(30)	gas	PE	6
	2	C=C stretch	1590(20)	gas	PE	3,6
	3	CD ₂ scissors	865(10)	gas	PE	3,6

References⁶K. M. Ervin, J. Ho, and W. C. Lineberger, J. Chem. Phys. **91**, 5974 (1989).**HCNH⁺** $\tilde{X}$ $C_{\infty v}$ Structure: LD³

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ	1	NH stretch	3482.84	gas	LD	1,2
	2	CH stretch	3187.86	gas	LD	1,2
	3	CN stretch	2155.70	gas	DL	6,7
Π	4	HCN bend	801.59	gas	DL	4
	5	HNC bend	645.92	gas	DL	5

 $B_0 = 1.236$ LD^{1,2}

References

- ¹R. S. Altman, M. W. Crofton, and T. Oka, *J. Chem. Phys.* **80**, 3911 (1984).
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⁴K. Tanaka, K. Kawaguchi, and E. Hirota, *J. Mol. Spectrosc.* **117**, 408 (1986).
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H₂C=C⁻

Threshold for electron detachment from ground-state H₂C=C⁻ = 3950(50) gas PE¹

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a ₁	2	CC stretch	1485(30)	gas	PE	1
	3	CH ₂ scissors	1305(10)	gas	PE	1

D₂C=C⁻

Threshold for electron detachment from ground-state D₂C=C⁻ = 3970(50) gas PE¹

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a ₁	3	CD ₂ scissors	960(20)	gas	PE	1

References

- ¹K. M. Ervin, J. Ho, and W. C. Lineberger, *J. Chem. Phys.* **91**, 5974 (1989).

HGaOH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OH stretch	3675	Ar	IR	1
		HGa stretch	1669.8	Ar	IR	1
		HGaO bend	784.9	Ar	IR	1
		⁶⁹ GaO stretch	646.4 ^a	Ar	IR	1
		GaOH bend	520.5	Ar	IR	1

DGaOD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OD stretch	2708	Ar	IR	1
		DGa stretch	1213.8	Ar	IR	1
		⁶⁹ GaO stretch	644.6	Ar	IR	1
		DGaO bend	582.9	Ar	IR	1

References

- ¹R. H. Hauge, J. W. Kauffman, and J. L. Margrave, *J. Am. Chem. Soc.* **102**, 6005 (1980).

HInOH

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OH stretch	3663	Ar	IR	1
		HIn stretch	1486.3	Ar	IR	1
		HInO bend	713.4	Ar	IR	1
		InO stretch	548.0	Ar	IR	1

DInOD

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		DIn stretch	1080.1	Ar	IR	1
		InO stretch	550.9	Ar	IR	1

References

- ¹R. H. Hauge, J. W. Kauffman, and J. L. Margrave, *J. Am. Chem. Soc.* **102**, 6005 (1980).

H₂CSe

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

Structure: LF⁷

T₀ ~ 13555 gas LF^{5,6}

$\tilde{A}-\tilde{X}$ 685-720 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a ₁	3	C=Se stretch	662	gas	LF	6
b ₁	4	OPLA	~355	gas	LF	6

A^a = 9.015; B^a = 0.377; C^a = 0.360 LF⁷

$\tilde{a}^3A_2$ C_{2v} $T_0 = 12171.0$ gas $AB^1CL^3LF^{5,6}$ $\tilde{a}-\tilde{X}$ 658–822 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH ₂ scissors	1312	gas	LF	5,6
	3	C=Se stretch	704	gas	AB,CL	1,3,5,6
b_1	4	OPLA	297 ^b	gas	AB,LF	1,5,6
b_2	6	HCS _e bend	812 ^c	gas	LF	5,6

 $\tilde{X}^1A_1$ C_{2v} Structure: MW^{2,4}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	C=Se stretch	~901	gas	LF	6

 $A_0 = 9.690$; $B_0 = 0.414$; $C_0 = 0.396$ MW^{2,4}LF⁷**D₂CSe** $\tilde{A}^1A_2$ C_{2v} $T_0 = 13631.4$ gas LF⁶ $\tilde{A}-\tilde{X}$ 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

 $A_0 = 4.711$; $B_0 = 0.316$; $C_0 = 0.296$ LF⁷ $\tilde{a}^3A_2$ C_{2v} $T_0 = 12262.7$ gas LF⁶ $\tilde{a}-\tilde{X}$ 661–815 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD ₂ scissors	996	gas	LF	6
	3	C=Se stretch	667	gas	LF	6
b_1	4	OPLA	208 ^b	gas	LF	6
b_2	6	DCSe bend	563 ^c	gas	LF	6

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	C=Se stretch	~789	gas	LF	6

 $A_0 = 4.87(2)$; $B_0 = 0.344$; $C_0 = 0.321$ MW⁴LF⁷^a $v_4 = 1$.^bFrom fit to double minimum potential. Barrier to inversion 13.1 for H₂CSe, 16.2 for D₂CSe.⁶^c $\frac{1}{2}(2\nu_i)$.

References

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²R. D. Brown, P. D. Godfrey, and D. McNaughton, Chem. Phys. Lett. **118**, 29 (1985).

³R. J. Glinski, E. A. Mishalanie, and J. W. Birks, J. Am. Chem. Soc. **108**, 531 (1986).⁴R. D. Brown, P. D. Godfrey, D. McNaughton, and P. R. Taylor, J. Mol. Spectrosc. **120**, 292 (1986).⁵D. J. Clouthier, R. H. Judge, and D. C. Moule, Chem. Phys. **114**, 417 (1987).⁶R. H. Judge, D. J. Clouthier, and D. C. Moule, J. Chem. Phys. **89**, 1807 (1988).⁷D. J. Clouthier, R. H. Judge, and D. C. Moule, J. Mol. Spectrosc. **141**, 175 (1990).**H₂SiO** $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Si=O stretch	1202	Ar	IR	1,2
		SiH ₂ deform.	697	Ar	IR	2

D₂SiO $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Si=O stretch	1189	Ar	IR	1,2
		SiD ₂ deform.	533	Ar	IR	2

References

¹R. Withnall and L. Andrews, J. Am. Chem. Soc. **107**, 2567 (1985).²R. Withnall and L. Andrews, J. Phys. Chem. **89**, 3261 (1985).**HSiOH** $\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3661	Ar	IR	1,2
	2	SiH stretch	1882 ^a 1847	Ar	IR	1,2
	3	HSiO bend	937	Ar	IR	1,2
	4	SiO stretch	851	Ar	IR	1,2
	5	SiOH bend	723	Ar	IR	1,2
a''	6	Torsion	595	Ar	IR	1,2

DSiOD

 $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	1	OD stretch	2667	Ar	IR	2
	2	SiD stretch	1354	Ar	IR	1,2
	3	DSiO bend	715	Ar	IR	1,2
			701 ^b	Ar	IR	1
	4	SiO stretch	847 ^b	Ar	IR	1,2
<i>a''</i>			841	Ar	IR	1,2
	5	SiOD bend	521	Ar	IR	1,2
	6	Torsion	447	Ar	IR	1,2

^aFermi resonance splitting.^bLess stable rotamer, presumed to have the *cis*-structure.

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- ¹Z. K. Ismail, R. H. Hauge, L. Fredin, J. W. Kauffman, and J. L. Margrave, *J. Chem. Phys.* **77**, 1617 (1982).
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H₂GeO $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		GeH ₂ stretch	2079.6	Ar	IR	1
		GeH ₂ stretch	2076.6	Ar	IR	1
		Ge=O stretch	961.9	Ar	IR	1
		GeH ₂ scissors	803.8	Ar	IR	1

D₂GeO $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		GeD ₂ a-stretch	1495.7	Ar	IR	1
		GeD ₂ s-stretch	1490.1	Ar	IR	1
		Ge=O stretch	963.2	Ar	IR	1
		D ₂ GeO wag	615.4	Ar	IR	1
		GeH ₂ scissors	577	Ar	IR	1

References

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

HGeOH

 $\bar{\chi}$ *C_s*

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	1	OH stretch	3652.0	Ar	IR	2
	2	GeH stretch	1741.3	Ar	IR	1,2
	3	GeOH bend	885.2	Ar	IR	2
	4	HGeO bend	708.7	Ar	IR	2
	5	GeO stretch	657.6	Ar	IR	1,2
<i>a''</i>	6	Torsion	566.2	Ar	IR	1,2

DGeOD

 $\bar{\chi}$ *C_s*

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	1	OD stretch	2695.1	Ar	IR	2
	2	GeD stretch	1257.6	Ar	IR	2
	3	GeOD bend	685.4	Ar	IR	2
	4	GeO stretch	642.0	Ar	IR	2
	5	DGeO bend	503.0	Ar	IR	2
<i>a''</i>	6	Torsion	420.3	Ar	IR	2

References

- ¹J. W. Kauffman, R. H. Hauge, and J. L. Margrave, "Metal Bonding and Interactions in High Temperature Systems," J. L. Gole and W. C. Stwalley, Eds., ACS Symposium Ser. 179 (American Chemical Society, Washington, D. C., 1982), pp. 355-362.
²R. Withnall and L. Andrews, *J. Phys. Chem.* **94**, 2351 (1990).

HSnOH

 $\bar{\chi}$ *C_s*

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	2	SnH stretch	1608.0	Ar	IR	1
			1597.7			
	4	HSnO bend	782.6	Ar	IR	1
<i>a''</i>	5	SnO stretch	569.3	Ar	IR	1
	6	Torsion	475.5	Ar	IR	1

References

- ¹J. W. Kauffman, R. H. Hauge, and J. L. Margrave, "Metal Bonding and Interactions in High Temperature Systems," J. L. Gole and W. C. Stwalley, Eds., ACS Symposium Ser. 179 (American Chemical Society, Washington, D. C., 1982), pp. 355-362.

H₂NN

Photolyzes on irradiation of the sample by visible light; solid solution in 2-methyltetrahydrofuran at 80 K shows structured absorption between 500 and 730 nm, with maximum near 636 nm.¹

 $\bar{\chi}$ *C_{2v}*

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a₁</i>	1	NH stretch	2862.0s	Ar	IR	1,2
	2	NH ₂ scissors	1644.7w	Ar	IR	2
	3	N=N stretch	1574.2m	Ar	IR	1,2
<i>b₁</i>	4	OPLA	1002.7vs	Ar	IR	1,2
<i>b₂</i>	5	NH stretch	2804.6m	Ar	IR	1,2
	6	NH ₂ rock	1287.5vw	Ar	IR	2

D₂NN $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₁	1	ND stretch	2140.2vs	Ar	IR	2
	2	N=N stretch	1599.0wm	Ar	IR	1,2
<i>b</i> ₁	4	OPLA	793.5ms	Ar	IR	1,2
<i>b</i> ₂	5	ND stretch	2107.0s	Ar	IR	1,2

References

- ¹A. P. Sylwester and P. B. Dervan, *J. Am. Chem. Soc.* **106**, 4648 (1984).
²J. H. Teles, G. Maier, B. A. Hess, Jr., and L. J. Schaad, *Chem. Ber.* **122**, 749 (1989).

H₂CS⁻

Threshold for electron detachment from ground-state H₂CS⁻ = 3750(185) gas PE^{1,2}

 $\tilde{X}$ *C*_{2v}Structure: PE^{1,2}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₁	3	CS stretch	860(220)	gas	PE	1,2
<i>b</i> ₁	4	OPLA	450(120)	gas	PE	1,2

References

- ¹S. Moran and G. B. Ellison, *Int. J. Mass Spectrom. Ion Proc.* **80**, 83 (1987).
²S. Moran and G. B. Ellison, *J. Phys. Chem.* **92**, 1794 (1988).

H₂CCl $\tilde{X}$ *C*_{2v}Structure: ESR³MW⁴

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₁	2	CH ₂ scissors	1391wm	Ar	IR	2
	3	CCl stretch	827s	Ar	IR	1,2
<i>b</i> ₁	4	OPLA	402s	Ar	IR	1,2

*A*₀ = 9.152(3); *B*₀ = 0.532; *C*₀ = 0.502 MW⁴

D₂CCl $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₁	2	CD ₂ scissors	1045m	Ar	IR	1,2
	3	CCl stretch	788m	Ar	IR	1,2
<i>b</i> ₁	4	OPLA	291m	Ar	IR	1,2

References

- ¹M. E. Jacox and D. E. Milligan, *J. Chem. Phys.* **53**, 2688 (1970).
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H₂Cl $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CH stretch	~3050	gas	IR	2
		CH ₂ scissors	~1330	gas	IR	2
			1331.5s	Ar	IR	1
		Cl stretch	611wm	Ar	IR	1
		Umbrella	375s	Ar	IR	1

D₂Cl $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CD ₂ scissors	994m	Ar	IR	1
		Cl stretch	578w	Ar	IR	1
		Umbrella	271s	Ar	IR	1

References

- ¹D. W. Smith and L. Andrews, *J. Chem. Phys.* **58**, 5222 (1973).
²S. L. Baughcum and S. R. Leone, *J. Chem. Phys.* **72**, 6531 (1980).

H₂PO $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		PH stretch	2275.7	Ar	IR	1
			2273.8			
		P=O stretch	1153.1	Ar	IR	1
			1151.7			
			1147.7			
		PH ₂ rock	833.2	Ar	IR	1
		PH ₂ wag	791.6	Ar	IR	1

D₂PO $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		PD stretch	1648.2	Ar	IR	1
		P=O stretch	1147.3	Ar	IR	1
			1141.7			
			1137.7			
		PD ₂ rock	628.4	Ar	IR	1
		PD ₂ wag	602.9	Ar	IR	1

References

¹R. Withnall and L. Andrews, *J. Phys. Chem.* **92**, 4610 (1988).

HPOH

 $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		POH deform.	1094.4	Ar	IR	1
		HPO deform.	955.7	Ar	IR	1
		P-O stretch	817.7	Ar	IR	1
		Torsion	406.3	Ar	IR	1

DPOD

 $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OD stretch	2689.0	Ar	IR	1
		POD deform.	821.8	Ar	IR	1
			820.2			
		P-O stretch	816.6	Ar	IR	1
		DPO deform.	710.5	Ar	IR	1
		Torsion	303	Ar	IR	1

References

¹R. Withnall and L. Andrews, *J. Phys. Chem.* **92**, 4610 (1988).

NH₂F⁺ $\tilde{C}, \tilde{D}^2A', ^2A'$ C_s

$T^a = 52300(1000)$ gas PE¹

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

$T^a = 34500(1000)$ gas PE¹

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

$T^a = 21220(160)$ gas PE¹

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			~550	gas	PE	1

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			~300 ^b	gas	PE	1

^aFrom vertical ionization potentials.

^bSeparation characteristic of higher vibrational spacings.

References

¹H. Baumgärtel, H.-W. Jochims, E. Rühl, H. Bock, R. Dammel, J. Minkwitz, and R. Nass, *Inorg. Chem.* **28**, 943 (1989).

NH₂F $\tilde{X}$ C_sStructure: MW²

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	NH ₂ s-stretch	3269 ^a	Ar	IR	1
			3234	N ₂	IR	3
	2	NH ₂ scissors	1568 ^a	Ar	IR	1
			1564	N ₂	IR	3
	3	NH ₂ wag	1244 ^a	Ar	IR	1
a''			1241	N ₂	IR	3
			1233			
	4	NF stretch	934 ^a	Ar	IR	1
			891	N ₂	IR	3
	5	NH ₂ a-stretch	3346	N ₂	IR	3

Barrier to inversion = 5250 MW²

$A_0 = 8.782$; $B_0 = 0.879$; $C_0 = 0.845$ MW²

ND₂F $\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	ND ₂ s-stretch	2399 ^a	Ar	IR	1
	2	ND ₂ scissors	1151 ^a	Ar	IR	1
	3	ND ₂ wag	968 ^a	Ar	IR	1
	4	NF stretch	924 ^a	Ar	IR	1

$A_0 = 4.612$; $B_0 = 0.784$; $C_0 = 0.726$ MW²

^aHF or DF trapped in adjacent site.

References

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

²D. Christen, R. Minkwitz, and R. Nass, *J. Am. Chem. Soc.* **109**, 7020 (1987).

³H. Baumgärtel, H.-W. Jochims, E. Rühl, H. Bock, R. Dammel, J. Minkwitz, and R. Nass, *Inorg. Chem.* **28**, 943 (1989).

PH₂F $\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	PH ₂ s-stretch	2304	Ar	IR	1
	2	PH ₂ scissors	1090	Ar	IR	1
	3	PH ₂ s-deform.	934	Ar	IR	1
	4	PF stretch	795 ^{vs}	Ar	IR	1
a''	5	PH ₂ a-stretch	2310	Ar	IR	1

PD₂F

$\bar{\chi}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	PD ₂ s-stretch	1673	Ar	IR	1
	3	PF stretch	798	Ar	IR	1
	4	PD ₂ s-deform.	701	Ar	IR	1
a''	5	PD ₂ a-stretch	1680	Ar	IR	1

References

¹L. Andrews and R. Withnall, *Inorg. Chem.* **28**, 494 (1989).

H₂O₂

Continuous absorption, 120–300 nm.^{1,2,7,12}

$\bar{\chi}$	C_2					
	Structure: IR ^{4,10} MW ⁸					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a	1	OH s-stretch	3617.95 ^a	gas	IR,Ra	3,4,10,17
			3609.8			
			3593	Ar	Ra	11
	2	OH s-bend	1393.5	gas	Ra	10
			1385	Ar	Ra	11
	3	OO stretch	863.5	gas	Ra	10
			869	Ar	Ra	11
	4	Torsion	370.89 ^a	gas	IR	6,17,18,19
			254.55			
			372br	Ar	IR	9
b	5	OH a-stretch	264			
			378vs,br	N ₂	IR	5,9
			3618.84 ^a	gas	IR	3,4,17
			3610.66			
			3597	Ar	IR	9
			3589			
			3587s	N ₂	IR	5,9
			3582s			
			1273.68 ^a	gas	IR,DL	3,16
			1264.58			
	6	OH a-bend	1277ms	Ar	IR	9
			1271vs			
			1294vs	N ₂	IR	5,9

$A_0 = 10.069$; $B_0 = 0.874$; $C_0 = 0.838$ IR^{4,17}MW^{8,13–15}

D₂O₂

$\bar{\chi}$	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

 $\bar{\chi}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
b	5	OD a-stretch	2661m	gas	IR	3
			2646	Ar	IR	9
			2646	N ₂	IR	9
	6	OD a-bend	947s	gas	IR	3
			951vs	Ar	IR	9
			966vs	N ₂	IR	9

^aTransitions to two lowest torsional levels associated with this fundamental are given.

References

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HFe₂F $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		HFe stretch	1713.9	Ar	IR	1
		FeF stretch	651.6	Ar	IR	1

References

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HC₃ $\tilde{X}^2\Pi_{1/2}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3238.0 ^a	Ar	IR	5
	2	C ₃ a-stretch	1832.3 1824.8	Ar	IR	1,5
	3	C ₃ s-stretch	1167br 1159.7	Ar	IR	5
Π	4	HCC bend	28 ^b	gas	MW	4

$A = 14.44$ gas MW²⁻⁴

$B_0 = 0.373$ MW²⁻⁴

DC₃ $\tilde{X}^2\Pi_{1/2}$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2424.2 ^a	Ar	IR	5
	2	C ₃ a-stretch	1779.3 1770.6	Ar	IR	1,5
	3	C ₃ s-stretch	1148.0 1140.3	Ar	IR	5

$A = 12.53$ gas MW⁴

$B_0 = 0.337$ MW⁴

^aTentative assignment.

^b Σ^u component.

References

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HNCN $\tilde{A}^2A'$ C_s Structure: AB¹

$T_0 = 28994.1$ gas AB¹ $\tilde{A}-\tilde{X}$ 344 nm

$A_0 = 22.438$; $B_0 = 0.376$; $C_0 = 0.369$ AB¹

$\tilde{X}^2A''$ C_s Structure: AB¹

$A_0 = 21.220$; $B_0 = 0.370$; $C_0 = 0.362$ AB¹

References

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HCCO

On flash photolysis of oxazole or isoxazole (C₃H₃NO), absorption band systems appear between 367 and 340 nm and between 340 and 308 nm which have tentatively been assigned to HCCO.¹ Band separations of 1057 and 1074 were identified in the first of these transitions and of 423 and 969 in the second, with some evidence for a "hot band" at 505 in the second transition.

Analysis of the submillimeter-wave spectrum² indicates that HCCO possesses a low-lying excited electronic state which, together with the ground state, is derived from a Π state by Renner-Teller interaction.

 $\tilde{X}$ C_s Structure: MW²

$A_0 = 41.5(1.5)$; $B_0 = 0.363$; $C_0 = 0.359$ MW²

DCCO $\tilde{X}$ C_s

$A_0 = 21.75(12)$; $B_0 = 0.331$; $C_0 = 0.325$ MW²

References

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HCNN $\tilde{A}$

$T_0 = 30500$ gas AB^{1,2,4,5} $\tilde{A}-\tilde{X}$ 289–328 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			1048	gas	AB	4

 $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CH stretch	3233wm 3229m	Ar N ₂	IR	3
		CNN a-stretch	1787s 1784s 1800s	Ar Kr N ₂	IR	3
		H deform.	861vs 860vs 871m 863m	Ar Kr N ₂	IR	3

DCNN

$\tilde{X}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CNN a-stretch	1771vs	Ar	IR	3
		D deform.	725vs	Ar	IR	3

References

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HNCO

Between 132.5 and 120 nm, continuous absorption, with some diffuse bands.⁵

Relatively sharp absorption bands at 72940, 73910, and 74680 (137.1, 135.3, and 133.9 nm), which may be contributed by a Rydberg transition.⁵

Between 147 and 163 nm, diffuse bands are superposed on a continuum, with maximum near 157 nm.⁵

Continuous absorption between 163 and 185 nm, with a maximum near 166 nm.⁵

Continuous absorption has its onset near 41000 (244 nm), and extends beyond 200 nm.⁴

$\tilde{A}'A''$ C _s			$\tilde{A}-\tilde{X}$ 228–282 nm			
gas AB ⁴						

Complicated group of progressions, possibly resulting from the occurrence of *cis*- and *trans*- rotamers in the excited state.

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'		NCO bend	~555	gas	AB	4

$A \sim 4.37$; $B \sim 0.388$; $C \sim 0.357$ AB⁴

$\tilde{X}'A'$ C _s			Structure: MW ⁷			
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	NH stretch	3538.25s	gas	IR	1,2,12
			3516.8wm	Ar	IR	14
			3505.7wm			12
	2	NCO a-stretch	2268.89vs	gas	IR	1,2,9,10
			2259.0vs	Ar	IR	12,13
	3	NCO s-stretch	1327vw	gas	IR	1,2
	4	HNC, NCO bend	776.62wm	gas	IR	6
			769.8wm	Ar	IR	12,13
	5	HNC, NCO bend	577.35w	gas	IR	1,2,6
			573.7wm	Ar	IR	12,13
a''	6	Torsion	656.29	gas	IR	6,11

$A_0 = 30.638$; $B_0 = 0.369$; $C_0 = 0.364$ MW⁷IR¹⁴

DNCO

$\tilde{X}'A'$ 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

$A_0 = 17.09$; $B_0 = 0.344$; $C_0 = 0.336$ MW⁷

References

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HOCN

$\tilde{X}$ C _s			Structure: MO ²⁻⁴			
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	OH stretch	3610	Ne	IR	5
			3569.6s	Ar	IR	1,6
			3506s	N ₂	IR	1
	2	C≡N stretch	2294	Ne	IR	5
			2286.3vs	Ar	IR	1,6,7
			2294s	N ₂	IR	1
	3	OH deform.	1227	Ne	IR	5
			1227.9s	Ar	IR	1,6,7
			1241m	N ₂	IR	1
	4	C-O stretch	1082	Ne	IR	5
			1081.3m	Ar	IR	1,6,7
			1098s	N ₂	IR	1
	5	OCN deform.	460wm	N ₂	IR	1

DOCN

$\tilde{\chi}$	C_∞					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2635.0vs 2590sh	Ar N ₂	IR	1,6 1
	2	C≡N stretch	2284.6vs 2292s	Ar N ₂	IR	1,6 1
	3	OD deform.	1077.8ms 1093m	Ar N ₂	IR	1,6 1
	4	C-O stretch	949.4m 957m	Ar N ₂	IR	1,6 1
	5	OCN deform.	437wm	N ₂	IR	1

References

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HCNO

A	C_s		
$T_0 \leq 35053$	gas	AB ⁸	$\tilde{A}-\tilde{X}$ 244–285 nm
Underlying absorption continuum, with increasing intensity at shorter wavelengths. ⁸			

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Bend	345(5)	gas	AB	8

$\tilde{\chi}$	C_∞ ^a		Structure: MW, IR ¹³ MO ¹⁵			
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3336.1	gas	IR	1,10
			3338	Ne	IR	14
			3317.2s	Ar	IR	17
			3311	N ₂	IR	17
			2195.8	gas	IR	1,2,10
	2	CNO a-stretch	2200	Ne	IR	14
			2192.7vs	Ar	IR	17
			2200	N ₂	IR	17
			1253.4	gas	IR	1,2,10
			1250	Ne	IR	14
Π	3	CNO s-stretch	1244.1m	Ar	IR	17
			1232	N ₂	IR	17
	4	CNO bend	537.25	gas	IR	1,2,9,16
			539	Ne	IR	14
			538.2w	Ar	IR	17
			536.9w			
			528	N ₂	IR	17
	5	HCN bend	224.11	gas	IR	9,11
			560	Ne	IR	17
			566.6m	Ar	IR	17
			582	N ₂	IR	17

$B_0 = 0.383$ MW^{3,4}

DCNO

$\tilde{\chi}$	C_∞ ^a					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2620.73 2612.7vs	gas Ar	IR	7 17
	2	CNO a-stretch	2070.92 2063.2s	gas Ar	IR	12 17
	3	CNO s-stretch	1254 1218.5m	gas Ar	IR	2,6 17
	Π	DCN bend	162.7	gas	IR	9
			418.5wm	Ar	IR	17

$B_0 = 0.343$ MW^{3,5} IR⁷

^aQuasilinear. See discussion in Refs. 13, 15, and 17.

References

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HONC

$\tilde{\chi}$	C_∞					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3443.7vs	Ar	IR	1,2
	2	NC stretch	2190.1wm	Ar	IR	1,2
	3	HON bend	1232.4m	Ar	IR	1,2
	4	NO stretch	628.4w	Ar	IR	1,2
	5	ONC bend	361.2w	Ar	IR	1,2
a''	6	Torsion	379.3w	Ar	IR	1,2

DONC

$\tilde{X}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2545.2vs	Ar	IR	1,2
	2	NC stretch	2190.3wm	Ar	IR	1,2
	3	DON bend	902.6m	Ar	IR	1,2
	4	NO stretch	623.1w	Ar	IR	1,2
	5	ONC bend	357.3w	Ar	IR	2
a''	6	ONC bend	362.1w	Ar	IR	1,2

References

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HOCO⁺

$\tilde{X}$	C_s	Structure:	MW ⁵			
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3375.37	gas	LD	2,3
	2	OCO a-stretch	~2300	gas	PI	6
	3	OCO s-stretch	~1500	gas	PI	6

$A_0 = 26.350$; $B_0 = 0.359$; $C_0 = 0.354$ MW^{1,4,5}LD^{2,3}

DOCO⁺

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

References

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HOCS⁺

$\tilde{X}$						
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OH stretch	3435.16	gas	LD	1

$A_0 = 26.11$; $B_0 = 0.192$; $C_0 = 0.190$ LD¹

References

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HONN⁺

$\tilde{X}$						
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OH stretch	3330.91	gas	LD	1

$A_0 = 20.88$; $B_0 = 0.377$; $C_0 = 0.370$ LD¹MW^{2,3}

DONN⁺

$\tilde{X}$						
$A_0 = 11.64$; $B_0 = 0.358$; $C_0 = 0.347$		MW ³				

References

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HFCN

$\tilde{X}$						
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CH stretch	3016	Ar	IR	1
	2	C=N stretch	1672s	Ar	IR	1
		CF stretch	1057vs	Ar	IR	1
		FCN bend	536m	Ar	IR	1

DFCN

$\tilde{X}$						
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CD stretch	2252	Ar	IR	1
	2	C=N stretch	1651m	Ar	IR	1
		CF stretch	1047vs	Ar	IR	1
		FCN bend	530wm	Ar	IR	1

References

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***t*-HOCO**

$\tilde{X}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	1	OH stretch	3602.9	Ar	IR	2
			3456	CO	IR	1
	2	C=O stretch	1843.6	Ar	IR	2
			1833	CO	IR	1
	3	HOC bend	1211.2	Ar	IR	2
<i>a''</i>			1261	CO	IR	1
	4	C-O stretch	1064.6	Ar	IR	2
			1077	CO	IR	1
	5	OCO bend	615	CO	IR	1
	6	Torsion	515	Ar	IR	2

***t*-DOCO**

$\tilde{X}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	1	OD stretch	2558	CO	IR	1
	2	C=O stretch	1841.7	Ar	IR	2
			1825	CO	IR	1
	3	C-O stretch + DOC bend	1092.6	Ar	IR	2
			1117	CO	IR	1
<i>a''</i>	5	OCO bend	610m	CO	IR	1
	6	Torsion	472wm	CO	IR	1

References¹D. E. Milligan and M. E. Jacox, J. Chem. Phys. **54**, 927 (1971).²M. E. Jacox, J. Chem. Phys. **88**, 4598 (1988).***t*-HONO*****B***

An intense, unstructured absorption between 200 and 275 nm, with a maximum near 46500 (215 nm), has been attributed¹³ to HONO.

$\tilde{A}'\tilde{A}''$ C_s
 $T_0 = 26034$ gas AB^{1-3,6} $\tilde{A}-\tilde{X}$ 315-385 nm

Diffuse bands; predissociated into OH + NO.

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>		NO stretch	1117	gas	AB	6

$\tilde{X}'\tilde{A}'$ C_s Structure: MW^{9,11,12}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	1	OH stretch	3590.71m	gas	IR	4,5,8,16 17
			3558	N ₂	IR	7
	2	N=O stretch	1699.76s	gas	IR,LS DL	4,5,8,14 16-18
			1688.0	Ar	IR	10,20
			1684	N ₂	IR	7
<i>a''</i>	3	HON bend	1263.21s	gas	IR,DL	4,5,8,16 17,19
			1298	N ₂	IR	7
	4	O-N stretch	790.12s	gas	IR	4,5,8,16 17
<i>a''</i>			795.1	Ar	IR	10,20
			815	N ₂	IR	7
	5	ONO bend	595.6s	gas	IR	4,5,8,17
			625	N ₂	IR	7
	6	Torsion	543.0m	gas	IR	4,5,8,17
			550	Ar	IR	10
			583	N ₂	IR	7

$A_0 = 3.099$; $B_0 = 0.418$; $C_0 = 0.367$ MW^{9,11,15}

***t*-DONO**

$\tilde{X}'\tilde{A}''$ 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.
<i>a'</i>		NO stretch	1147(20)	gas	AB	6

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	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
<i>a''</i>			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
<i>a''</i>			618	N ₂	IR	7
	6	Torsion	416.1	gas	IR	4,8,17
			444	N ₂	IR	7

$A_0 = 2.981$; $B_0 = 0.389$; $C_0 = 0.344$ MW^{9,11}

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c-HONO

B

An intense, unstructured absorption between 200 and 275 nm, with a maximum near 46500 (215 nm), has been attributed¹³ to HONO.

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

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

Structure: MW^{10,11}

141(35) higher in energy than *t*-HONO ($\tilde{X}$). MW¹²

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	OH stretch	3426.22w	gas	IR	4,5,8,16
			3412	Ar	IR	9
			3410	N ₂	IR	7
	2	N=O stretch	1640.52m	gas	IR,LS	4,5,8,14
			1632.6	Ar	IR	9,19
	3	HON bend	1633	N ₂	IR	7
			1261w	gas	IR	8
	4	O-N stretch	1263.3	Ar	IR	9,19
			851.94s	gas	IR,DL	4,5,8
a''	5	ONO bend	16–18			16–18
			849.6	Ar	IR	9,19
			865	N ₂	IR	7
			609.0w	gas	IR	8,17
			608	Ar	IR	9,19
	6	Torsion	638.5m	gas	IR	4,5,8,17
			637	Ar	IR	9,19
			658	N ₂	IR	7

$A_0 = 2.805$; $B_0 = 0.439$; $C_0 = 0.379$ MW^{10,15}DL¹⁸

c-DONO

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

gas $AB^{2,3}$

$\tilde{A}-\tilde{X}$ 315–385 nm

Diffuse bands; predissociated into OD + NO.

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	4	O-N stretch	~660	gas	AB	6

$\tilde{X} \text{ } ^1A'$ 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
a''	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
	6	Torsion	508.2	gas	IR	4,8,17
			522	N ₂	IR	7

$A_0 = 2.362$; $B_0 = 0.430$; $C_0 = 0.363$ MW¹⁰

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- ¹⁷C. M. Deeley and I. M. Mills, *J. Mol. Struct.* **100**, 199 (1983).
- ¹⁸A. G. Maki and R. L. Sams, *J. Mol. Struct.* **100**, 215 (1983).
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c-HOPO

$\tilde{\chi}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OH stretch	3550.7	Ar	IR	1
	2	P=O stretch	1252.6	Ar	IR	1
	4	P-O stretch	841.5	Ar	IR	1
a''	6	Torsion	523.9	Ar	IR	1

c-DOPO

$\tilde{\chi}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2620.4	Ar	IR	1
	2	P=O stretch	1253.0	Ar	IR	1

References

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HCOBr

$\tilde{\chi}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	2912.5	gas	IR	1
	2	CO stretch	1798.4 ^a	gas	IR	1
	3	H deform.	1271.2 ^b	gas	IR	1
	4	BrCO deform.	646.0	gas	IR	1
a''	6	OPLA	894vw	gas	IR	1

DCOBr

$\tilde{\chi}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CD stretch	2207.1	gas	IR	1
	2	CO stretch	1748.6	gas	IR	1
	3	D deform.	975.8 ^c	gas	IR	1
	4	BrCO deform.	605.9	gas	IR	1
a''	6	OPLA	747vw	gas	IR	1

^aIn Fermi resonance with $2\nu_6$.

^bIn Fermi resonance with $2\nu_4$.

^cIn Fermi resonance with $(\nu_4 + \nu_3)$.

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6.7. Four-Atomic Nonhydrides**C₄**

$\tilde{\chi}$	$D_{\infty h}$?					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1543.4	Ar	IR	1

References

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CNCN⁺ ^a

$\tilde{\nu}$	$C_{\infty v}$					
$T_0 = 26080(80)$ gas PE ¹						
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			710(40)	gas	PE	1

B $C_{\infty v}$

$T_0 = 12240(80)$ gas PE¹

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2075(40)	gas	PE	1
			1160(40)	gas	PE	1

A $C_{\infty v}$

$T_0 = 310(80)$ gas PE¹

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2270(40)	gas	PE	1
			1300(40)	gas	PE	1

^aThe molecule studied in Ref. 1 was at that time believed to be CNNC. Subsequent infrared studies² demonstrated that it is CNCN.

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B₂O₂

$\tilde{\chi}$	$D_{\infty h}$		Structure: MO, PE ³			
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	BO stretch	1897.8	Ar	IR	1,2
Π_u	5	Bend	213	Ar	IR	1,2

References

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CNCN

$\tilde{X}$	$C_{\infty v}$	Structure: MW ⁴				
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ^+	1	C≡N s-stretch	2302.00	gas	IR	1
			2294.4	Ar	IR	2
	2	C≡N a-stretch	2059.73	gas	IR	1
			2053.7	Ar	IR	2
	3	N-C stretch	975 ^a	gas	IR	1
Π			979.2	Ar	IR	2
	4	Bend	463.5 ^a	gas	IR	2
			468.5	Ar	IR	2
			467.2			
	5	Bend	194.75	gas	IR	1
			~200 ^b	Ar	IR	1

$$B_0 = 0.173 \text{ IR}^{1,3} \text{ MW}^{1,3,4}$$

^aPreliminary value.

^bFrom combination bands.

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CNNC

$\tilde{X}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			1996.4 ^a	Ar	IR	1

^aTentative assignment.

References

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CCCO

 $\tilde{X}$

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

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t-OCCO⁺ $\tilde{B}$

gas PD² $\tilde{B}-\tilde{X}$ 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, MO¹

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_g	1	CO s-stretch	~2076 ^a	Ne	IR	4
			526(30) ^b	gas	PD	2
b_u	5	CO a-stretch	2056.6	Ne	IR	3,4

^aCalculated using observed values for asymmetrically substituted species.

^bTentative assignment.

References

- ¹L. B. Knight, Jr., J. Steadman, P. K. Miller, D. E. Bowman, E. R. Davidson, and D. Feller, *J. Chem. Phys.* **80**, 4593 (1984).
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 $N\frac{1}{2}$ $\tilde{A}, \tilde{B}$

A broad, unstructured absorption¹⁻³ between 270 and 650 nm, with a maximum near 330 nm, leads to the formation of $N\frac{1}{2} + N_2$. Detection of the fluorescence of $N\frac{1}{2}$ ($\tilde{B}$) at the higher energies in this range suggests that the potential energy surface for a bound excited state of $N\frac{1}{2}$ which correlates with $N\frac{1}{2}$ ($\tilde{B}$) has an avoided crossing with the surface for the dissociative $\tilde{A}$ state.³

$\tilde{X}^2\Sigma_u$	$D_{\infty h}$	Structure: ESR, MO ⁴				
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ_g^+	1	N≡N s-stretch	~2283 ^a	Ne	IR	6
Σ_u^+	3	N≡N a-stretch	2237.6	Ne	IR	5,6

^aCalculated using observed values for asymmetrically ¹⁵N-substituted species.

References

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P⁺

B^2A_1 T_d

$T_0^a = 21860(500)$ gas PE^{1,2}
22936(5) Ar AB³ $\tilde{B}-\tilde{X}$ 398–436 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	540(40) 550(10)	gas Ar	PE AB	1,2 3

$\tilde{A}^2T_2^b$ T_d

$T_0^a = 8880(800)$ gas PE^{1,2}

A weak, broad absorption maximum observed³ in an argon matrix at 9570 has been tentatively assigned to the $\tilde{A}-\tilde{X}$ transition of P⁺.

Jahn-Teller splitting ~ 1130 gas PE^{1,2}

$\tilde{X}^2E^b$ T_d

Jahn-Teller splitting ~ 2820 gas PE^{1,2}

^aThe first ionization potential of P₄ is taken as 9.10(5) eV, as in Ref. 2. T_0 values are given with respect to onset of the transition.

^bRef. 2 reverses the assignment of these two bands.

References

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Si₂O₂

$\tilde{X}$	D_{2h}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
b_{1u}	4	Deformation	79	Ar	IR	2
b_{2u}	5	SiO stretch	809.5 803.2 804.7	Ne Ar N ₂	IR IR IR	2 1–3 1
b_{3u}	6	SiO stretch	766.7 768.2 766.3	Ne Ar N ₂	IR IR IR	2 1–3 1

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Ge₂O₂

$\tilde{X}$	D_{2h}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
b_{2u}	5	GeO stretch	666 667	Ar N ₂	IR IR	1 1
B_{3u}	6	GeO stretch	601 599	Ar N ₂	IR IR	1 1

References

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Sb₄

$\tilde{X}$	T_d					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1		242.1(5) Ne 241.5(3) Ar 239.6(3) Kr		Ra Ra Ra	1,2 2 2
e	2		137.1(3) Ar 135.8(3) Kr		Ra Ra	2 2
t_2	3		179.1(5) Ne 178.5(3) Ar 177.1(3) Kr		Ra Ra Ra	1,2 2 2

References

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Bi₄**B** T_d

$T_0 = 15312$ Ne LF¹ $\tilde{B}-\tilde{X}$ 600–710 nm
 15250 Ar LF¹ $\tilde{B}-\tilde{X}$ 600–670 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1		129.1	Ne	LF	1
			131	Ar	LF	1
e	2		82.4	Ne	LF	1
t_2	3		104.9	Ne	LF	1

 $\tau < 20$ ns Ne LF¹

A weak emission band system with origin at 13424 which terminates in Bi₄ ($\tilde{X}$) was observed by Ref. 4 in neon matrix studies of the laser excitation of Bi₄ ($\tilde{B}$).

A T_d

$T_0 = 12535$ Ne AB²LF² $\tilde{A}-\tilde{X}$ 725–765 nm
 12396 Ar LF¹ $\tilde{A}-\tilde{X}$ 740–765 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1		123	Ar	LF	1

 $\tau \sim 1.5$ μ s Ne LF¹**X** T_d

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1		149.7	Ne	LF	1
			151	Ar	LF, Ra	1,4
			152	Kr	Ra	3
e	2		89.8	Ne	LF	1
t_2	3		120.4	Ne	LF	1

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***t*-OCCO⁻**

In solid neon, threshold for electron detachment < 18000 .^{1,2}

X C_{2h}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_g	3	Bend	524 ^a	Ne	IR	2
b_u	5	CO a-stretch	1517.7	Ne	IR	1,2

^a ($\nu_3 + \nu_5$) – ν_5 . Tentative assignment of combination band.

References

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FN $\frac{1}{2}$ **E²A''** C_s $T^a = 58000(1050)$ gas PE¹**D²A'** C_s $T^a = 45670(480)$ gas PE¹**C²A''** C_s $T^a = 39450(1050)$ gas PE¹**B²A'** C_s $T^a = 37030(1050)$ gas PE¹**A²A'** C_s $T^a = 21860(480)$ gas PE¹

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	N ₃ a-stretch	~ 1800	gas	PE	1

X²A'' C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	2	N ₃ s-stretch	~ 800	gas	PE	1

^aFrom vertical ionization potentials.

References

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c-(NO)₂

$\bar{X}$	C _{2v}	Structure:	MW ⁷			
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a ₁	1	NO s-stretch	1868.25	gas	IR,DL	3,11
			1867.2	Ne	IR	12
			1866m	Ar	IR	1
			1870	N ₂	IR	2
			1862m	CO ₂	IR,Ra	1,6
	2	N...N stretch	1866	NO	IR,Ra	4,5,8
			262	CO ₂	Ra	6
			266	NO	IR,Ra	4,5,8
	3	NNO s-bend	161	CO ₂	Ra	6,8
			187	NO	Ra	4,5,8
a ₂	4	Torsion	88.2 ^a	gas	IR	9
b ₂	5	NO a-stretch	97	NO	IR,Ra	4,5,8
			1789	gas	IR,DL	3,9,10
						11
			1780.6	Ne	IR	12
			1778.7			
	6	NNO a-bend	1776s	Ar	IR	1
			1785	N ₂	IR	2
			1768s	CO ₂	IR	1
			1762	NO	IR,Ra	5,8
			202	CO ₂	Ra	6,8
			214	NO	Ra	4,5,8

$A_0 = 0.862$; $B_0 = 0.187$; $C_0 = 0.154$ MW⁷

^aFrom observation of $\nu_3 - \nu_4 = 1700.8$ cm⁻¹.

References

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- ¹²M. E. Jacox and W. E. Thompson, *J. Chem. Phys.* **93**, (Dec. 1990).

(PO)₂

$\bar{X}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		PO stretch	1155.0	Ar	IR	1

References

- ¹Z. Mielke, M. McCluskey, and L. Andrews, *Chem. Phys. Lett.* **165**, 146 (1990).

C₂F₂

$\bar{X}$	D _{∞h}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ_u^+	3	CF stretch	1149 ^a	gas	IR	1
			1341 ^a	Ar	IR	2

^aTentative value. Further experimental studies are needed to resolve this conflicting assignment.

References

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FNCO

$\bar{X}$	C _s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	NCO a-stretch	2177s	Ar	IR	1
			2167s			
	3	NF stretch	861s	Ar	IR	1
	4	NCO deform.	695wm	Ar	IR	1
	5	FNC deform.	529m	Ar	IR	1
a''	6	NCO deform.	646wm	Ar	IR	1

References

- ¹K. Gholivand, H. Willner, D. Bielefeldt, and A. Haas, *Z. Naturforsch.* **39B**, 1211 (1984).

CINCO

$\bar{X}$	C _s	Structure:	MW ^{3,4}			
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	NCO a-stretch	2212.2vs	gas	IR	1,2,5
	2	NCO s-stretch	1306.6w	gas	IR	1,2,5
	3		707.7wm	gas	IR	1,2,5
	4		607.7vw	gas	IR	5
a''	6	NCO bend	559.0wm	gas	IR	1,2,5

$A_0 = 1.720$; $B_0 = 0.104$; $C_0 = 0.098$ MW^{3,4}

References

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- ⁵T. C. DeVore, *J. Mol. Struct.* **162**, 287 (1987).

BrNCO

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

$\tilde{\chi}$	C_s	Structure: MW ^{2,3} IR ⁵				
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	NCO a-stretch	2198.0vs	gas	IR	1,4,5
			2196	Ne	IR	5
			2191.9	Ar	IR	5
	2	NCO s-stretch	1294.5w	gas	IR	1,4,5
			1290.9	Ne	IR	5
			1296.9	Ar	IR	5
	3	NCO bend	687.7w	gas	IR	1,4,5
			691.1	Ne	IR	5
			686.6	Ar	IR	5
			506.0vw	Ne	IR	5
a''	4	NBr stretch	506.0vw	Ne	IR	5
	5	BrNC bend	137.4w	Ne	IR	5
	6	NCO bend	569.9w	gas	IR	1,4,5
			572.2	Ne	IR	5
			563.1	Ar	IR	5

$$A_0 = 1.374; B_0 = 0.073; C_0 = 0.069 \quad MW^{2,3}$$

References

- ¹W. Gottardi, *Monatsh. Chem.* **103**, 1150 (1972).
²H. M. Jemson, W. Lewis-Bevan, N. P. C. Westwood, and M. C. L. Gerry, *Chem. Phys. Lett.* **108**, 496 (1984).
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⁵M. Gerke, G. Schatte, and H. Willner, *J. Mol. Spectrosc.* **135**, 359 (1989).

INCO

$\tilde{\chi}$	C_s	Structure: MW ¹				
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			2201.1vs	gas	IR	2
			1298.1w	gas	IR	2
			667.0w	gas	IR	2
			462.3vw	gas	IR	2
			583.3w	gas	IR	2

$$A_0 = 1.354; B_0 = 0.057; 0.055 \quad MW^1$$

References

- ¹H. M. Jemson, W. Lewis-Bevan, N. P. C. Westwood, and M. C. L. Gerry, *J. Mol. Spectrosc.* **119**, 22 (1986).
²T. C. DeVore, *J. Mol. Struct.* **162**, 287 (1987).

CISCN

$\tilde{\chi}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
	1	CN stretch	2170w	gas	IR	2
	2	CS stretch	678.9wm	gas	IR	2
	3	SCI stretch	533.6wm	gas	IR	2

$$A_0 = 0.404; B_0 = 0.097; C_0 = 0.078 \quad MW^1$$

References

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BrSCN

$\tilde{\chi}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
	1	CN stretch	2145.1wm	gas	IR	1
	2	CS stretch	674.2ms	gas	IR	1
	3	BrS stretch	455.8m	gas	IR	1

References

- ¹T. C. DeVore, *J. Mol. Struct.* **162**, 287 (1987).

ISCN

$\tilde{\chi}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
	1	CN stretch	2124.2vs	gas	IR	1
		CS stretch	668.0wm	gas	IR	1

References

- ¹T. C. DeVore, *J. Mol. Struct.* **162**, 287 (1987).

CICNO

$\tilde{\chi}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CNO a-stretch	2281.4	Ar	IR	1
			2261.7			
		CNO s-stretch	1326.3	Ar	IR	1

References

- ¹G. Maier and J. H. Teles, *Angew. Chem.* **99**, 152 (1987); *Angew. Chem. Int. Ed. Engl.* **26**, 155 (1987).

BrCNO $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CNO a-stretch	2271.3	Ar	IR	1
			2252.5			
		CNO s-stretch	1305.6	Ar	IR	1

References

¹G. Maier and J. H. Teles, *Angew. Chem.* **99**, 152 (1987); *Angew. Chem. Int. Ed. Engl.* **26**, 155 (1987).

BCl $\frac{1}{2}$ $\tilde{D}^2E'$ D_{3h} $T_0 = 29700(320)$ gas PE¹

A shoulder 1450(160) above the band maximum may result from spin-orbit coupling or from the Jahn-Teller effect.

Emission which is observed between 330 and 420 nm on excitation of BCl $\frac{1}{2}$ by radiation of wavelength shorter than 81 nm has been attributed to the $\tilde{D}-\tilde{X}$ transition of BCl $\frac{1}{2}$, and emission between 420 and 580 nm, with vibrational spacings of ~ 445 , has been attributed to the $\tilde{D}-\tilde{A}, \tilde{B}$ transitions of this species.³

A broad absorption with maximum at 320 nm (31200) which appears on argon-resonance photolysis of BCl $\frac{1}{2}$ isolated in an argon matrix and which can be destroyed by prolonged exposure of the sample to 340–600 nm radiation has been assigned² to the $\tilde{D}-\tilde{X}$ transition of BCl $\frac{1}{2}$.

 $\tilde{C}^2A_2'$ D_{3h} $T_0 = 20800(320)$ gas PE¹

Emission which is observed between 400 and 550 nm on excitation of BCl $\frac{1}{2}$ by radiation of wavelength shorter than 88 nm has been attributed to the $\tilde{C}-\tilde{X}$ transition of BCl $\frac{1}{2}$, and emission between 550 and 750 nm has been attributed to the $\tilde{C}-\tilde{A}$ transition of this species.³

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1'	1	BCl stretch	440(30)	gas	PE	1

References

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

NO $\frac{3}{2}$ $\tilde{X}^2A_2'$ D_{3h} Structure: DL¹¹

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	1050	gas	LF	8,9
a_2''	2	OPLA	762.33	gas	IR	12
e'	3	NO stretch ^a	1492.39	gas	LF, DL	8,9,11
					IR	12
	4	Deformation	360	gas	LF	8,9

 $B_0 = 0.459$ DL^{11,13}IR¹²

"Arguments of Ref. 3 suggest that NO $\frac{3}{2}$ should have a very low-lying $\tilde{A}^2E''$ state. Ref. 12 presents experimental evidence consistent with the presence of such a state. Ref. 13 has suggested that the 1492 cm⁻¹ absorption may possibly be contributed by the $\tilde{A}$ state.

References

¹³K. Kawaguchi, E. Hirota, T. Ishiwata, and I. Tanaka, *J. Chem. Phys.* **93**, 951 (1990).

PO $\frac{3}{2}$ $\tilde{B}^2E'$ D_{3h} $T_0 = 14378$ Ar AB² $\tilde{A}-\tilde{X}$ 589–696 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1'	1	PO $\frac{3}{2}$ s-stretch	913(10)	Ar	IR	2
e'	4	Deformation	525(10)	Ar	IR	2

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_2''	2	OPLA	480.3	Ar	IR	1
e'	3	PO stretch	1273.3	Ar	IR	1
	4	Deformation	435.2	Ar	IR	1

^aTentative assignment, by analogy with NO $\frac{3}{2}$.

References

¹R. Withnall and L. Andrews, *J. Phys. Chem.* **92**, 4610 (1988).

²R. Withnall, M. McCluskey, and L. Andrews, *J. Phys. Chem.* **93**, 126 (1989).

t-O $\frac{1}{2}$

In the gas phase, the high frequency tail of a photo dissociation continuum, resulting in the formation of O $\frac{1}{2}$ + O $\frac{1}{2}$, 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
			1320.3 ^b	Ne	IR	4
b_u	5	O=O a-stretch	1164.4	Ne	IR	4

^a($\nu_1 + \nu_5$) – ν_5 .

^bIn a neon matrix, almost as intense as ν_5 , and with very similar isotopic shift pattern. Probably results from interaction of ν_5 with combination bands of B_u symmetry.

References

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²M. L. Vestal and G. H. Mauclaire, *J. Chem. Phys.* **67**, 3767 (1977).

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⁴W. E. Thompson and M. E. Jacox, *J. Chem. Phys.* **91**, 3826 (1989).

F₂GeO

$\tilde{X}$	C_{2v}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	GeO stretch	989.9	Ar	IR	1
	2	GeF s-stretch	731.7	Ar	IR	1
b_1	4	OPLA	209.4	Ar	IR	1
b_2	5	GeF a-stretch	746.7	Ar	IR	1
	6	FGeO bend	226.9	Ar	IR	1

References

¹H. Schnöckel, J. Mol. Struct. **70**, 183 (1981).

ClONO

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

References

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²H. Niki, P. D. Maker, C. M. Savage, and L. P. Breitenbach, Chem. Phys. Lett. **59**, 78 (1978).
³J. P. Burrows, G. S. Tyndall, and G. K. Moortgat, J. Phys. Chem. **92**, 4340 (1988).

BrNO₂

$\tilde{X}$	C_{2v}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	NO ₂ s-stretch	1292	gas	IR	3
			1289s	Ar	IR	1,2
	2	NO ₂ deform.	787	gas	IR	3
			784s ^a	Ar	IR	2
	3	NBr stretch	496m	Ar	IR	1
b_1	4	OPLA	574s	Ar	IR	2
b_2	5	NO ₂ a-stretch	~1660	gas	IR	3
			1660m ^a	Ar	IR	2
	6	NO ₂ wag	402w ^b	Ar	IR	2

^aPartially obscured by nearby N₂O₄ absorption.

^bThis fundamental assigned to a moderately intense 360-cm⁻¹ absorption by Ref. 1.

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PO₂Cl

$\tilde{X}$	C_{2v}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	PO ₂ s-stretch	1122	Ar	IR	1
	2	PCl stretch	586	Ar	IR	1
b_2	5	PO ₂ a-stretch	1429	Ar	IR	1

References

¹R. Ahlrichs, C. Ehrhard, M. Lakenbrink, S. Schunck, and H. Schnöckel, J. Am. Chem. Soc. **108**, 3596 (1986).

SeO₃

$\tilde{X}$	D_{3h} Structure: Ra ¹					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_2''	2	Deform.	356	Ar	IR	2
			358	N ₂	IR	2
e'	3	SeO stretch	995 ^a	Ar	IR	2
			1005.5 ^a	N ₂	IR	2

^a⁸⁰Se.

References

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

CF₂Cl

3p Rydberg state C_{2v}

$T_0 \leq 49220$ gas MPI³

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
b_1	4	OPLA	745(25)	gas	MPI	3

$\tilde{X}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	CF stretch	1148vs	Ar	IR	1,2
	2	CCl stretch	761s	Ar	IR	1,2
	3	CF ₂ scissors	599m	Ar	IR	1,2
a''	5	CF stretch	1208vs	Ar	IR	1,2

References

- ¹D. E. Milligan, M. E. Jacox, J. H. McAuley, and C. E. Smith, J. Mol. Spectrosc. **45**, 377 (1973).
²F. T. Prochaska and L. Andrews, J. Chem. Phys. **68**, 5577 (1978).
³B. P. Tsai, R. D. Johnson, III, and J. W. Hudgens, J. Phys. Chem. **93**, 5334 (1989).

CFCl₂**3p Rydberg state** C_{2v}*T*₀ < 49850 gas MPI³

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₁	3	CCl ₂ scissors	270(30)	gas	MPI	3
<i>b</i> ₁	4	OPLA	590(20)	gas	MPI	3

X̃ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	1	CF stretch	1143vs	Ar	IR	1,2
	2	CCl stretch	747m	Ar	IR	1,2
<i>a''</i>	5	CCl stretch	919vs	Ar	IR	1,2

References

- ¹D. E. Milligan, M. E. Jacox, J. H. McAuley, and C. E. Smith, *J. Mol. Spectrosc.* **45**, 377 (1973).
²F. T. Prochaska and L. Andrews, *J. Chem. Phys.* **68**, 5568 (1978).
³B. P. Tsai, R. D. Johnson, III, and J. W. Hudgens, *J. Phys. Chem.* **93**, 5334 (1989).

CCl₃***M̃*²E' (4d)^a** D_{3h}*T*₀ = 57733(10) gas MPI⁹

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₂ ^{''}	2	OPLA	542(3)	gas	MPI	9

***L̃*²A₂' (4p)** D_{3h}*T*₀ = 56409(10) gas MPI⁹

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₂ ^{''}	2	OPLA	533(15)	gas	MPI	9

***K̃*²E' (4p)** D_{3h}*T*₀ = 56236(10) gas MPI⁹

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₂ ^{''}	2	OPLA	526(16)	gas	MPI	9

***J̃*²A₁' (4s)** D_{3h}*T*₀ = 53471(10) gas MPI⁹

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₂ ^{''}	2	OPLA	530(20)	gas	MPI	9

***G̃*²E' (3d)^a** D_{3h}*T*₀ = 51218(10) gas MPI⁹

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₂ ^{''}	2	OPLA	520(17)	gas	MPI	9

***F̃*²A₂' (3p)** D_{3h}*T*₀ = 47868(10) gas MPI⁹

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₂ ^{''}	2	OPLA	528(3)	gas	MPI	9

***Ẽ*²E' (3p)** D_{3h}*T*₀ = 47170(10) gas MPI⁹

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	1	Sym. stretch	544(6)	gas	MPI	9
<i>a</i> ₂ ^{''}	2	OPLA	509(21)	gas	MPI	9

A = 33(5) gas MPI⁹

An unstructured gas-phase absorption between 195 and 260 nm, with a maximum at 211(2) nm, has been assigned⁸ to CCl₃.

A broad emission observed in radiofrequency discharges between 420 and 700 nm, with a maximum near 490 nm, has been attributed⁷ to a transition between two electronically excited states of CCl₃.

***X̃*²A₁** C_{3v} Structure: ESR⁵

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₂	2	Umbrella	290 ^b 251	gas	MPI	9
<i>e</i>	3	CCl stretch	898vs	Ar	IR	1-4,6

^aTentative symmetry assignment.^bInversion doublet. Barrier to inversion = 460(40) gas MPI⁹**References**

- ¹L. Andrews, *J. Phys. Chem.* **71**, 2761 (1967).
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⁵C. Hesse, N. Leray, and J. Roncin, *Mol. Phys.* **22**, 137 (1971).
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⁸F. Danis, F. Caralp, B. Veyret, H. Loirat, and R. Lesclaux, *Int. J. Chem. Kinet.* **21**, 715 (1989).
⁹J. W. Hudgens, R. D. Johnson III, B. P. Tsai, and S. Kafafi, *J. Am. Chem. Soc.* **112**, 5763 (1990).

SiF₃

Unstructured emission bands between 350 and 800 nm and between 290 and 340 nm which appear with varying relative intensities on photoexcitation of SiF₄ by radiation at 99.1, 95.5, or 92.2 nm have been attributed³ to SiF₃. 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 SiF₄. Although that band system was initially assigned² to SiF₃, subsequent studies⁴ have demonstrated that it is entirely contributed by SiF₂.

$\tilde{X}$	C_{3v}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	SiF stretch	832s	Ar	IR	1
	2	Umbrella	406s	Ar	IR	1
e	3	SiF stretch	954vs	Ar	IR	1
	4	Deformation	290wm	Ar	IR	1

References

- ¹D. E. Milligan, M. E. Jacox, and W. A. Guillory, *J. Chem. Phys.* **49**, 5330 (1968).
²J. L.-F. Wang, C. N. Krishnan, and J. L. Margrave, *J. Mol. Spectrosc.* **48**, 346 (1973).
³M. Suto, J. C. Han, L. C. Lee, and T. J. Chuang, *J. Chem. Phys.* **90**, 2834 (1989).
⁴W. B. Griffith, Jr., and C. W. Mathews, private communication.

GeCl₃

$\tilde{X}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
e	3	GeCl ₃ stretch	420	Ar	IR	1

References

- ¹J. H. Miller and L. Andrews, *J. Mol. Struct.* **77**, 65 (1981).

OPCl₂

$\tilde{X}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		P=O stretch	1300 ^a	Ar	IR	1
		PCl ₂ a-stretch	621 ^a	Ar	IR	1

^aTentative assignment.

References

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

OPBr₂

$\tilde{X}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			558 ^a	Ar	IR	1

^aTentative assignment.

References

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

t-O₄

An unstructured absorption which appears near 270 nm in Ar:O₂ samples in which an alkali metal is also present and which grows on controlled warmup of the sample has been attributed⁷ to M⁺O₄⁻.

Threshold for photodestruction near 900 nm, and increasing cross section for photodestruction, probably by photodetachment, in the 850–400 nm spectral region.⁸ Photoelectron studies⁹ suggest that both photodetachment and photodissociation occur at 532 and 355 nm.

$\tilde{X}$	C_{2h}		Structure: MO ¹			
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_g	1	O=O stretch	1292 ^c	Ar	IR	10
	2	O...O stretch	287 ^a	Ar	Ra	6
			298 ^b	Ar	Ra	6
			305 ^c	Ar	Ra	5
b_u	5	O=O a-stretch	973.1	Ne	IR	11
			1001 ^a	Ar	IR	4
			992 ^b	Ar	IR	3
			993 ^c	Ar	IR	3,10
			1001 ^d	Ar	IR	2,4
	6	Asym. bend	991			
			131 ^c	Ar	IR	10

^aCs⁺ present.

^bRb⁺ present.

^cK⁺ present.

^dNa⁺ present.

References

- ¹D. C. Conway, *J. Chem. Phys.* **50**, 3864 (1969).
²L. Andrews, *J. Phys. Chem.* **73**, 3922 (1969).
³L. Andrews, *J. Chem. Phys.* **54**, 4935 (1971).
⁴M. E. Jacox and D. E. Milligan, *Chem. Phys. Lett.* **14**, 518 (1972).
⁵R. R. Smardzewski and L. Andrews, *J. Chem. Phys.* **57**, 1327 (1972).
⁶R. R. Smardzewski and L. Andrews, *J. Phys. Chem.* **77**, 801 (1973).
⁷L. Andrews, *J. Mol. Spectrosc.* **61**, 337 (1976).
⁸L. C. Lee and G. P. Smith, *J. Chem. Phys.* **70**, 1727 (1979).
⁹L. A. Posey, M. J. Deluca, and M. A. Johnson, *Chem. Phys. Lett.* **131**, 170 (1986).
¹⁰L. Manceron, A.-M. Le Quéré, and J.-P. Perchard, *J. Phys. Chem.* **93**, 2960 (1989).
¹¹W. E. Thompson and M. E. Jacox, *J. Chem. Phys.* **91**, 3826 (1989).

SO₃⁻ **$\bar{X}$**

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		S=O stretch	1191 ^a	Ar	IR	1
		S-O stretch	1093 ^a	Ar	IR	1
			1091 ^a			
		S-O stretch	965 ^a	Ar	IR	1
			585 ^a	Ar	IR	1
			504 ^a	Ar	IR	1
			4747 ^a	Ar	IR	1

^aCs⁺ trapped in adjacent site.**References**¹D. M. Stanbury, T. A. Holme, Z. H. Kafafi, and J. L. Margrave, *Chem. Phys. Lett.* **129**, 181 (1986).**ClOOCi**An unstructured gas-phase absorption with maximum at 40800 (245 nm) has been assigned^{1,4} to ClOOCi. **$\bar{X}$** C₂ Structure: MW³

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			750	gas	IR	4
			752.6	Ar	IR	2
			653	gas	IR	4
			649.8	Ar	IR	2
			647.6			

 $A_0 = 0.437$; $B_0 = 0.080$; $C_0 = 0.071$ MW³**References**¹R. A. Cox and G. D. Hayman, *Nature* **332**, 796 (1988).²B.-M. Cheng and Y.-P. Lee, *J. Chem. Phys.* **90**, 5930 (1989).³M. Birk, R. R. Friedl, E. A. Cohen, H. M. Pickett, and S. P. Sander, *J. Chem. Phys.* **91**, 6588 (1989).⁴J. B. Burkholder, J. J. Orlando, and C. J. Howard, *J. Phys. Chem.* **94**, 687 (1990).**O₂ICI** **$\bar{X}$** C_{2v}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	IO s-stretch	844.7	Ar	IR	1
			845.5	Kr	IR	1
			852.2	N ₂	IR	1
			421.1	Ar	IR	1
			330.5	Ar	IR	1
	2	IO ₂ scissors	327.5	Kr	IR	1
			331.9	N ₂	IR	1
			886.5	Ar	IR	1
			879.5			
			883.5	Kr	IR	1
b_2	5	IO a-stretch	879.6			
			883.7	N ₂	IR	1
			879.7			

References¹M. Hawkins, L. Andrews, A. J. Downs, and D. J. Drury, *J. Am. Chem. Soc.* **106**, 3076 (1984).**6.8. H₃⁺ and Five-Atomic Tetra- and Trihydrides****H₃⁺** **$\bar{X}$** C_{2v}

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

^aVibrational predissociation of mass-selected beam.**References**¹M. Okumura, L. I. Yeh, and Y. T. Lee, *J. Chem. Phys.* **83**, 3705 (1985).**SiH₄⁺** **$\bar{X}$ ^{bc}** C_s Structure: MO^{3,5,6}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			760(10)	gas	PE,PI	1,2,4

References⁵M. N. Paddon-Row and S. S. Wong, *J. Chem. Soc., Chem. Commun.* 1585 (1987).⁶R. F. Frey and E. R. Davidson, *J. Chem. Phys.* **89**, 4227 (1988).**NH₄⁺** **$\bar{X}$** T_d Structure: LD^{1,4}CC²

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
t_2	3	NH stretch	3343.14	gas	LD,CC	1-3
	4	Deformation	1447.22	gas	DL	5

 $B_0 = 5.929$ LD^{1,4}CC²**ND₄⁺** **$\bar{X}$** T_d

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
t_2	3	ND stretch	2495.0	gas	LD	4

 $B_0 = 2.979(3)$ LD⁴**References**¹M. Crofton and T. Oka, *J. Chem. Phys.* **79**, 3157 (1983).²E. Schaeffer, M. H. Begemann, C. S. Gudeman, and R. J. Saykally, *J. Chem. Phys.* **79**, 3159 (1983).

³E. Schafer, R. J. Saykally, and A. G. Robiette, *J. Chem. Phys.* **80**, 3969 (1984).

⁴M. W. Crofton and T. Oka, *J. Chem. Phys.* **86**, 5983 (1987).

⁵M. Polak, M. Gruebele, B. W. DeKock, and R. J. Saykally, *Mol. Phys.* **66**, 1193 (1989).

CaCH₃

$\bar{B}^2A_1$ C_{3v}

$T_0 = 16003(10)$ gas LF¹ $\bar{B}-\bar{X}$ 620–630 nm

$\bar{A}^2E$ C_{3v}

$T_0 = 14743.174^a$ gas LF^{1,2} $\bar{A}-\bar{X}$ 630–730 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	2	CH ₃ umbrella	1048(10)	gas	LF	1
	3	CaC stretch	413(10)	gas	LF	1
e	6	CaCH deform.	391(5) ^b	gas	LF	1

$A = 73.13$ gas LF^{1,2}

$A_0 = 5.384$; $B_0 = 0.254$ LF²

$\bar{X}^2A_1$ C_{3v} Structure: LF²

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	2	CH ₃ umbrella	1085(10)	gas	LF	1
	3	CaC stretch	419(10)	gas	LF	1
e	6	CaCH deform.	319(5) ^b	gas	LF	1

$A_0 = 5.448$; $B_0 = 0.252$ LF²

^aPredissociated above ~ 16200 .¹

^b $\frac{1}{2}(2\nu_6)$.

References

¹C. R. Brazier and P. F. Bernath, *J. Chem. Phys.* **86**, 5918 (1987).

²C. R. Brazier and P. F. Bernath, *J. Chem. Phys.* **91**, 4548 (1989).

ZnCH₃

$\bar{B}^2E$ C_{3v}

$T_0 = 36510$ gas AB¹ $\bar{B}-\bar{X}$ 260–274 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	2	CH ₃ deform.	~ 950	gas	AB	1

$\bar{A}^2E$ C_{3v}

$T_0 = 23949$ gas AB¹ $\bar{A}-\bar{X}$ 379–418 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	2	CH ₃ deform.	~ 1060	gas	AB	1
	3	ZnC stretch	~ 265	gas	AB	1

References

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

CdCH₃

$\bar{B}^2E$ C_{3v}

$T_0 = 34916$ gas AB¹ $\bar{B}-\bar{X}$ 264–287 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	2	CH ₃ deform.	~ 960	gas	AB	1
	3	CdC stretch	~ 360	gas	AB	1

$\bar{A}^2E$ C_{3v}

$T_0 = 22507$ gas AB¹ $\bar{A}-\bar{X}$ 400–445 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	2	CH ₃ deform.	~ 1000	gas	AB	1
	3	CdC stretch	~ 400	gas	AB	1

References

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

HFeNH₂

$\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		NH stretch	3381	Ar	IR	1
		FeH stretch	1717.4	Ar	IR	1
		NH ₂ bend	1517.8	Ar	IR	1
		FeN stretch	649.8	Ar	IR	1
		FeNH bend	536.8	Ar	IR	1

DFeND₂

$\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		FeD stretch	1236.4	Ar	IR	1
		ND ₂ bend	1131.7	Ar	IR	1
		FeN stretch	614.3	Ar	IR	1

References

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

HNiNH₂ $\tilde{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		NH ₂ stretch	3367.5	Ar	IR	1
			3358.2	Kr	IR	1
		NiH stretch	1918.1	Ar	IR	1
			1918.1	Kr	IR	1
		NH ₂ scissors	1533.3	Ar	IR	1
			1531.7	Kr	IR	1
		NiN stretch	676.5	Ar	IR	1
			671.7	Kr	IR	1
		NH ₂ wag	619.2	Ar	IR	1
			618.7	Kr	IR	1

DNiND₂ $\tilde{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		ND ₂ stretch	2522.9	Ar	IR	1
		NiD stretch	1431.3	Ar	IR	1
		ND ₂ scissors	1177.1	Ar	IR	1
		NiN stretch	653.6	Ar	IR	1

References

¹D. W. Ball, R. H. Hauge, and J. H. Margrave, *High Temp. Sci.* **25**, 95 (1988).

HCuNH₂

In an argon matrix, threshold for photodecomposition into Cu + NH₃ near 400 nm.¹

 $\tilde{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		NH stretch	3329.5	Ar	IR	1
		CuH stretch	1851.2	Ar	IR	1
		NH ₂ deform.	1524.1	Ar	IR	1
		NH ₂ wag	592.2	Ar	IR	1

DCuND₂ $\tilde{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		ND stretch	2444.1	Ar	IR	1
		CuD stretch	1334.2	Ar	IR	1
		ND ₂ deform.	1133.4	Ar	IR	1

References

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

C₂H⁺₃ $\tilde{\chi}$ C_{2v} (bridged)Structure: CE¹LD^{2,3}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
A ₁ ⁺		CH stretch	3142.2	gas	LD	3

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

References

¹E. P. Kanter, Z. Vager, G. Both, and D. Zajfman, *J. Chem. Phys.* **85**, 7487 (1986).

²T. Oka, *Phil. Trans. Roy. Soc. (London)* **A324**, 81 (1988).

³M. W. Crofton, M.-F. Jagod, B. D. Rehfuss, and T. Oka, *J. Chem. Phys.* **91**, 5139 (1989).

C₂H₃*Rydberg state* $T_0 = 59410$ gas AB³

164–169 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			1306	gas	AB	3

 $\tilde{\chi}$ C_s^a

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a''	7	Mixed OPLA	895.16	gas	DL	4
			900	Ar	IR	2

$A_0 = 7.913$; $B_0 = 1.083$; $C_0 = 0.949$ DL⁴

C₂D₃ $\tilde{\chi}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a''	7	Mixed OPLA	704	Ar	IR	2

^aRapid tunneling, giving effective C_{2v} symmetry.⁴

References

²R. A. Shepherd, T. J. Doyle, and W. R. M. Graham, *J. Chem. Phys.* **89**, 2738 (1988).

³A. Fahr and A. H. Laufer, *J. Phys. Chem.* **92**, 7229 (1988).

⁴H. Kanamori, Y. Endo, and E. Hirota, *J. Chem. Phys.* **92**, 197 (1990).

CH₃N $\tilde{A}^3E$ C_{3v} Structure: EM⁴

$T_0 = 31823.915(7)$ gas AB¹, EM^{1,2,4,5} $\tilde{A}-\tilde{X}$ 288–356 nm
 31576(20) N₂ AB³ $\tilde{A}-\tilde{X}$ 284–317 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1		CN stretch	758(4)	gas	UV	1,2
			755(22)	N ₂	AB	3
e	6	CH ₃ rock	728(4)	gas	EM	5

 $A = -22.872(7)$ gas EM⁴ $B_0 = 0.846$ EM⁴ $\tilde{X}^3A_2$ C_{3v} Structure: EM⁴

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	CH ₃ s-stretch	2943(4)	gas	EM	2,5
	2	CH ₃ deform.	1349(4)	gas	EM	2,5
	3	CN stretch	1040(4)	gas	EM	2,5
			1029	N ₂	AB	3
e	4	CH ₃ a-stretch	2989(4)	gas	EM	5
	5	CH ₃ deform.	1490(4)	gas	EM	5
	6	CH ₃ rock	903(8)	gas	EM	2,5

 $B_0 = 0.931$ EM⁴**CD₃N** $\tilde{A}^3E$ C_{3v}

$T_0 = 31774.158(2)^b$ gas AB¹, EM^{2,4,5} $\tilde{A}-\tilde{X}$ 294–365 nm
 31516(30) N₂ AB³ $\tilde{A}-\tilde{X}$ 295–318 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1		CN stretch	759(4)	gas	UV	1,2
			805(53)	N ₂	AB	3
		CD ₃ rock	579(4) ^a	gas	EM	2

 $B_0 = 0.691$ EM⁴ $\tilde{X}^3A_2$ 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

 $B_0 = 0.744$ EM⁴^aObserved as sequence band.^bCalculated assuming $A(\text{CD}_3\text{N}) = A(\text{CH}_3\text{N})$.**References**⁵E. L. Chappell and P. C. Engelking, J. Chem. Phys. **89**, 6007 (1988).**HSiNH₂**

In an argon matrix, a prominent absorption maximum at 208 nm and a shoulder at 220 nm have been assigned¹ to HSiNH₂.

In an argon matrix, a weak, broad, unstructured absorption with maximum at 348 nm is associated with the photolysis of HSiNH₂ to produce HNSi + H₂.¹ Subsequent irradiation at 254 nm reverses this photodecomposition.

 $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		NH ₂ stretch	3494.5wm	Ar	IR	1
		NH ₂ stretch	3408.7w	Ar	IR	1
		SiH stretch	1975.3vs	Ar	IR	1
		NH ₂ scissors	1562.6m	Ar	IR	1
		SiN stretch	866.4s	Ar	IR	1
		NH ₂ wag	570.4vs	Ar	IR	1

DSiND₂ $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		ND ₂ stretch	2611.2wm	Ar	IR	1
		ND ₂ stretch	2500.8wm	Ar	IR	1
		SiD stretch	1432.4vs	Ar	IR	1
		ND ₂ scissors	1179.3vs	Ar	IR	1
		SiN stretch	814.3m	Ar	IR	1
		ND ₂ wag	443.6ms	Ar	IR	1

References¹G. Maier, J. Glatthaar, and H. P. Reisenauer, Chem. Ber. **122**, 2403 (1989).**CH₂OH⁺** $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OH stretch	3422.802	gas	LD	2
		CO stretch	1650(30)	gas	PE	1
		CH ₂ deform.	1370(30)	gas	PE	1

 $A_0 = 6.590$; $B_0 = 1.146$; $C_0 = 0.973$ LD²**References**¹J. M. Dyke, A. R. Ellis, N. Jonathan, N. Keddar, and A. Morris, Chem. Phys. Lett. **111**, 207 (1984).²T. Amano and H. E. Warner, Astrophys. J. **342**, L99 (1989).**CH₃O** $3s^2A_1$ C_{3v}

Resonance-enhanced MPI spectrum of CH₃O between 313 and 328 nm has been tentatively assigned to a two-photon absorption into this Rydberg state, accompanied by a single-photon ionization.¹⁵

1^2A_1 C_{3v} Structure: $LF^{23,24}$

$\lambda = 31614.51(4)$ gas $EM^{1,2,11,12}AB^5$
 $LF^{6,8,19,20,23-25}$ $\tilde{A}-\tilde{X}$ 271–421 nm
 31291(3) Ar LF^{22} $\tilde{A}-\tilde{X}$ 270–420 nm
 Evidence for predissociation above 36800.¹³

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
i_1	1	CH ₃ stretch	3079	gas	LF	20
	2	Umbrella	1315	gas	LF	20
			1308(4)	Ar	LF	22
e	3	CO stretch	660	gas	AB,EM	5,12,20
					LF	
			657(2)	Ar	LF	22
e	4	CH ₃ stretch	2962	gas	LF	20
	5	CH ₂ scissors	1407	gas	LF	20
			1410(3)	Ar	LF	22
	6	HCO deform.	595	gas	LF	20

$\tau = 2.2(2)\mu s$ gas $EM^{2,9}LF^{4,14,16,17,19,21}$
 $A_0 = 4.981(3)$; $B_0 = 0.743$ LF^{23-25}

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

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

$A = -61.97(7)$ gas $LMR^7MW^{10}EM^{11,12}LF^{20,23,24}$
 $A_0 = 5.206(4)$; $B_0 = 0.932$ $LMR^7MW^{10,18}LF^{23,24}$

CD₃O

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

Resonance-enhanced MPI spectrum of CD₃O between 313 and 328 nm has been tentatively assigned to a two-photon absorption into this Rydberg state, accompanied by a single-photon ionization.¹⁵

 $\tilde{A}^2A_1$

$T_0 = 31554$ gas $LF^{6,20}EM^{12}$ $\tilde{A}-\tilde{X}$ 282–410 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	CD ₃ stretch	2015	gas	LF	20
	2	CD ₃ umbrella	971	gas	LF	20
	3	CO stretch	663	gas	EM,LF	12,20
e	5	CD ₂ scissors	1047	gas	LF	20

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

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

$A = -56(2)$ gas EM^{12}

$B_0 = 0.740$ MW¹⁸

^aSomewhat distorted by Jahn-Teller coupling.

^bTentative assignment.

References

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- ²³X. Liu, C. P. Damo, T.-Y. D. Lin, S. C. Foster, P. Misra, L. Yu, and T. A. Miller, *J. Phys. Chem.* **93**, 2266 (1989).
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CH₂OH

 $3p$ Rydberg state C_s

$T_0 = 41064$ gas $MPI^{3,4}AB^5$ $3p-\tilde{X}$ 217–244 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	4	CH ₂ scissors	1459	gas	MPI	3
	5	COH bend + CH ₂ rock	1091	gas	MPI	3
e	6	CO stretch	1623	gas	MPI	3,4
	7	CH ₂ rock + COH bend	1351	gas	MPI	3
a''	8	CH ₂ wag	950	gas	MPI	3
	9	Torsion	573	gas	MPI	3

Threshold for photodecomposition into H₂CO + H near 280 nm.^{1,2}

 $3s$ Rydberg state C_s

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

CD₂OD**3p Rydberg state** C_s $T_0 = 40913$ gas MPI^{3,4}AB⁶ $3p-\tilde{X}$ 216–244 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	4	CD ₂ scissors	1109	gas	MPI,AB	3,6
	5	COD bend + CD ₂ rock	803	gas	MPI	3
a''	6	CO stretch	1565	gas	MPI,AB	3,4,6
	9	Torsion	440	gas	MPI	3

3s Rydberg state C_s $T_0 = 35124$ gas AB⁶**References**

- ⁵P. Pagsberg, J. Munk, A. Sillesen, and C. Anastasi, Chem. Phys. Lett. **146**, 375 (1988).
⁶P. Pagsberg, J. Munk, C. Anastasi, and V. Simpson, Chem. Phys. Lett. **157**, 271 (1989).

CH₃S $\tilde{A}^2A_1$ C_{3v}Structure: LF⁹ $T_0 = 26399$ gas EM²LF^{6,9} $\tilde{A}-\tilde{X}$ 365–520 nmPredissociation threshold < 27300.⁶ In an argon matrix, CH₂SH is formed.⁵

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

 $\tau_0 = 310(20)$ ns gas LF⁶; 760(60) ns gas LF⁸ $A_0 = 5.343(47)$; $B_0 = 0.346$ LF⁹ $\tilde{X}^2E$ C_{3v}Structure: MW⁷LF⁹

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	2	CH ₃ umbrella	1316(4)	gas	PD,LF	4,6
	3	CS stretch	740(4)	gas	EM,PE	2–4,6
					PD,LF	

 $A = -255.5$ gas LF⁹ $A_0 = 5.68(4)$; $B_0 = 0.450$ MW⁷LF⁹**References**

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

CH₃Te $\tilde{B}$ C_{3v} $T_0 = 41068$ gas AB^{1,2} $\tilde{B}-\tilde{X}$ 225–245 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	2	CH ₃ deform.	~1100	gas	AB	2

References

- ¹J. Connor, G. Greig, and O. P. Strausz, J. Am. Chem. Soc. **91**, 5695 (1969).
²P. J. Young, R. K. Gosavi, J. Connor, O. P. Strausz, and H. E. Gunning, J. Chem. Phys. **58**, 5280 (1973).

CH₃I⁺ $\tilde{A}^2A_1$ 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 CH₃I isolated in solid argon and which has a photodecomposition threshold between 500 and 650 nm has been assigned⁵ to the $\tilde{A}-\tilde{X}$ transition of CH₃I⁺.

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	CH ₃ stretch	2810	gas	PF	7
	2	CH ₃ umbrella	1192	gas	PF	9–11
	3	CI stretch	294.2	gas	PE,PF	3,9–11

 $A^b = 5.07(5)$; $B^b = 0.185$ PF^{6,8} $\tilde{X}^2E$ C_{3v}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	CH ₃ stretch ^c	2970(50)	gas	PE	2,3
	2	CH ₃ umbrella	1254	gas	PE,PF	1–3,9
	3	CI stretch	492(50)	gas	PE	1,3
e	4	CH ₃ stretch	3060(50)	gas	PE	3,4
	6	CH ₃ rock	920(50)	gas	PE	3

Spin-orbit splitting = 5050 gas PE^{1–4}PF^{9,11}**CD₃I⁺** $\tilde{A}^2A_1$ C_{3v} $T_0 = 16982$ gas PE,PF^{7,9–11}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	CD ₃ stretch	2100	gas	PF	9
	2	CD ₃ umbrella	918	gas	PF	10,11
	3	CI stretch	276.3	gas	PF	10,11

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	CD ₃ stretch	2125	gas	PF	11
	2	CD ₃ umbrella	952	gas	PF	7
	3	CI stretch	442	gas	PF	11

Spin-orbit splitting = 5036 gas PF¹¹^aFrom vertical ionization potential.^bFrom study of band at 16978 in $\tilde{A} \leftarrow \tilde{X}^2E_{1/2}$ transition.^cIdentified for ²E_{1/2}, but not for ²E_{3/2}.

References

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

CH₃S⁻

Threshold for electron detachment from ground-state CH₃S⁻ = 15020(30) gas PD²PE^{1,3}

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a ₁	3	CS stretch	770(190)	gas	PE	3

References

¹P. C. Engelking, G. B. Ellison, and W. C. Lineberger, *J. Chem. Phys.* **69**, 1826 (1978).

²B. K. Janousek and J. I. Brauman, *J. Chem. Phys.* **72**, 694 (1980).

³S. Moran and G. B. Ellison, *J. Phys. Chem.* **92**, 1794 (1988).

PH₃O

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a ₁	1	PH ₃ stretch	2359.0 ^a	Ar	IR	1
	2	PO stretch	1240.2	Ar	IR	1
	3	PH ₃ umbrella	1143.5	Ar	IR	1
e	4	PH ₃ stretch	2371.5	Ar	IR	1
	5	PH ₃ deform.	1114.3	Ar	IR	1
	6	HPO deform.	853.0	Ar	IR	1

PD₃O

$\bar{X}$ 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

^aIn Fermi resonance with $\nu_2 + \nu_3$.

References

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

c-H₂POH

$\bar{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	OH stretch	3643.6	Ar	IR	1
	2	PH ₂ s-stretch	2304.8	Ar	IR	1

 $\bar{X}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
	3	PH ₂ scissors	1123.9	Ar	IR	1
	4	POH deform.	1074.8	Ar	IR	1
	5	PH ₂ wag	915.0	Ar	IR	1
	6	PO stretch	797.1	Ar	IR	1
a''	7	PH ₂ a-stretch	2278.1	Ar	IR	1
	8	PH ₂ rock	848.1	Ar	IR	1
	9	Torsion	375.3	Ar	IR	1

c-D₂POD

$\bar{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	OD stretch	2688.5	Ar	IR	1
	2	PD ₂ s-stretch	1679.1	Ar	IR	1
	3	POD deform.	828.5	Ar	IR	1
	4	PD ₂ scissors	813.6	Ar	IR	1
	5	PO stretch	796.1	Ar	IR	1
	6	PD ₂ wag	681.6	Ar	IR	1
a''	7	PD ₂ a-stretch	1658.5	Ar	IR	1
	8	PD ₂ rock	622.6	Ar	IR	1

References

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

H₃AsO

$\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		AsH stretch	2173.5s	Ar	IR	1
		AsH stretch	2170.1s	Ar	IR	1
		AsH ₃ deform.	983.4s	Ar	IR	1
		AsH ₃ deform.	979.8s	Ar	IR	1
		As=O stretch	937.9vs	Ar	IR	1
		HAsO deform.	817.1m	Ar	IR	1

D₃AsO

$\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		AsD stretch	1568.2	Ar	IR	1
		AsD stretch	1559.8	Ar	IR	1
		As=O stretch	938.2vs	Ar	IR	1
		AsD ₃ deform.	707.8	Ar	IR	1
		AsD ₃ deform.	704.9	Ar	IR	1
		DAsO deform.	576.3	Ar	IR	1

References

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

H₂AsOH $\tilde{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OH stretch	3652.2	Ar	IR	1
		AsH stretch	2092 ^a	Ar	IR	1
		AsH stretch	2086.3	Ar	IR	1
		AsH stretch	2080.7	Ar	IR	1
		AsH ₂ scissors	976 ^a	Ar	IR	1
		AsH ₂ scissors	974.5	Ar	IR	1
		HAsO deform.	813 ^a	Ar	IR	1
		HAsO deform.	806.7	Ar	IR	1
		AsH ₂ rock	687.2	Ar	IR	1
		AsO stretch	647.9s	Ar	IR	1
		Torsion	366 ^a	Ar	IR	1
		Torsion	297.5	Ar	IR	1

D₂AsOD $\tilde{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OD stretch	2694.6	Ar	IR	1
		AsD stretch	1504.2	Ar	IR	1
		AsD stretch	1498.9	Ar	IR	1
		AsOD deform.	762.0	Ar	IR	1
		AsD ₂ scissors	697.7	Ar	IR	1
		AsO stretch	647.8	Ar	IR	1
		AsD ₂ rock	516.1	Ar	IR	1

^aBelieved to be contributed by the other rotamer of the *cis-trans* pair.**References**¹L. Andrews, R. Withnall, and B. W. Moores, *J. Phys. Chem.* **93**, 1279 (1989).**H₃SbO** $\tilde{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₁	3	SbH ₃ deform.	791.8	Ar	IR	1
<i>e</i>	4	SbH ₃ stretch	1970	Ar	IR	1

D₃SbO $\tilde{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₁	2	Sb=O stretch	824.6	Ar	IR	1
	3	SbD ₃ deform.	568	Ar	IR	1
<i>e</i>	4	SbD ₃ stretch	1413	Ar	IR	1
	6	DSbO a-deform.	402.0	Ar	IR	1

References¹L. Andrews, B. W. Moores, and K. K. Fonda, *Inorg. Chem.* **28**, 290 (1989).**H₂SbOH** $\tilde{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OH stretch	3654	Ar	IR	1
		SbH ₂ stretch	1836.8	Ar	IR	1
		SbO stretch	583.5	Ar	IR	1

D₂SbOD $\tilde{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OD stretch	2697	Ar	IR	1
		SbD ₂ stretch	1320.6	Ar	IR	1
		SbO stretch	598	Ar	IR	1

References¹L. Andrews, B. W. Moores, and K. K. Fonda, *Inorg. Chem.* **28**, 290 (1989).**6.9. Five-Atomic Dihydrides****Cu₃H₂** $\tilde{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			1082.1	Ar	IR	1
			1039.7	Ar	IR	1
			537.1	Ar	IR	1

Cu₃D₂ $\tilde{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			781	Ar	IR	1
			755.7	Ar	IR	1

References¹R. H. Hauge, Z. H. Kafafi, and J. L. Margrave, in "Physics and Chemistry of Small Clusters," P. Jena, B. K. Rao, and S. N. Khanna, Eds., p. 787 (Plenum, New York, 1987).

LiC₂H₂

$\tilde{\chi}$	C_{2v}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	CH s-stretch	2952	Ar	IR	1
	2	C=C stretch	1655	Ar	IR	1
	4	CLi s-stretch	600	Ar	IR	1
b_1	6	CH deform.	479	Ar	IR	1
b_2	7	CH a-stretch	2908	Ar	IR	1
	8	CH a-deform.	714	Ar	IR	1

LiC₂D₂

$\tilde{\chi}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	CD s-stretch	2272	Ar	IR	1
	2	C=C stretch	1561	Ar	IR	1
b_1	6	CD deform.	366	Ar	IR	1
b_2	7	CD a-stretch	2161	Ar	IR	1
	8	CD deform.	576	Ar	IR	1

References

¹L. Manceron and L. Andrews, J. Am. Chem. Soc. **107**, 563 (1985).

HFeCCH

$\tilde{\chi}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CH stretch	3276.2	Ar	IR	1
		C≡C stretch	1976.4	Ar	IR	1
			1974.8			
		FeH stretch	1765.0	Ar	IR	1
			1762.6			

DFeCCD

$\tilde{\chi}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CD stretch	2432.8	Ar	IR	1
		C≡C stretch	1862.7	Ar	IR	1
			1861.0			
		FeD stretch	1269.4	Ar	IR	1
			1267.2			

References

¹E. S. Kline, Z. H. Kafafi, R. H. Hauge, and J. L. Margrave, J. Am. Chem. Soc. **107**, 7559 (1985).

HMgOMgH

$\tilde{\chi}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		MgH stretch	1561.3	Ar	IR	1
		MgO stretch	936.7	Ar	IR	1

DMgOMgD

$\tilde{\chi}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		MgD stretch	1145.1	Ar	IR	1
		MgO stretch	925.6	Ar	IR	1

References

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

HMg₂OH

$\tilde{\chi}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		MgH stretch	1524.4	Ar	IR	1
		MgO stretch	736.2	Ar	IR	1
		MgOH bend	692	Ar	IR	1
		MgMg stretch	544.2	Ar	IR	1

DMg₂OD^a

$\tilde{\chi}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		MgD stretch	1109.6	Ar	IR	1
		MgO stretch	704.4	Ar	IR	1
		MgOD bend	569	Ar	IR	1
		MgMg stretch	536.6	Ar	IR	1

^a ¹⁸O-substituted species.

References

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

HCaOCaH $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CaH stretch	1179.0	Ar	IR	1
		CaO stretch	726.1	Ar	IR	1
		HCaO bend	515.1	Ar	IR	1

DCaOCaD $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CaD stretch	851.6	Ar	IR	1
		CaO stretch	715.0	Ar	IR	1

References

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

HCa₂OH $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CaH stretch	1239.2	Ar	IR	1
		CaO stretch	588.6	Ar	IR	1

References

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

HMnOMnH $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		MnH stretch	1648.7 ^a 1643.2 ^a 1637.7	Ar	IR	1
		MnOMn stretch	874.5 ^a 872.3 ^a 870.4	Ar	IR	1

DMnOMnD $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		MnD stretch	1174.5	Ar	IR	1
		MnOMn stretch	870.3	Ar	IR	1

^aDiminished in intensity when matrix was annealed.

References

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

HMn₂OH $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		MnH stretch	1562.0 1556.4	Ar	IR	1
		MnO stretch	640.1	Ar	IR	1

References

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

HFeOFeH $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		FeH stretch	1724.0 ^a 1708.2	Ar	IR	1
		FeO stretch	914.5 ^a 911.8	Ar	IR	1

DFeOFeD $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		FeD stretch	1239.2 ^a 1231.8 ^a 1228.7	Ar	IR	1
		FeO stretch	914.3 ^a 911.7	Ar	IR	1

^aDiminished in intensity when matrix was annealed.

References

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

HFe₂OH $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		FeH stretch	1713.1	Ar	IR	1
		FeO stretch	649.9 522.4	Ar	IR	1

DFe₂OD $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		FeD stretch	1215.8	Ar	IR	1
		FeO stretch	630.4	Ar	IR	1
			521.7	Ar	IR	1

References

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

HNi₂OH $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OH stretch	3660.5	Ar	IR	1
		NiHNi stretch	1187.0	Ar	IR	1
			1134.2	Ar	IR	1
		NiONi stretch	662.7	Ar	IR	1
		Deformation	593.2	Ar	IR	1

DNi₂OD $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OD stretch	2717.5	Ar	IR	1
		NiDNi stretch	868.5	Ar	IR	1
			830.9	Ar	IR	1

References

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

cyc-C₃H₂

Photodecomposition threshold in an argon matrix near 360 nm; linear C₃H₂ formed.^{1,6,7}

 $\bar{X}$ C_{2v}Structure: MW^{4,5}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			1278.6	Ar	IR	1,6,7
			1277.7			
			1063.6 ^a	Ar	IR	1,6,7
			887.1 ^a	Ar	IR	1,6,7
			787.8 ^a	Ar	IR	1,6,7

A₀ = 1.171; B₀ = 1.075; C₀ = 0.559 MW²⁻⁵

cyc-C₃D₂ $\bar{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			1261.8	Ar	IR	7

^aDid not diminish in intensity on mercury-arc irradiation at wavelengths longer than 345 nm,⁷ calling into question the assignment to cyc-C₃H₂.

References

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

H₂C=C=C:

Photoisomerization to HCCCH occurs at 254 nm.^{1,2}

 $\bar{X}^a$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a ₁	1	CH ₂ s-stretch	3059.6	Ar	IR	1,2
			3049.5			
	2	C ₃ a-stretch	1963.2	Ar	IR	1,2
			1952.2			
	3	CH ₂ scissors	1449.3	Ar	IR	1,2
			1446.9			
b ₁	5	H ₂ CC OPLA	1003.0	Ar	IR	1,2
			999.2			
b ₂	8	CH ₂ rock	1025.0	Ar	IR	1

^aSinglet state.

References

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

HCCCH $\bar{X}^aA'$ C_sStructure: ESR¹IR,MO⁶

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'		CH stretch	3266.0s	Ar	IR	5-7
			3285	Kr	IR	3
		C ₃ a-stretch	1619.4w	Ar	IR	6,7
		CCH s-bend	550.4m	Ar	IR	6
			402.6	Ar	IR	4-7
			401.5wm			
			408	Kr	IR	3
a''	7	HCC wag	248.5	Ar	IR	4-7
			245.9s			
			258	Kr	IR	3

DCCCD

$\tilde{X}^3A'$	C_s					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CD stretch	2457.9s	Ar	IR	4,6,7
			2482	Kr	IR	3
		C_3 a-stretch CCD, C_3 bend	1529.0w	Ar	IR	6,7
			384.0m	Ar	IR	6,7
a''	7	DCC wag	392	Kr	IR	3
			171m	Ar	IR	4

References

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

HCCH=C:

On exposure of the sample to radiation of wavelength longer than 250 nm, the 1959.5 cm^{-1} absorption decreases and the 3292.4 cm^{-1} absorption grows. This process is reversed on irradiation of the sample at wavelengths longer than 295 nm.

$\tilde{X}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3292.4 ^a	Ar	IR	1
		CC stretch	1959.5 ^b	Ar	IR	1

DCCD=C:

$\tilde{X}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD stretch	2472.1 ^a	Ar	IR	1
		CC stretch	1938.6 ^b	Ar	IR	1

^aTentatively assigned to *cis*- isomer.

^bTentatively assigned to *trans*- isomer.

References

- ¹J. W. Huang and W. R. M. Graham, *J. Chem. Phys.* **93**, 1583 (1990).

H₂CCN

$\tilde{X}^1B_1$	C_{2v}					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_1	5	H_2CC OPLA	680 ^a	gas	PE	1

D₂CCN

$\tilde{X}^2B_1$	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

^aFrom computer fit.

References

- ¹S. Moran, H. B. Ellis, Jr., D. J. DeFrees, A. D. McLean, and G. B. Ellison, *J. Am. Chem. Soc.* **109**, 5996 (1987).

H₂CNC

$\tilde{X}^2B_1$	C_{2v}					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_1	5	H_2CN OPLA	615 ^a	gas	PE	1

D₂CNC

$\tilde{X}^2B_1$	C_{2v}					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_1	5	D_2CN OPLA	486 ^a	gas	PE	1

^aFrom computer fit.

References

- ¹S. Moran, H. B. Ellis, Jr., D. J. DeFrees, A. D. McLean, S. E. Paulson, and G. B. Ellison, *J. Am. Chem. Soc.* **109**, 6004 (1987).

Ca(OH)₂

$\tilde{X}$						
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CaO a-stretch	591.9	Ar	IR	1

Ca(OD)₂

$\tilde{X}$						
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CaO a-stretch	594.6	Ar	IR	1

References

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

Ba(OH)₂ $\tilde{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		BaO a-stretch	482.1	Ar	IR	1

Ba(OD)₂ $\tilde{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		BaO a-stretch	472.0	Ar	IR	1

References

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

Fe(OH)₂ $\tilde{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OFeO stretch	735.5	Ar	IR	1

Fe(OD)₂ $\tilde{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OFeO stretch	721.7	Ar	IR	1

References

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

Ni(OH)₂ $\tilde{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		ONiO stretch	800.8 795.5	Ar	IR	1

Ni(OD)₂ $\tilde{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		ONiO stretch	777.4 770.4	Ar	IR	1

References

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

H₂CCN⁻*Dipole-Bound State* C_{2v}T₀ = 12428.665(2) gas PD^{3,4}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			951(10)	gas	PD	4
b ₁	5	H ₂ CC deform.	692(10)	gas	PD	4

A₀ = 9.510; B₀ = 0.341; C₀ = 0.329 PD³**References**

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

HN=C=NH $\tilde{\chi}$ C₂

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

A₀ = 12.650; B₀ = 0.346; C₀ = 0.346 IR, MW^{3,4}**DN=C=ND** $\tilde{\chi}$

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

^aCalculated from (ν₂ + ν₈) combination band.

^bBoth ND-stretching frequencies presumed equal.

References

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

HCCOH

 $\bar{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	1	OH stretch	3501.3s	Ar	IR	1
	2	CH stretch	3339.6m	Ar	IR	1
	3	C≡C stretch	2198.3vs	Ar	IR	1
	4	COH bend	1232.1m	Ar	IR	1
	5	CO stretch	1072.1m	Ar	IR	1
	6	Bend	~599	Ar	IR	1
	7	Bend	~523	Ar	IR	1
	8	Bend	~383	Ar	IR	1
	9	Bend	~346	Ar	IR	1

DCCOD

 $\bar{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	1	OD,CD stretch	2620.4vs	Ar	IR	1
	2	OD,CD stretch	2586.8v	Ar	IR	1
	3	C≡C stretch	2035.1s	Ar	IR	1
	4	CO stretch	1046.9wm	Ar	IR	1
	5	COD bend	944.5m	Ar	IR	1

References

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

HC≡CSH

 $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CH stretch	3315s	Ar	IR	1-3
		SH stretch	2575vw	Ar	IR	2
		C≡C stretch	2065w	Ar	IR	1,2
			1112m	Ar	IR	2
			959w	Ar	IR	2,3
		CCH bend (⊥ plane)	558w	Ar	IR	1-3

DC≡CSD

 $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CD stretch	2580s	Ar	IR	1
		C≡C stretch	1925vw	Ar	IR	1
		SD stretch	1835vw	Ar	IR	1
		CCD bend (⊥ plane)	430m	Ar	IR	1

References

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

cyc-C₂H₂S $\bar{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a₁</i>	1	CH stretch	3207w	Ar	IR	2-4
			3202	N ₂	IR	6
	2	C=C stretch	1663w	Ar	IR	1-4
			1660	N ₂	IR	6
<i>b₁</i>	4	C-S stretch	657m ^b	Ar	IR	3,4,7
	6	OPLA	563m	Ar	IR	1-4,7
<i>b₂</i>			570	N ₂	IR	6
	7	CH stretch	3169m	Ar	IR	1-4
			3166m			
			3161	N ₂	IR	6
	8	CH deform.	912m	Ar	IR	1-4,7
			910	N ₂	IR	6

cyc-C₂D₂S $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a₁</i>	1	CD stretch	2485w	Ar	IR	2,4,6
	2	C=C stretch	1567w	Ar	IR	2,4,6
	3	C-S stretch	681m	Ar	IR	4
<i>b₁</i>	6	OPLA	423m	Ar	IR	2,4,6
<i>b₂</i>	7	CD stretch	2355m	Ar	IR	4
	8	CD deform.	716s	Ar	IR	4,6

^aFor assignment, see Ref. 8.^bTentative. See Refs. 5 and 6.

References

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

⁶A. Krantz and J. Laureni, *J. Am. Chem. Soc.* **103**, 486 (1981).

⁷M. Hawkins, M. J. Almond, and A. J. Downs, *J. Phys. Chem.* **89**, 3326 (1985).

⁸W. D. Allen, J. E. Bertie, M. V. Falk, B. A. Hess, Jr., G. B. Mast, D. A. Othen, L. J. Schaad, and H. F. Schaefer III, *J. Chem. Phys.* **84**, 4211 (1986).

HGe₂OH

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			784.8	Ar	IR	1
			710.8	Ar	IR	1
			683.0	Ar	IR	1

References

¹J. W. Kauffman, R. H. Hauge, and J. L. Margrave, "Metal Bonding and Interactions in High Temperature Systems," J. L. Gole and W. C. Stwalley, Eds., ACS Symposium Ser. 179 (American Chemical Society, Washington, D. C., 1982), pp. 355-362.

HSn₂OH

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			1100	Ar	IR	1
			748.9	Ar	IR	1
			690.0	Ar	IR	1
			620.3	Ar	IR	1

References

¹J. W. Kauffman, R. H. Hauge, and J. L. Margrave, "Metal Bonding and Interactions in High Temperature Systems," J. L. Gole and W. C. Stwalley, Eds., ACS Symposium Ser. 179 (American Chemical Society, Washington, D. C., 1982), pp. 355-362.

CHBr=CH

$\bar{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'		CH stretch	3094wm	Ar	IR	1
		C=C stretch	1564wm	Ar	IR	1
		H deform.	1120w	Ar	IR	1
		CBr stretch	495m	Ar	IR	1
a''		H deform.	794vs	Ar	IR	1

CDBr=CD

$\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'		CD stretch	2288vw	Ar	IR	1
		C=C stretch	1506wm	Ar	IR	1
		D deform.	828w	Ar	IR	1
		CBr stretch	480wm	Ar	IR	1
a''			600wm	Ar	IR	1
			573m	Ar	IR	1

References

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

CH₂=NCl

$\bar{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	3	C=N stretch	1611w	gas	IR	1
	4	CH ₂ scissors	1420w	gas	IR	1
	5	CH ₂ rock	1150m	gas	IR	1
	6	NCl stretch	619s	gas	IR	1
a''	8	OPLA	1006s	gas	IR	1

References

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

CH₂=PCI

$\bar{X}$ C_s Structure: MW^{1,2}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	CH ₂ a-stretch	3095.6vw	gas	IR	3
	2	CH ₂ s-stretch	2974.3vw	gas	IR	3
	3	CH ₂ scissors	1372.3m	gas	IR	3
	4	C=P stretch	979.7w	gas	IR	3
	5	CH ₂ rock	792.4s	gas	IR	3
	6	PCI stretch	499.7vs	gas	IR	3
	7	PCCl deform.	340.2w	gas	IR	3
a''	8	CH ₂ wag	804.7vs	gas	IR	3
	9	Torsion	609.4vw	gas	IR	3

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

CD₂=PCI

$\bar{X}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	3	CP stretch + CD ₂ scissors	1120.8m	gas	IR	3
	4	CP stretch + CD ₂ scissors	847.9w	gas	IR	3
	5	CD ₂ rock	642.9s	gas	IR	3
a''	6	PCI stretch	490.0vs	gas	IR	3
	8	CD ₂ wag	634.5s	gas	IR	3
	9	Torsion	431.6vw	gas	IR	3

$A_0 = 0.655$; $B_0 = 0.144$; $C_0 = 0.118$ gas MW^{1,2}

References

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

HSiOOH

$\bar{X}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		Si=O stretch	1249	Ar	IR	1,2

DSiOOD

$\bar{X}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		Si=O stretch	1245	Ar	IR	1,2
		Si-O stretch	891	Ar	IR	2

References

- ¹R. Withnall and L. Andrews, J. Am. Chem. Soc. **107**, 2567 (1985).
²R. Withnall and L. Andrews, J. Phys. Chem. **89**, 3261 (1985).

6.10. Five-Atomic Monohydrides**C₄H**

$\bar{X} \ ^2\Sigma$	$C_{\infty v}$					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3307.4w	Ar	IR	6
	2	C≡C stretch	2083.9wm	Ar	IR	6
	3	C≡C stretch	2060.6ms	Ar	IR	1,6

$B_0 = 0.165$ MW²⁻⁵

C₄D

$\bar{X} \ ^2\Sigma$	$C_{\infty v}$					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2579.3w	Ar	IR	6
	2	C≡C stretch	2056.5wm	Ar	IR	6
	3	C≡C stretch	2049.6ms	Ar	IR	1,6

References

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

HCOOCa

$\bar{B}, \bar{C} \ ^2B_2, \ ^2B_1 \ C_{2v}$

$T_0 = 15913(20)$ gas LF¹

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		Ca stretch	354(10)	gas	LF	1

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

$T_0 = 14715(20)$ gas LF¹

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		Ca stretch	356(10)	gas	LF	1

$\bar{X} \ ^2A_2 \ C_{2v}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		Ca stretch	349(10)	gas	LF	1

References

- ¹L. C. O'Brien, C. R. Brazier, S. Kinsey-Nielsen, and P. F. Bernath, J. Phys. Chem. **94**, 3543 (1990).

HCOOSr

$\bar{C} \ ^2B_1 \ C_{2v}$

$T_0 = 14903(20)$ gas LF¹

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		Sr stretch	285(10)	gas	LF	1

B²B₂ C_{2v}T₀ = 14749(20) gas LF¹

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		Sr stretch	291(10)	gas	LF	1

A²A₁ C_{2v}T₀ = 13624(20) gas LF¹

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		Sr stretch	307(10)	gas	LF	1

X²A₁ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		Sr stretch	275(10)	gas	LF	1

References

¹L. C. O'Brien, C. R. Brazier, S. Kinsey-Nielsen, and P. F. Bernath, J. Phys. Chem. **94**, 3543 (1990).**HCOCN****X¹A'** C_s

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

A₀ = 2.251; B₀ = 0.167; C₀ = 0.155 MW³

References

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

(Formylperoxy)

X

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		C=O stretch	1790.2	O ₂	IR	1,2
		C—O stretch	1089.9	O ₂	IR	1,2

DC(O)OO**X**

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		C=O stretch	1759.5	O ₂	IR	2

References

¹T-L. Tso, M. Diem, and E. K. C. Lee, Chem. Phys. Lett. **91**, 339 (1982).²T-L. Tso and E. K. C. Lee, J. Phys. Chem. **88**, 5475 (1984).**c-HFC=NF****X**

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		C=N stretch	1647wm	Ar	IR	1
		CF stretch	1205s	Ar	IR	1
		NF stretch	951wm	Ar	IR	1

c-DFC=NF**X**

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		C=N stretch	1624?	Ar	IR	1
		CF stretch	1217wm	Ar	IR	1
		NF stretch	968wm	Ar	IR	1

References

¹R. D. Hunt and L. Andrews, Inorg. Chem. **26**, 3051 (1987).**CF₂=PH****X**C_sStructure: MW²

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	PH stretch	2326.9m	gas	IR	3,4
	2	C=P stretch	1349.5vs	gas	IR	3,4
	3	CF ₂ a-stretch	1228.5s	gas	IR	3,4
	4	CPH deform.	884.4m	gas	IR	3,4
	5	CF ₂ s-stretch	729.3m	gas	IR	3,4
	6	CF ₂ scissors	485.5m	gas	IR	3,4
	7	CF ₂ rock	418.3w	gas	IR	4
a''	8	CPH deform.	1088.8w	gas	IR	4
	9	CF ₂ wag	568.0w	gas	IR	3,4

A₀ = 0.370; B₀ = 0.159; C₀ = 0.111 MW^{1,2}

CF₂=PD

$\tilde{X}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	PD stretch	1690.6m	gas	IR	4
	2	C=P stretch	1350.2vs	gas	IR	4
	3	CF ₂ a-stretch	1219.9s	gas	IR	4
	4	CF ₂ s-stretch	736.6m	gas	IR	4
	5	CPD deform.	661.5w	gas	IR	4
	6	CF ₂ scissors	483.5m	gas	IR	4
	7	CF ₂ rock	401.2w	gas	IR	4
a''	9	CF ₂ wag	544.7vw	gas	IR	4

$A_0 = 0.356$; $B_0 = 0.156$; $C_0 = 0.108$ MW^{1,2}

References

- ¹M. J. Hopkinson, H. W. Kroto, J. F. Nixon, and N. P. C. Simmons, J. Chem. Soc., Chem. Commun. 513 (1976).
²H. W. Kroto, Chem. Soc. Rev. **11**, 435 (1982).
³K. Ohno, H. Matsuura, H. W. Kroto, and H. Murata, Chem. Lett. 981 (1982).
⁴K. Ohno, E. Kurita, M. Kawamura, and H. Matsuura, J. Am. Chem. Soc. **109**, 5614 (1987).

HCF $\frac{1}{2}$

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

$T^a \sim 54400$ gas PE¹⁻⁴

Broad emission bands between about 230 and 580 nm which appear on excitation of HCF₃ by synchrotron radiation in the 48–62 nm spectral region have been attributed⁵ to the $\tilde{D}-\tilde{X}, \tilde{A}, \tilde{B}, \tilde{C}$ transitions of HCF $\frac{1}{2}$.

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1			480(80)	gas	PE	1

References

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

HOPO₂

$\tilde{X}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	OH stretch	3585.4	Ar	IR	1
	2	PO ₂ a-stretch	1451.3	Ar	IR	1
	3	PO ₂ s-stretch	1192.6	Ar	IR	1
	4	POH deform.	1044.8	Ar	IR	1
	5	P—O stretch	913.4	Ar	IR	1
	6	PO ₂ scissors	447.2	Ar	IR	1
	7	PO ₂ rock	412.0	Ar	IR	1
a''	8	OH torsion	492.0	Ar	IR	1
	9	OPO ₂ OPLA	428.0	Ar	IR	1

DOPO₂

$\tilde{X}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	OD stretch	2646.9	Ar	IR	1
	2	PO ₂ a-stretch	1450.9	Ar	IR	1
	3	PO ₂ s-stretch	1190.7	Ar	IR	1
	6	PO ₂ scissors	445.6	Ar	IR	1
	7	PO ₂ rock	386.5	Ar	IR	1
	8	OPO ₂ OPLA	434.4	Ar	IR	1
a''	9	OD torsion	366.0	Ar	IR	1

References

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

HOPO

$\tilde{X}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	OH stretch	3227	Ar	IR	1
		P=O stretch	1226.3	Ar	IR	1
		O—O stretch	1052.3	Ar	IR	1
		P—O stretch	915.3	Ar	IR	1
		POO bend	742.1	Ar	IR	1
a''		HOOP torsion	492.0	Ar	IR	1

References

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

HP(O₂)O

$\tilde{X}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		PH stretch	2490.1	Ar	IR	1
		P=O stretch	1370.3	Ar	IR	1,2
		PO ₂ s-stretch	974.1	Ar	IR	1
		PO stretch	587.3	Ar	IR	1
		OPO ₂ deform.	436.7	Ar	IR	1

DP(O₂)O

$\tilde{X}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		P=O stretch	1368.3	Ar	IR	1
		PO ₂ s-stretch	973.5	Ar	IR	1
		PO stretch	585.6	Ar	IR	1

References

- ¹R. Withnall and L. Andrews, *J. Phys. Chem.* **91**, 784 (1987).
²R. Withnall and L. Andrews, *J. Phys. Chem.* **92**, 4610 (1988).

HOAsO₂ $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OH stretch	3613	Ar	IR	1
		AsO ₂ a-stretch	1061.4	Ar	IR	1
		HOAs deform.	948	Ar	IR	1
		AsO ₂ s-stretch	932.2	Ar	IR	1
		As—O stretch	725	Ar	IR	1
		Torsion	424	Ar	IR	1
			414			

DOAsO₂ $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OD stretch	2664	Ar	IR	1
		AsO ₂ s-stretch	951.3	Ar	IR	1
		As—O stretch	778	Ar	IR	1

References

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

HSbO₃ $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		SbH stretch	2027	Ar	IR	1
		SbH a-deform.	872.7	Ar	IR	1
		O ₃ a-stretch	767.4	Ar	IR	1
		Sb—O ₃ stretch	727	Ar	IR	1
		SbH s-deform.	472.4	Ar	IR	1
		O ₃ s-bend	425.6	Ar	IR	1

DSbO₃ $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		SbD stretch	1457	Ar	IR	1
		O ₃ a-stretch	796.7	Ar	IR	1
		Sb—O ₃ stretch	731.8	Ar	IR	1
		SbD a-deform.	617.6	Ar	IR	1
		O ₃ s-bend	437.9	Ar	IR	1
		SbD s-deform.	387	Ar	IR	1

References

- ¹L. Andrews, B. W. Moores, and K. K. Fonda, *Inorg. Chem.* **28**, 290 (1989).

HOSbO₂ $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OH stretch	3604	Ar	IR	1
		SbO stretch	635	Ar	IR	1
		Torsion	370	Ar	IR	1

DOSbO₂ $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OD stretch	2658	Ar	IR	1
		SbO ₂ s-stretch	778.5	Ar	IR	1
		Torsion	276	Ar	IR	1

References

- ¹L. Andrews, B. W. Moores, and K. K. Fonda, *Inorg. Chem.* **28**, 290 (1989).

HOSO₂ $\bar{\chi}$

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

References

- ¹S. Hashimoto, G. Inoue, and H. Akimoto, *Chem. Phys. Lett.* **107**, 198 (1984).
²S. Nagase, S. Hashimoto, and H. Akimoto, *J. Phys. Chem.* **92**, 641 (1988).

6.11. Five-Atomic Nonhydrides

References

C₅

¹G. Maier and J. H. Teles, *Angew. Chem.* **99**, 152 (1987); *Angew. Chem. Int. Ed. Engl.* **26**, 155 (1987).

$\bar{X}$	$^3\Sigma_g^-$	$D_{\infty h}$	Structure: ESR ²			
Vib. No. sym.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.	
Σ_u^+ 3	Asym. stretch	2169.441	gas	IR,DL	4-7	
		2168(3)	Ne	IR	2	
		2164	Ar	IR	1-3	
Π_g 5	Bend	~218(13)	gas	DL	7	
Π_u 7	Bend	~118(3)	gas	DL	7	
$B_0 = 0.0853$		IR ⁴ DL ⁵⁻⁷				

References

- ¹K. R. Thompson, R. L. DeKock, and W. Weltner, Jr., *J. Am. Chem. Soc.* **93**, 4688 (1971).
²W. R. M. Graham, K. I. Dismuke, and W. Weltner, Jr., *Astrophys. J.* **204**, 301 (1976).
³M. Vala, T. M. Chandrasekhar, J. Szczepanski, R. Van Zee, and W. Weltner, Jr., *J. Chem. Phys.* **90**, 595 (1989).
⁴P. F. Bernath, K. H. Hinkle, and J. J. Keady, *Science* **244**, 562 (1989).
⁵N. Moazzen-Ahmadi, A. R. W. McKellar, and T. Amano, *Chem. Phys. Lett.* **157**, 1 (1989).
⁶J. R. Heath, A. L. Cooksy, M. H. W. Gruebele, C. A. Schmuttenmaer, and R. J. Saykally, *Science* **244**, 564 (1989).
⁷N. Moazzen-Ahmadi, A. R. W. McKellar, and T. Amano, *J. Chem. Phys.* **91**, 2140 (1989).

C₄O $\bar{X}$

Vib. No. sym.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		2221.7vs	Ar	IR	1
		1922.7s	Ar	IR	1
		1431.5wm	Ar	IR	1
		774.8w	Ar	IR	1
		484.0wm	Ar	IR	1

References

- ¹G. Maier, H. P. Reisenauer, U. Schäfer, and H. Balli, *Angew. Chem.* **100**, 590 (1988); *Angew. Chem. Int. Ed. Engl.* **27**, 566 (1988).

N≡C—CNO $\bar{X}$ $C_{\infty v}$

Vib. No. sym.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
	CNO a-stretch	2356vs	Ar	IR	1
		2192w	Ar	IR	1
	CNO s-stretch	1445wm	Ar	IR	1
		717vw	Ar	IR	1
		407vw	Ar	IR	1

NC—NCO $\bar{X}$ C_s Structure: MW^{3,4}

Vib. No. sym.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		~2280vs	gas	IR	1,5
		2233.1ms	gas	IR	1,5
		1429.4wm	gas	IR	1,5
		1165w	gas	IR	1
		1073.5wm	gas	IR	1,5
		727.3	gas	IR	5
		610.2s	gas	IR	1,5
		455s	gas	IR	1
		365s	gas	IR	1

$A_0 = 2.480$; $B_0 = 0.090$; $C_0 = 0.087$ MW^{2,3}

References

- ¹E. Mayer, *Monatsh. Chem.* **101**, 834 (1970).
²W. H. Hocking and M. C. L. Gerry, *J. Chem. Soc., Chem. Commun.* **47** (1973).
³W. H. Hocking and M. C. L. Gerry, *J. Mol. Spectrosc.* **59**, 338 (1976).
⁴B. Bak, H. Svanholt, and A. Holm, *Acta Chem. Scand.* **A33**, 597 (1979).
⁵T. C. DeVore, *J. Mol. Struct.* **162**, 287 (1987).

NC—NCS $\bar{X}$ $C_s (C_{\infty v})^a$ Structure: MW²

Vib. No. sym.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
1	CN stretch	2260.9	gas	IR	3
2	CN stretch	2016.4	gas	IR	3
	Skel. bend	97(11)	gas	MW	2

$B_0 = 0.051$ MW^{1,2}

^aBarrier to linearity 308(34). MW²

References

- ¹M. A. King and H. W. Kroto, *J. Chem. Soc., Chem. Commun.* **606** (1980).
²M. A. King, H. W. Kroto, and B. M. Landsberg, *J. Mol. Spectrosc.* **113**, 1 (1985).
³T. C. DeVore, *J. Mol. Struct.* **162**, 287 (1987).

P₄O $\bar{X}$ C_{3v}

Vib. No. sym.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1 P=O stretch	1241s	Ar	IR	1
	2 P ₄ s-stretch	603	Ar	IR	1
	3	441	Ar	IR	1
e	4	501	Ar	IR	1
	5	393	Ar	IR	1
	6 P—P=O deform.	243w	Ar	IR	1

References

¹L. Andrews and R. Withnall, *J. Am. Chem. Soc.* **110**, 5605 (1988).

br-P₄O

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

Vib. No. sym.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		856s	Ar	IR	1
		553w	Ar	IR	1

References

¹L. Andrews and R. Withnall, *J. Am. Chem. Soc.* **110**, 5605 (1988).

As₄O

$\bar{X}$

Vib. No. sym.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		981.5 ^a	Ar	IR	1

^aTentative assignment.

References

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

br-As₄O

$\bar{X}$

Vib. No. sym.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
	AsOAs a-stretch	590.3s 565.4s	Ar	IR	1
	AsOAs s-stretch	301.5w	Ar	IR	1
	As-As stretch	240.5	Ar	IR	1

References

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

O₂N—NO

In nitrogen- and neon-matrix studies,^{4,7} excitation in the region of a weak absorption between 700 and 900 nm, with maximum near 720 nm, leads to isomerization forming O=N—O—N=O.

$\bar{X}$ C_s Structure: MW³

Vib. No. sym.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i> 1	N=O stretch	1832	gas	IR	1,5
		1830.2s	Ne	IR	7
		1840m	N ₂	IR	4
		1867vs	O ₂	IR	2
		1861	NO	IR, Ra	6

$\bar{X}$ — Continued

Vib. No. sym.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
2	NO ₂ a-stretch	1652 1643.3s 1630vs 1596s 1593	gas Ne N ₂ O ₂ NO	IR IR IR IR IR,Ra	5 7 4 2 6
3	NO ₂ s-stretch	1305 1302.5vs 1302s 1303 1298	gas Ne N ₂ O ₂ NO	IR IR IR IR IR,Ra	1,5 7 4 2 6
4	NO ₂ deform.	773 773.1wm 776wm 788 787	gas Ne N ₂ O ₂ NO	IR IR IR IR IR,Ra	1,5 7 4 2 6
5	NO ₂ rock	414 420w 405	gas N ₂ NO	IR IR Ra	5 4 6
6	N—N stretch	241 266	gas NO	IR Ra	5 6
7	NO ₂ wag	205	NO	Ra	6
a'' 8	NNO ₂ OPLA	627	NO	Ra	6
9	Torsion	63 70	gas NO	IR Ra	5 6

A₀ = 0.415; B₀ = 0.141; C₀ = 0.105 MW³

References

¹L. D'Or and P. Tarte, *Bull. Soc. Roy. Sci. Liege* **22**, 276 (1953).

²W. G. Fateley, H. A. Bent, and B. Crawford, Jr., *J. Chem. Phys.* **31**, 204 (1959).

³A. H. Brittain, A. P. Cox, and R. L. Kuczkowski, *Trans. Faraday Soc.* **65**, 1963 (1969).

⁴E. L. Varette and G. C. Pimentel, *J. Chem. Phys.* **55**, 3813 (1971).

⁵C. H. Bibart and G. E. Ewing, *J. Chem. Phys.* **61**, 1293 (1974).

⁶E. M. Nour, L.-H. Chen, and J. Laane, *J. Phys. Chem.* **87**, 1113 (1983).

⁷M. E. Jacox and W. E. Thompson, *J. Chem. Phys.* **93** (in press).

O=N—O—N=O

In nitrogen-matrix studies,¹ absorption maxima were observed at 398, 381, and 363 nm. Excitation in the 370–480 nm spectral region resulted in photoisomerization to O₂N—NO.^{1,3}

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

Vib. No. sym.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a ₁ 1	N=O s-stretch	1740	NO	Ra	2
2	N—O s-stretch	973.6m 969w 973m	Ne N ₂ NO	IR IR IR,Ra	3 1 2
3	NON bend	387m 395	N ₂ NO	IR Ra	1 2
4	Sym. O=NO bend	366s	N ₂	IR	1
a ₂ 5	Torsion	140	NO	Ra	2
b ₁ 6	Torsion	105 ^a	NO	Ra	2
b ₂ 7	N=O a-stretch	1697.2vs 1690s 1687vs 1661w	Ne N ₂ NO N ₂	IR IR IR IR	3 1 2 1

$\bar{X}$ — Continued

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

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

References

¹E. L. Varetto and G. C. Pimentel, *J. Chem. Phys.* **55**, 3813 (1971).²E. M. Nour, L.-H. Chen, and J. Laane, *J. Phys. Chem.* **87**, 1113 (1983).³M. E. Jacox and W. E. Thompson, *J. Chem. Phys.* **93**, (in press).

ON—NSO

 $\bar{X}$

Vib. No. sym.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
	NO stretch	1827m	Ar	IR	1
		1823m			
	NO stretch	1499wm	Ar	IR	1
		1495wm			
	NS stretch	826w	Ar	IR	1
		822w			

References

¹M. Hawkins and A. J. Downs, *J. Phys. Chem.* **88**, 2042 (1984).ONSNO ^a $\bar{X}$

Vib. No. sym.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
	NO stretch	1669m	Ar	IR	1
	NO stretch	1567m	Ar	IR	1
	Deformation	323w	Ar	IR	1

^aAlternative assignment of absorptions to SNONO cannot be definitively excluded.

References

¹M. Hawkins and A. J. Downs, *J. Phys. Chem.* **88**, 3042 (1984).cyc-F₂SiO₂ $\bar{X}$

Vib. No. sym.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
	SiF ₂ s-stretch	1155.2s	O ₂	IR	1
	SiF ₂ a-stretch	1013.7s	O ₂	IR	1
	SiO ₂ s-stretch	862.6w	O ₂	IR	1

References

¹A. Patyk, W. Sander, J. Gauss, and D. Cremer, *Chem. Ber.* **123**, 89 (1990).cyc-Cl₂SiO₂ $\bar{X}$

Vib. No. sym.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
	SiO ₂ s-stretch	1054.4s	O ₂	IR	1
	SiCl ₂ stretch	649.9ms	O ₂	IR	1
	O—O stretch	576.1wm	O ₂	IR	1

References

¹A. Patyk, W. Sander, J. Gauss, and D. Cremer, *Chem. Ber.* **123**, 89 (1990).F₂CSO $\bar{X}$ C_s

Vib. No. sym.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
	C=S stretch	1373vs	Ar	IR	1
	CF ₂ a-stretch	1296s	Ar	IR	1
	S=O stretch	1117.5s	Ar	IR	1
		724.5w	Ar	IR	1

References

¹W. Sander, R. Henn, and W. Sundermeyer, *Spectrochim. Acta* **42A**, 1281 (1986).CIFCSO ^a $\bar{X}$

Vib. No. sym.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
	C=S stretch	1297	Ar	IR	1
	CF stretch	1131	Ar	IR	1
	S=O stretch	1050	Ar	IR	1
		640	Ar	IR	1

^aMore stable isomer.

References

¹W. Sander, R. Henn, and W. Sundermeyer, *Spectrochim. Acta* **42A**, 1281 (1986).

CIFCSO^a $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		C=S stretch	1246	Ar	IR	1
		CF stretch	1145	Ar	IR	1
		S=O stretch	1082	Ar	IR	1

^aLess stable isomer.

References

¹W. Sander, R. Henn, and W. Sundermeyer, *Spectrochim. Acta* **42A**, 1281 (1986).BrONO₂ $\bar{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	1	NO ₂ a-stretch	1714vs	gas	IR	1
			1709vs	Ne	IR	1
			1702vs	N ₂	IR	1
	2	NO ₂ s-stretch	1288vs	gas	IR	1
			1285vs	Ne	IR	1
			1285vs	N ₂	IR	1
3	NO ₂ scissors		806vs	gas	IR	1
			802vs	Ne	IR	1
			805vs	N ₂	IR	1
			750w	Ne	IR	1
			750w	N ₂	IR	1
4	OBr stretch		564s	gas	IR	1
			563s	Ne	IR	1
			574s	N ₂	IR	1
			569s			
<i>a''</i>	8	ONO ₂ OPLA	728wm	gas	IR	1
			723vw	Ne	IR	1
			725wm	N ₂	IR	1

References

¹W. W. Wilson and K. O. Christe, *Inorg. Chem.* **26**, 1573 (1987).Cl₂O₃An unstructured gas-phase absorption with maximum at 37700 (265 nm) has been assigned^{2,4} to Cl₂O₃. $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			1225vs	gas	IR	1,4
			1226.1	Ar	IR	3
			1057s	gas	IR	4
			1058.4	Ar	IR	3
			740w	gas	IR	4
			560wm	gas	IR	4

References

¹A. J. Schell-Sorokin, D. S. Bethune, J. R. Lankard, M. M. T. Loy, and P. P. Sorokin, *J. Phys. Chem.* **86**, 4653 (1982).²G. D. Hayman and R. A. Cox, *Chem. Phys. Lett.* **155**, 1 (1989).³B.-M. Cheng and Y.-P. Lee, *J. Chem. Phys.* **90**, 5930 (1989).⁴J. B. Burkholder, J. J. Orlando, and C. J. Howard, *J. Phys. Chem.* **94**, 687 (1990).CF₃O $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CF ₃ stretch	1221.6	Ar	IR	1,2

References

¹L. Andrews, M. Hawkins, and R. Withnall, *Inorg. Chem.* **24**, 4234 (1985).²K. C. Clemmshaw and J. R. Sodeau, *J. Phys. Chem.* **93**, 3552 (1989).CF₄⁺ $\bar{D}^2A_1$ T_dStructure: PE,EF⁷ $T_0^a = 78830(160)$ gas PE^{2,3,5}
gas EF⁶ $\bar{D}-\bar{C}$ 350–420 nmBroad, unstructured emission maxima at 189 and 160 nm (52900 and 62500) which appear on He⁺ or electron impact on CF₄ have been interpreted as arising from the $\bar{D}-\bar{B}$ and $\bar{D}-\bar{A}$ transitions of CF₄⁺, respectively.⁶

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₁	1	CF stretch	800(1)	gas	PE,EF	3,5,6

 $\tau = 2.1(2)$ ns gas EF¹ $B_0 = 0.180(3)^b$ EF⁷ $\bar{C}^2T_2$ T_dStructure: PE,EF⁷ $T_0^a = 51230(160)$ gas PE^{2,3,5}
gas EF⁶ $\bar{D}-\bar{C}$ 350–420 nmBroad, unstructured emission maxima at 290 and 230 nm (34500 and 43500) which result from He⁺ or electron impact⁶ on CF₄ and from exposure of CF₄ to synchrotron radiation¹⁰ of wavelength shorter than 57.4 nm have been interpreted as arising from the $\bar{C}-\bar{A}$ and $\bar{C}-\bar{X}$ transitions of CF₄⁺, respectively.

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₁	1	CF stretch	729	gas	PE,EF	2,3,5,6

Spin-orbit splitting = +16(1) EF⁶⁻⁸ $\tau = 9.0(9)$ ns gas EF¹EM⁹ $B_0 \sim 0.168^c$ PE,EF⁷

B^2E $T_0^a = 23800(1000)$ gas PE^{2-5}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF stretch	810(80)	gas	PE	3-5
e		Deformation	500(100)	gas	PE	3-5

 $\tilde{A}^2T_2$ $T_0^a = 14100(1000)$ gas PE^{2-5} **$\tilde{X}^2T_1$** ^aMeasured with respect to onset of first photoelectron band, estimated by Ref. 3 at 15.35 eV.^bFrom computer simulation of emission bands.^cFrom Franck-Condon analysis of photoelectron spectrum.**References**

- ¹J. E. Hesser and K. Dressler, J. Chem. Phys. **47**, 3443 (1967).
- ²A. W. Potts, H. J. Lempka, D. G. Streets, and W. C. Price, Phil. Trans. Roy. Soc. (London) **A268**, 59 (1970).
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- ⁶J. F. M. Aarts, S. M. Mason, and R. P. Tuckett, Mol. Phys. **60**, 761 (1987).
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- ⁸R. N. Dixon and R. P. Tuckett, Chem. Phys. Lett. **140**, 553 (1987).
- ⁹I. R. Lambert, S. M. Mason, R. P. Tuckett, and A. Hopkirk, J. Chem. Phys. **89**, 2683 (1988).
- ¹⁰L. C. Lee, J. C. Han, C. Ye, and M. Suto, J. Chem. Phys. **92**, 133 (1990).

 CF_3Cl^+ **$\tilde{D}^2E$** C_{3v} $T_0^a = 39720(400)$ gas $PE^{1,2,4}$

Broad emission bands in the 200–600 nm spectral region which appear on excitation of CF_3Cl by synchrotron radiation of wavelength less than about 62 nm have been tentatively attributed⁸ to transitions arising from the $\tilde{D}$ state of CF_3Cl^+ .

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF_3 umbrella	726(80)	gas	PE	4
	3	CCl stretch	387(80)	gas	PE	4
e	4	CF_3 stretch	1130(80)	gas	PE	4

References

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

 CF_3Br^+ **$\tilde{D}^2E$** C_{3v} $T^a = 44300(800)$ gas $PE^{1,2}$

Emission bands between about 200 and 700 nm which result from the excitation of CF_3Br by synchrotron radiation of wavelength shorter than about 75 nm have been attributed⁶ to the $\tilde{D}-\tilde{X}$, $\tilde{A}-\tilde{B}$, transitions of CF_3Br^+ .

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF_3 stretch	1080(80)	gas	PE	2
	2	CF_3 umbrella	690(80)	gas	PE	2

References

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

 CF_2Cl^+ **$\tilde{D}^2B_2$** C_{2v} $T_0^a = 19150(110)$ gas $PE^{1,2,4,5}$

It has been proposed⁸ that an unstructured emission in the 200–400 nm region, with its principal contribution at wavelengths longer than 300 nm, which appears on electron bombardment of CF_2Cl_2 at electron energies greater than that for the onset of the $\tilde{D}$ state of CF_2Cl^+ may be contributed by the $\tilde{D}-\tilde{X}$ transition of CF_2Cl^+ .

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CF_2 scissors	370(40)	gas	PE	1,4,5

References

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

 SiF_4^+ **$\tilde{D}^2A_1$** T_d Structure: PE, EF^9 $T^{ab} = 50800(200)$ gas PE^2 $EF^7EM^{8,10}$ $\tilde{D}-\tilde{C}$ 530–590 nm

$\tilde{D}-\tilde{C}$ band origin measured at 18146.8 in emission studies on a cooled beam.⁷

Continuous emission between 570 and 730 nm, with a maximum near 610 nm (16400), has been assigned to the $\tilde{D}-\tilde{C}$ transition.^{8,10,12}

Broad, unstructured emission maxima at 370 and 304 nm (27000 and 32900) which appear on ion, electron, or photon impact on SiF_4 have been interpreted as arising from the $\tilde{D}-\tilde{B}$ and $\tilde{D}-\tilde{A}$ transitions of SiF_4^+ , respectively.^{6,8}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiF stretch	743.4(5)	gas	EF	7

 $\tau = 9.30(4)$ ns gas EF^1EM^{12} $B_0 = 0.136(1)^c$ EF^9

$\tilde{C}^2T_2$ T_d^d Structure: PE,EF⁹ $T_0^a = 33130(100)$ gas PE^{2,3,5}
EF⁷EM^{8,10} $\tilde{D}-\tilde{C}$ 530–590 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	SiF stretch	706.6(5)	gas	PE,EF	3,5,7
e	2	Deformation	159.0(5)	gas	EF	7
t_2	4	Deformation	431.0(5)	gas	PE,EF	3,5,7

Spin-orbit splitting = +6.9(2) EF^{7,9,11} $B_0 = 0.132^c$ PE,EF⁹ $\tilde{B}^2E$ $T_0^a = 22580(100)$ gas PE^{2,3,5}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	SiF stretch	685(50)	gas	PE	5

 $\tilde{A}^2T_2$ $T_0^a = 17000(1000)$ gas PE^{2,3,5} $\tilde{X}^2T_1$ ^aMeasured with respect to a first ionization potential of 15.19 eV, estimated⁴ by extrapolation of the photoionization efficiency curve for SiF₄.^bFrom vertical ionization potential.^cFrom Franck-Condon analysis of the photoelectron spectrum and computer simulation of the $\tilde{D}-\tilde{C}$ emission.^dDynamic Jahn-Teller distortion, probably to C_{3v}.^{7,9}

References

- ¹J. E. Hesser and K. Dressler, J. Chem. Phys. **47**, 3443 (1967).
- ²T. P. Fehlner and D. W. Turner, Inorg. Chem. **13**, 754 (1974).
- ³D. R. Lloyd and P. J. Roberts, J. Electron Spectrosc. Relat. Phenom. **7**, 325 (1975).
- ⁴M. K. Murphy and J. L. Beauchamp, J. Am. Chem. Soc. **99**, 2085 (1977).
- ⁵R. Jadrny, L. Karlsson, L. Mattsson, and K. Siegbahn, Chem. Phys. Lett. **49**, 203 (1977).
- ⁶J. F. M. Aarts, Chem. Phys. **101**, 105 (1986).
- ⁷S. M. Mason and R. P. Tuckett, Mol. Phys. **60**, 771 (1987).
- ⁸M. Suto, X. Wang, L. C. Lee, and T. J. Chuang, J. Chem. Phys. **86**, 1152 (1987).
- ⁹S. M. Mason and R. P. Tuckett, Mol. Phys. **62**, 175 (1987).
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- ¹¹R. N. Dixon and R. P. Tuckett, Chem. Phys. Lett. **140**, 553 (1987).
- ¹²I. R. Lambert, S. M. Mason, R. P. Tuckett, and A. Hopkirk, J. Chem. Phys. **89**, 2683 (1988).

SiCl₄⁺ $\tilde{D}^2A_1$ T_d $T_0 = 48900(400)$ gas PE^{1,2}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	SiCl stretch	~290	gas	PE	3

 $\tilde{C}^2T_2$ $T_0 = 26620(160)$ gas PE^{1,2}

A broad, unstructured emission with maxima at 410 and 570 nm (24400 and 17500) has been assigned^{5,6} to the $\tilde{C}-\tilde{X}$ and $\tilde{C}-\tilde{A}$ transitions, respectively, of gas-phase SiCl₄⁺. Using pulsed synchrotron excitation of SiCl₄, a radiative lifetime of 38.4(1) ns has been determined⁶ for the $\tilde{C}$ state of SiCl₄⁺.

A broad absorption with maximum at 475 nm (21000) which appears on argon-resonance photolysis of SiCl₄ isolated in an argon matrix has been assigned⁴ to the $\tilde{C}-\tilde{X}$ transition of SiCl₄⁺. The energy difference is attributed to structural relaxation in the argon matrix. The absorption can be destroyed by exposure of the sample to 290–1000 nm radiation.

 $\tilde{B}^2E$ $T^a = 13880(400)$ gas PE^{1,2} $\tilde{A}^2T_2$ $T_0 = 7750(160)$ gas PE^{1,2} $\tilde{X}^2T_1$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		SiCl ₂ a-stretch	717 ^b	Ar	IR	4

^aFrom vertical ionization potential.^bTentative assignment.

References

- ¹J. C. Green, M. L. H. Green, P. J. Joachim, A. F. Orchard, and D. W. Turner, Phil. Trans. Roy. Soc. (London) **A268**, 111 (1970).
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- ⁵I. R. Lambert, S. M. Mason, R. P. Tuckett, and A. Hopkirk, J. Chem. Phys. **89**, 2675 (1988).
- ⁶I. R. Lambert, S. M. Mason, R. P. Tuckett, and A. Hopkirk, J. Chem. Phys. **89**, 2683 (1988).

SiBr₄⁺ $\tilde{D}^2A_1$ T_d $T^a = 50600(320)$ gas PE¹

$\tilde{C}^2T_2$ T_d $T^a = 24300(400)$ gas PE¹

A broad, unstructured emission with maxima at 435 and 550 nm (23000 and 18200) has been assigned² to the $\tilde{C}-\tilde{X}$ and $\tilde{C}-\tilde{A}$ transitions, respectively, of gas-phase SiBr₄, excited by electron impact. Using pulsed synchrotron excitation of SiBr₄, a radiative lifetime of 47.6(3) ns has been determined² for the $\tilde{C}$ state of SiBr₄.

 $\tilde{B}^2E$ T_d $T^a = 10400(320)$ gas PE¹ $\tilde{A}^2T_2$ T_d $T^a = 6000(400)$ gas PE¹ $\tilde{X}^2T_1$ T_d ^aFrom vertical ionization potentials.

References

- ¹J. C. Green, M. L. H. Green, P. J. Joachim, A. F. Orchard, and D. W. Turner, Phil. Trans. Roy. Soc. (London) **A268**, 111 (1970).
- ²J. C. Creasey, I. R. Lambert, R. P. Tuckett, and A. Hopkirk, J. Chem. Soc., Faraday Trans. **86**, 2021 (1990).

GeF₄⁺ $\tilde{D}^2A_1$ T_d $T^{ab} = 45300(1000)$ gas PE^{2,4}
EF⁶ $\tilde{D}-\tilde{C}$ 390–420 nm

Broad, unstructured emission maxima at 290 and 255 nm (34500 and 39200) which appear on ion impact on GeF₄ have been interpreted as arising from the $\tilde{D}-\tilde{B}$ and $\tilde{D}-\tilde{A}$ transitions of GeF₄⁺, respectively.⁵

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	GeF stretch	644.3	gas	EF	6

Biexponential. $\tau_1 = 3.1(3)$ ns, $\tau_2 = 6.3(4)$ ns EM⁷^aFirst ionization potential taken to be 15.69(2) eV, as in Ref. 1.^bFrom vertical ionization potential.^cDistorted by Jahn-Teller interaction.^dTentative value.

References

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

GeCl₄⁺ $\tilde{D}^2A_1$ T_d $T_0 = 51070(400)$ gas PE^{1,2} $\tilde{C}^2T_2$ T_d $T_0 = 21620(240)$ gas PE^{1,2}

A broad, unstructured emission with maxima at 495 and 615 nm (20200 and 16300) has been assigned^{3,4} to the $\tilde{C}-\tilde{X}$ and $\tilde{C}-\tilde{A}$ transitions, respectively, of gas-phase GeCl₄⁺. Using pulsed synchrotron excitation of GeCl₄, a radiative lifetime of 65.4(4) ns has been determined⁴ for the $\tilde{C}$ state of GeCl₄⁺.

 $\tilde{B}^2E$ $T^a = 9440(240)$ gas PE^{1,2} $\tilde{A}^2T_2$ $T^a = 6130(320)$ gas PE^{1,2} $\tilde{X}^2T_1$ ^aFrom vertical ionization potential.

References

- ¹J. C. Green, M. L. H. Green, P. J. Joachim, A. F. Orchard, and D. W. Turner, Phil. Trans. Roy. Soc. (London) **A268**, 111 (1970).
- ²P. J. Bassett and D. R. Lloyd, J. Chem. Soc. A **641** (1971).
- ³I. R. Lambert, S. M. Mason, R. P. Tuckett, and A. Hopkirk, J. Chem. Phys. **89**, 2675 (1988).
- ⁴I. R. Lambert, S. M. Mason, R. P. Tuckett, and A. Hopkirk, J. Chem. Phys. **89**, 2683 (1988).

GeBr₄⁺ $\tilde{D}^2A_1$ T_d $T^a = 53400(1000)$ gas PE¹ $\tilde{C}^2T_2$ T_d $T^a = 21660(160)$ gas PE¹

A broad, unstructured emission maximum at 475 nm (21000) has been assigned² to the $\tilde{C}-\tilde{X}$ transition of gas-phase GeBr₄⁺, excited by Penning ionization in collisions of GeBr₄ with He*. Using pulsed synchrotron excitation of GeBr₄, a radiative lifetime of 67(4) ns has been determined² for the $\tilde{C}$ state of GeBr₄⁺.

 $\tilde{B}^2E$ T_d $T^a = 7340(160)$ gas PE¹ $\tilde{A}^2T_2$ T_d $T^a = 4680(400)$ gas PE¹ $\tilde{X}^2T_1$ T_d ^aFrom vertical ionization potentials.

References

- ¹J. C. Green, M. L. H. Green, P. J. Joachim, A. F. Orchard, and D. W. Turner, Phil. Trans. Roy. Soc. (London) **A268**, 111 (1970).
- ²J. C. Creasey, I. R. Lambert, R. P. Tuckett, and A. Hopkirk, J. Chem. Soc., Faraday Trans. **86**, 2021 (1990).

SCIF₃ $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		SF eq. stretch	841wm	Ar	IR	1
		SF ax. a-str.	668s	Ar	IR	1
		SF ax. s-str.	606m	Ar	IR	1
		SCl stretch	506m	Ar	IR	1

References

- ¹R. Minkwitz, U. Nass, and J. Sawatzki, J. Fluorine Chem. **31**, 175 (1986).

SCI₂F₂

$\tilde{\chi}$	C_{2v}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	SF ax. stretch	592	Ar	IR,Ra	1
	2	SCI eq. stretch	527	Ar	IR	1
	4	Deformation	162	Ar	Ra	1
b_1	6	SF ax. stretch	770	Ar	IR	1
	7	Deformation	296	Ar	IR,Ra	1
b_2	8	SCI eq. stretch	533	Ar	IR	1
	9	Deformation	274	Ar	IR,Ra	1

References

¹R. Minkwitz, U. Nass, and J. Sawatzki, *J. Fluorine Chem.* **31**, 175 (1986).

SCI₃F

$\tilde{\chi}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		SF stretch	656m	Ar	IR	1
		SCI eq. a-str.	458m	Ar	IR	1
		SCI eq. s-str.	420m	Ar	IR	1
		SCI ax. stretch	332m	Ar	IR	1

References

¹R. Minkwitz, U. Nass, and J. Sawatzki, *J. Fluorine Chem.* **31**, 175 (1986).

XeO₂F₂

$\tilde{\chi}$	C_{2v} Structure: ND ²					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	XeO stretch	849wm	Ar	IR	1,3
	2	XeF stretch	537w	Ar	IR	3
	3	XeO ₂ scissors	331sh	Ar	IR	3
	4	XeF ₂ scissors	202w	Ar	IR	3
a_2	5	XeO ₂ twist	329sh	Ar	IR	3
b_1	6	XeO stretch	906s	Ar	IR	1,3
b_2	8	XeF stretch	585vs	Ar	IR	1
	9	XeO ₂ rock	324m	Ar	IR	1,3

References

¹H. H. Claassen, E. L. Gasner, H. Kim, and J. L. Huston, *J. Chem. Phys.* **49**, 253 (1968).

²S. W. Peterson, R. D. Willett, and J. L. Huston, *J. Chem. Phys.* **59**, 453 (1973).

³K. O. Christe and W. W. Wilson, *Inorg. Chem.* **27**, 3763 (1988).

6.12. Six-Atomic Molecules**B₂H₄**

$\tilde{\chi}$	C_{2v}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1			1300(100)	gas	PI	1

References

¹B. Rušćić, M. Schwarz, and J. Berkowitz, *J. Chem. Phys.* **91**, 4576 (1989).

HFeCH₃

$\tilde{\chi}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		FeH stretch	1684.2	Ar	IR	1
		FeCH rock	540.2	Ar	IR	1
		CFe stretch	524.3	Ar	IR	1

DFeCD₃

$\tilde{\chi}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		FeD stretch	1210.8	Ar	IR	1
		CFe stretch	480.2	Ar	IR	1

References

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

HNiCH₃

Threshold for dissociation into Ni + CH₄ near 400 nm.¹

$\tilde{\chi}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CH stretch	2950.5	Ar	IR	1
		CH stretch	2861.0	Ar	IR	1
		NiH stretch	1945.1	Ar	IR	1
		CH ₃ deform.	1139.0	Ar	IR	1
		CH ₃ deform.	1120.3	Ar	IR	1
		CH ₃ rock	642.7	Ar	IR	1
		NiC stretch	554.9	Ar	IR	1

DNICD₃ $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CD stretch	2197.5	Ar	IR	1
		NiD stretch	1406.8	Ar	IR	1
		CD ₃ deform.	895.8	Ar	IR	1
		CD ₃ deform.	891.9	Ar	IR	1

References

¹S.-C. Chang, R. H. Hauge, W. E. Billups, J. L. Margrave, and Z. H. Kafafi, *Inorg. Chem.* **27**, 205 (1988).

H₂BNH₂ $\tilde{X}$ C_{2v}Structure: MW¹

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a ₁	1	NH stretch	3451	gas	IR	2
	2	BH stretch	2495	gas	IR	2
	3	NH ₂ scissors	1625	gas	IR	2
	4	BN stretch	1337.47	gas	IR	2
	5	BH ₂ scissors	1225	gas	IR	2
a ₂	6	Torsion	~820 ^a	gas	IR	3
b ₁	7	NH ₂ wag	1005	gas	IR	2
	8	BH ₂ wag	612s	gas	IR	3
b ₂	9	NH stretch	3534	gas	IR	2
	10	BH stretch	2564	gas	IR	2
	11	NH ₂ rock	1131	gas	IR	2
	12	BH ₂ rock	~742vw	gas	IR	3

A₀ = 4.610; B₀ = 0.917; C₀ = 0.763 MW¹

^aValue estimated from appearance of perturbation.

References

¹M. Sugie, H. Takeo, and C. Matsumura, *Chem. Phys. Lett.* **64**, 573 (1979).

²M. C. L. Gerry, W. Lewis-Bevan, A. J. Merer, and N. P. C. Westwood, *J. Mol. Spectrosc.* **110**, 153 (1985).

³W. D. Anderson, M. C. L. Gerry, W. Lewis-Bevan, A. J. Merer, and D. M. Steunenbergh, 41st Symposium on Molecular Spectroscopy, Columbus, Ohio, June 1986.

CH₂NH₂[‡] $\tilde{X}$ ¹A₁C_{2v}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a ₁	3	CN stretch	1810(50)	gas	PE	1
b ₁		CH ₂ OPLA	1190(50)	gas	PE	1

References

¹J. M. Dyke, E. P. F. Lee, and M. H. Zamanpour Niavaran, *Int. J. Mass Spectrom. Ion Proc.* **94**, 221 (1989).

SiH₃OH^a $\tilde{X}$

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

SiD₃OD^a $\tilde{X}$

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

^aTentative identification.

References

¹R. Withnall and L. Andrews, *J. Phys. Chem.* **89**, 3261 (1985).

GeH₃OH $\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'		GeOH bend	924	Ar	IR	1
		GeH ₃ deform.	877.2	Ar	IR	1
		GeH ₃ deform.	867.6	Ar	IR	1
		Ge—O stretch	688.6	Ar	IR	1
a''		GeH ₃ deform.	871.7	Ar	IR	1

GeD₃OD $\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'		Ge—O stretch	710.6	Ar	IR	1
		GeD ₃ deform.	623.4	Ar	IR	1
a''		GeD ₃ deform.	635	Ar	IR	1

References

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

HFe₂NH₂^a $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		FeH stretch	1687	Ar	IR	1
		FeN stretch	581	Ar	IR	1

^a¹⁵N.

References

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

SrOCH₃

References

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

CH₂CCH $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CH stretch	3308.8m	Ar	IR	2,4
		CCH bend	686.5m ^b	Ar	IR	2
		CCH OPLA bend	510(10)	gas	PE	3
		C ₃ deformation	483.5m	Ar	IR	2,4

CD₂CCD $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CD stretch	2546.8m	Ar	IR	2,4
		CCD bend	552.9m ^b	Ar	IR	2
			479.8	Ar	IR	4

^bRef. 4 presents arguments for the reassignment of this absorption to *cyc*-C₃H₃.

References

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

CH₂=C=NH⁺ B^2A' C_s

$T^a = 30340(160)$ gas PE¹

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	7	CH ₂ wag	600(40)	gas	PE	1

 A^2A'' C_s

$T^a = 21220(160)$ gas PE¹

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	3	CCN a-stretch	1900(40)	gas	PE	1
	5	CCN s-stretch	860(40)	gas	PE	1

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₁		CCN s-stretch	1040(40)	gas	PE	1
		CNH bend	550(40)	gas	PE	1

^aFrom vertical ionization potentials.

References

- ¹H. W. Kroto, G. Y. Matti, R. J. Suffolk, J. D. Watts, M. Rittby, and R. J. Bartlett, *J. Am. Chem. Soc.* **112**, 3779 (1990).

CH₂=C=NH $\tilde{X}$ C_s Structure: MO²MW⁵

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	3	CCN a-stretch	2043.58	gas	IR	6
			2040vs	Ar	IR	1,3
	5	CCN s-stretch; NH deform.	1124wm	Ar	IR	1,3
	6	NH deform.	1000s	Ar	IR	1,3
	7	H ₂ CC OPLA	690m	Ar	IR	1,3
<i>a''</i>	11	Torsion	872m	Ar	IR	1,3

$A_0 = 6.719$; $B_0 = 0.322$; $C_0 = 0.316$ MW^{4,5}IR⁶

CD₂=C=ND $\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	3	CCN a-stretch	1998vs	Ar	IR	1,3
	5	CD ₂ scissors	921m	Ar	IR	1,3
	6	ND deform.	800s	Ar	IR	1,3
<i>a''</i>	11	Torsion	648m	Ar	IR	1,3

References

- ¹M. E. Jacox and D. E. Milligan, *J. Am. Chem. Soc.* **85**, 278 (1963).
²A. C. Hopkinson, M. H. Lien, K. Yates, P. G. Mezey, and I. G. Csizmadia, *J. Chem. Phys.* **67**, 517 (1977).
³M. E. Jacox, *Chem. Phys.* **43**, 157 (1979).
⁴M. Rodler, R. D. Brown, P. D. Godfrey, and L. M. Tack, *Chem. Phys. Lett.* **110**, 447 (1984).
⁵M. Rodler, R. D. Brown, P. D. Godfrey, and B. Kleibömer, *J. Mol. Spectrosc.* **118**, 267 (1986).
⁶F. Ito, T. Nakanaga, K. Sugawara, H. Takeo, M. Sugie, C. Matsumura, and Y. Hamada, *J. Mol. Spectrosc.* **140**, 177 (1990).

HC≡CNH₂ $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		C≡C stretch	2162	Ar	IR	1

References

¹C. Wentrup, H. Briehl, P. Lorencak, U. J. Vogelbacher, H.-W. Winter, A. Maquestiau, and R. Flammang, *J. Am. Chem. Soc.* **110**, 1337 (1988).

CH₃CP

$\bar{X}$	C _{3v}	Structure: MW ¹				
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a ₁	2	C≡P stretch	1558.74	gas	IR	2,3
e	6	CH ₃ deform.	1437.47	gas	IR	4

B₀ = 0.166 MW¹

CD₃CP

$\bar{X}$	C _{3v}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a ₁	2	C≡P stretch	1554.96	gas	IR	2

B₀ = 0.143 MW¹

References

- ¹H. W. Kroto, J. F. Nixon, and N. P. C. Simmons, *J. Mol. Spectrosc.* **77**, 270 (1979).
²K. Ohno, Y. Yamamoto, H. Matsuura, and H. Murata, *Chem. Lett.* 413 (1984).
³K. Ohno, H. Matsuura, D. McNaughton, and H. W. Kroto, *J. Mol. Spectrosc.* **124**, 82 (1987).
⁴K. Ohno, H. Matsuura, D. McNaughton, and H. W. Kroto, *J. Mol. Spectrosc.* **126**, 245 (1987).

HCr(OH)₂^a

$\bar{X}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CrH stretch	1601.8	Ar	IR	1
		OCrO stretch	735.7	Ar	IR	1

DCr(OD)₂^a

$\bar{X}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OCrO stretch	721	Ar	IR	1

^aAlternatively, peaks may be contributed by an H₂Cr(OH)₂ species with $\times > 1$.

References

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

CH₂NOH

$\bar{X}$	C _s	Structure: MW ³				
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	OH stretch	3650.29vs	gas	IR	1,4,7
	2	CH ₂ stretch	3109.72w	gas	IR	1,4,7
	3	CH ₂ stretch	2973.17wm	gas	IR	1,4,7
	4	C=N stretch	1647wm	gas	IR	1,4
	5	CH ₂ scissors	1410ms	gas	IR	1,4
	6	OH bend	1318vs	gas	IR	1,4
	7	CH ₂ rock	1166m	gas	IR	1,4
	8	NO stretch	892.6s	gas	IR	1,4,6
	9	CNO deform.	530w	gas	IR	1,4
a''	10	CH ₂ OPLA	952.61s	gas	IR	1,4,6
	11	CH ₂ torsion	774.1m	gas	IR	1,4,6
	12	OH torsion	~400	gas	IR	1,4

A₀ = 2.258; B₀ = 0.396; C₀ = 0.336 MW^{2,3,5}

References

- ¹S. Califano and W. Lüttke, *Z. Phys. Chem.* **6**, 83 (1956).
²I. N. Levine, *J. Mol. Spectrosc.* **8**, 276 (1962).
³I. N. Levine, *J. Chem. Phys.* **38**, 2326 (1963).
⁴A. Azman, D. Hadzi, J. Kidric, B. Orel, and C. Trampuz, *Spectrochim. Acta* **27A**, 2499 (1970).
⁵V. K. Kaushik and K. Takagi, *J. Phys. Soc. Japan* **45**, 1975 (1978).
⁶G. Duxbury, R. M. Percival, D. Devoy, and M. R. M. Mahmoud, *J. Mol. Spectrosc.* **132**, 380 (1988).
⁷G. Duxbury, *J. Mol. Spectrosc.* **132**, 393 (1988).

CH₃O₂

On photolysis of CH₃NNCH₃:O₂ or CH₄:O₂:Cl₂ mixtures, an unstructured absorption which has been assigned^{1,3,4,6,7} to CH₃O₂ appears between 200 and 280 nm, with a maximum at ~240 nm. In an argon matrix, CH₃O₂ photolyzes on exposure to 254-nm radiation.⁵

References

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

CH₃S₂

$\bar{X}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'		SS stretch	610(160)	gas	PE	1

CD₃S₂

$\bar{X}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'		SS stretch	610(140)	gas	PE	1

References

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

CH₃S₂⁻

Threshold for electron detachment from ground-state CH₃S₂⁻ = 14180(180) gas PE¹

 $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'		SS stretch	530(220)	gas	PE	1

CD₃S₂⁻

Threshold for electron detachment from ground-state CD₃S₂⁻ = 14100(180) gas PE¹

 $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'		SS stretch	500(230)	gas	PE	1

References

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

CH₃IO $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CH ₃ s-stretch	2945	Ar	IR	1
		CH ₃ deform.	1400s	Ar	IR	1
		CH ₃ deform.	1223ms	Ar	IR	1
		CH ₃ rock	859m	Ar	IR	1
		CH ₃ rock	848m	Ar	IR	1
		IO stretch	724vs	Ar	IR	1
		CI stretch	497w	Ar	IR	1

CD₃IO $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CD ₃ s-stretch	2132	Ar	IR	1
		CD ₃ deform.	939	Ar	IR	1
		IO stretch	723	Ar	IR	1
		CD ₃ rock	646	Ar	IR	1
		CD ₃ rock	640	Ar	IR	1
		CI stretch	460	Ar	IR	1

References

¹M. Hawkins and L. Andrews, *Inorg. Chem.* **24**, 3285 (1985).

CH₃OI $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CO stretch	1074	Ar	IR	1
		OI stretch	528	Ar	IR	1

CD₃OI $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OI stretch	509	Ar	IR	1

References

¹M. Hawkins and L. Andrews, *Inorg. Chem.* **24**, 3285 (1985).

ICH₂OH $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OH stretch	3350	Ar	IR	1
		CH stretch	2937	Ar	IR	1
		CH stretch	2815	Ar	IR	1
		CH ₂ deform.	1466	Ar	IR	1
		CO stretch	999	Ar	IR	1

ICD₂OD $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OD stretch	2478	Ar	IR	1
		CD stretch	2234	Ar	IR	1
		CD stretch	2063	Ar	IR	1
		CO stretch	972	Ar	IR	1
		CD deform.	845	Ar	IR	1

References

¹M. Hawkins and L. Andrews, *Inorg. Chem.* **24**, 3285 (1985).

NH₂NHF $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		HNF wag	1311s ^a	Ar	IR	1
		HNF rock	1282s ^a	Ar	IR	1
		NH ₂ wag	1091w ^a	Ar	IR	1
		NF stretch	1013w,br ^a	Ar	IR	1

^aMolecule hydrogen-bonded to HF.**References**¹R. Lascola, R. Withnall, and L. Andrews, *Inorg. Chem.* **27**, 642 (1988).**CH₃ClF** $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		ClF stretch	599vs	Ar	IR	1

CD₃ClF $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		ClF stretch	595vs	Ar	IR	1

References¹M. E. Jacox, *J. Chem. Phys.* **83**, 3255 (1985).**CH₃BrF** $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		BrF stretch	538vs 533vs	Ar	IR	1

CD₃BrF $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		BrF stretch	536vs	Ar	IR	1

References¹M. E. Jacox, *J. Chem. Phys.* **83**, 3255 (1985).**CH₃IF** $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		IF stretch	520s	Ar	IR	1

CD₃IF $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		IF stretch	518s	Ar	IR	1

References¹M. E. Jacox, *J. Chem. Phys.* **83**, 3255 (1985).**PH₃F₂** $\bar{X}$ D_{3h}

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

PD₃F₂ $\bar{X}$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a ₂ '	4	PF ₂ a-stretch	749	Ar	IR	2
e'	6	PD ₃ deform.	719	Ar	IR	2

References¹F. Seel and K. Velleman, *Z. Anorg. Allg. Chem.* **385**, 123 (1971).²L. Andrews and R. Withnall, *Inorg. Chem.* **28**, 494 (1989).**C₄H₂⁺** $\bar{B}$ T₀ = 51960(160) gas PE²

$\tilde{A}^2\Pi_u$	$D_{\infty h}$	Structure: LF^9				
$T_0 = 19722.610(2)$	gas	$EM^1EF^7LF^{7,9}$	$\tilde{A}-\tilde{X}$ 485–650 nm			
19708(2)	Ne	LF^4	$\tilde{A}-\tilde{X}$ 443–604 nm			
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	CH stretch	2858	gas	EM	1
			2821(2)	Ne	LF	4
	2	$C\equiv C$ stretch	1860(40)	gas	PE	2
			2002(2)	Ne	LF	4
	3	$C-C$ stretch	820(10) ^a	gas	PE,EF	2,3
			807(2)	Ne	LF	4
Π_g	7	Skel. deform.	430 ^{ab}	Ne	LF	4
$\tau = 72(3)$ ns gas $EF^3PEFCO^5LF^6$						
$A_0 = -31.1(2.0)$ gas $EM^1LF^{7,9}$						
$-30(2)$ Ne LF^4						
$B_0 = 0.140$ $LF^{7,9}$						

$\tilde{X}^2\Pi_g$	$D_{\infty h}$	Structure: LF^9				
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	CH stretch	3136.9	gas	EM	1
			3143(2)	Ne	LF	4
	2	$C\equiv C$ stretch	2176.6	gas	EM	1
			2177(2)	Ne	LF	4
	3	$C-C$ stretch	971.5	gas	EM,LF	1,8
			973(3)	Ne	LF	4
Σ_u^+	4	CH stretch	2820(40) ^b	gas	PE	2
Π_g	7	Skel. deform.	432.2 ^b	gas	EM,LF	1,8
			430.3 ^b			
			432.5 ^b	Ne	LF	4
$A = -33.5(1.9)$ gas $EM^1LF^4EF^7$						
$B_0 = 0.147$ $EM^1EF^7LF^9$						

C₄D₂⁺**B** $T_0 = 52930(160)$ gas PE^2

$\tilde{A}^2\Pi_u$	$D_{\infty h}$	Structure: LF^9				
$T_0 = 19740.683(2)$	gas	$EM^1LF^{7,9}EF^7$	$\tilde{A}-\tilde{X}$ 485–640 nm			
19727(2)	Ne	LF^4	$\tilde{A}-\tilde{X}$ 468–600 nm			
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	CD stretch	2296	gas	EM	1
	2	$C\equiv C$ stretch	1770(40)	gas	PE	2
			1892(2)	Ne	LF	4
	3	$C-C$ stretch	800(40) ^a	gas	PE	2
			782(2)	Ne	LF	4
Π_g	7	Skel. deform.	418 ^{ab}	Ne	LF	4
$\tau = 79(4)$ ns gas $EF^5PEFCO^5LF^6$						
$A = -31.1(2.0)$ gas $LF^{7,9}$						
$B_0 = 0.122$ $LF^{7,9}$						

$\tilde{X}^2\Pi_g$	$D_{\infty h}$					
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	CD stretch	2531.1	gas	EM	1
			2534(2)	Ne	LF	4
	2	$C\equiv C$ stretch	2066.3	gas	EM	1
			2067(2)	Ne	LF	4
	3	$C-C$ stretch	939.6	gas	EM	1
			932(3)	Ne	LF	4
Σ_u^+	4	CD stretch	2180(40) ^b	gas	PE	2
Π_g	7	Deformation	412.8 ^b	gas	EM	1
			414(2) ^b	Ne	LF	4

 $A = -33.3(2.0)$ gas EF^7LF^9 $B_0 = 0.127$ EF^7LF^9 ^aAlternate assignment in which values of ν_3 and $2\nu_7$ are interchanged is also possible.^b $\frac{1}{2}(2\nu_i)$.**References**⁹J. Lecoultré, J. P. Maier, and M. Rösslein, J. Chem. Phys. **89**, 6081 (1988).**HCCCNH⁺****X**

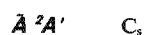
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	NH stretch	3513.96	gas	LD	1
$B_0 = 0.144$ LD^1						

References¹S. K. Lee and T. Amano, Astrophys. J. **323**, L145(1987).**HCONHCa** **$\tilde{C}^2A''$ C_s** $T_0 = 16248(20)$ gas LF^1 $\tilde{C}-\tilde{X}$ 600–630 nm

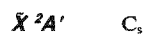
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Ca stretch	353(10)	gas	LF	1

 $\tilde{B}^2A'$ C_s $T_0 = 15083(20)$ gas LF^1 $\tilde{B}-\tilde{X}$ 645–680 nm

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Ca stretch	357(10)	gas	LF	1

 $T_0 = 14154(20)$ gas LF¹ $\tilde{A}-\tilde{X}$ 670–765 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		Ca stretch	355(10)	gas	LF	1

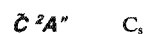


Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
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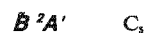
		Ca stretch	351(10)	gas	LF	1
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References

¹A. M. R. P. Bopegedera, W. T. M. L. Fernando, and P. F. Bernath, *J. Phys. Chem.* **94**, 3547 (1990).

 $T_0 = 14580(20)$ gas LF¹ $\tilde{C}-\tilde{X}$ 655–700 nm

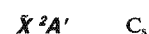
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		Sr stretch	315(10)	gas	LF	1

 $T_0 = 13917(20)$ gas LF¹ $\tilde{B}-\tilde{X}$ 700–750 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		Sr stretch	284(10)	gas	LF	1

 $T_0 = 13077(20)$ gas LF¹ $\tilde{A}-\tilde{X}$ 730–820 nm

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



Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
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		Sr stretch	288(10)	gas	LF	1
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References

¹A. M. R. P. Bopegedera, W. T. M. L. Fernando, and P. F. Bernath, *J. Phys. Chem.* **94**, 3547 (1990).



Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			2000(100)	gas	PE	1

References

¹D. McNaughton and R. J. Suffolk, *J. Chem. Research (S)* **32** (1985).

Structure: MW²

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CH stretch	3049	Ar	IR	3
			3024			
			3037	N ₂	IR	3
			3026			
		CH stretch	2978	Ar	IR	3
			2974			
			2978	N ₂	IR	3
			2968			
			2177	Ar	IR	3
			2172	N ₂	IR	3
		C=O stretch	2125	Ar	IR	3
			2124	N ₂	IR	3
			2079	Ar	IR	3
			2075	N ₂	IR	3
			1959	Ar	IR	3
			1973	N ₂	IR	3
			1690	Ar	IR	3
			1685	N ₂	IR	3
			1444	Ar	IR	3
			1457	N ₂	IR	3
			1046	Ar	IR	3
			1047	N ₂	IR	3
			980	Ar	IR	3
			988	N ₂	IR	3
			903	Ar	IR	3
			910	N ₂	IR	3
			668	Ar	IR	3
			674	N ₂	IR	3
			473	Ar	IR	3
			479	N ₂	IR	3

$A_0 = 4.998$; $B_0 = 0.146$; $C_0 = 0.142$ MW^{1,2}



$B_0 = 0.133$; $C_0 = 0.128$ MW¹

References

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³O. L. Chapman, M. D. Miller, and S. M. Pitzengerger, *J. Am. Chem. Soc.* **109**, 6867 (1987).

H₂C=C=C=S

$\bar{\chi}$	C _{2v}	Structure:	MW ¹			
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		C ₃ a-stretch	1999vs	Ar	IR	2
		CH ₂ deform.	1487wm	Ar	IR	2
		C ₃ s-stretch	1330m	Ar	IR	2
		CH ₂ OPLA	927m	Ar	IR	2
		C=S stretch	710w	Ar	IR	2

References

¹R. D. Brown, K. G. Dyall, P. S. Elmes, P. D. Godfrey, and D. McNaughton, *J. Am. Chem. Soc.* **110**, 789 (1988).

²E. Suzuki and F. Watari, *Chem. Phys. Lett.* **168**, 1 (1990).

H₂C=C=C=Se

$\bar{\chi}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		C ₃ a-stretch	1993s 1985vs 1981s	Ar	IR	1
		CH ₂ scissors	1467m	Ar	IR	1
		C ₃ s-stretch	1279s	Ar	IR	1
		CCH ₂ OPLA	909s	Ar	IR	1

References

¹W. W. Sander and O. L. Chapman, *J. Org. Chem.* **50**, 543 (1985).

HC≡C-CHSe

$\bar{\chi}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CH stretch	3322s	Ar	IR	1
		C≡C stretch	2072m	Ar	IR	1
		C=Se stretch ?	1058m	Ar	IR	1
		CH deform.	615m	Ar	IR	1

References

¹W. W. Sander and O. L. Chapman, *J. Org. Chem.* **50**, 543 (1985).

f-HN=CHCN

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

References

¹Y. Hamada, M. Tsuboi, T. Nakanaga, H. Takeo, and C. Matsumura, *J. Mol. Spectrosc.* **117**, 308 (1986).

H₂NNCO

$\bar{\chi}$	C _s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		NH ₂ a-stretch	3362m	Ar	IR	1
		NH ₂ s-stretch	3297w	Ar	IR	1
		NCO a-stretch	2262m 2210vs	Ar	IR	1
		NH ₂ scissors	1612w 1303vw 1026wm	Ar	IR	1
		NN stretch	844vw	Ar	IR	1
		NNC deform.	642w	Ar	IR	1
		NCO deform.	563w	Ar	IR	1

D₂NNCO

$\bar{\chi}$	C _s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		NCO a-stretch	2260vs 2213vs	Ar	IR	1
		ND ₂ scissors	1181w 876w 790w	Ar	IR	1
		NN stretch	843w	Ar	IR	1
		NNC deform.	638w	Ar	IR	1
		NCO deform.	563w	Ar	IR	1

References

¹J. H. Teles and G. Maier, *Chem. Ber.* **122**, 745 (1989).

CH₂COF⁻**Dipole-Bound State C_s**

$T_0 = 17709.646(3)$ gas PD¹ 547–588 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OCF deform.	571	gas	PD	1
		Torsion	~200 ^a	gas	PD	1

$A_0 = 0.382$; $B_0 = 0.358$; $C_0 = 0.184$ PD¹

 $\bar{\chi}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OCF deform.	694	gas	PD	1
		Torsion	494	gas	PD	1
		OCF deform.	475	gas	PD	1

$A_0 = 0.368$; $B_0 = 0.355$; $C_0 = 0.180$ PD¹

CD₂COF⁻*Dipole-Bound State* C_sT₀ = 17704 gas PD¹

549–586 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OCF deform.	491	gas	PD	1
		Torsion	172 ^a	gas	PD	1

 $\bar{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OCF deform.	650	gas	PD	1
		OCF deform.	419	gas	PD	1
		Torsion	385	gas	PD	1

^a $\frac{1}{2}(2\nu_1)$.**References**

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

H₂SiO₃ $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OH stretch	3677s	Ar	IR	2
		Si=O stretch	1270s	Ar	IR	1,2
		Si–O a-stretch	1023m	Ar	IR	2
		Torsion	453vs	Ar	IR	2
		SiO ₂ deform.	359wm	Ar	IR	2

D₂SiO₃ $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OD stretch	2710s	Ar	IR	2
		Si=O stretch	1267m	Ar	IR	1,2
		Si–O a-stretch	994ms	Ar	IR	2
		Si–O s-stretch	919m	Ar	IR	2
		Torsion	376s	Ar	IR	2
		SiO ₂ deform.	349m	Ar	IR	2

References

¹R. Withnall and L. Andrews, *J. Am. Chem. Soc.* **107**, 2567 (1985).

²R. Withnall and L. Andrews, *J. Phys. Chem.* **89**, 3261 (1985).

H₂GeO₃ $\bar{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OH stretch	3630.7	Ar	IR	1
		Ge=O stretch	971.4	Ar	IR	1
		GeOH deform.	955.1	Ar	IR	1
		GeOH deform.	926.0	Ar	IR	1
		Ge–O a-stretch	749.1	Ar	IR	1
		Ge–O s-stretch	732.3	Ar	IR	1
		OH torsion	396.9	Ar	IR	1

D₂GeO₃ $\bar{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OD stretch	2677.5	Ar	IR	1
		Ge=O stretch	972.2	Ar	IR	1
		Ge–O a-stretch	748.4	Ar	IR	1
		Ge–O s-stretch	733.8	Ar	IR	1
		OD torsion	295.4	Ar	IR	1
		GeO ₂ scissors	243.6	Ar	IR	1
		O ₂ GeO OPLA	209.5	Ar	IR	1

References

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

HOONO₂

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}

 $\bar{X}$ Structure: MW⁸

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
	1	OH stretch	3540.1wm	gas	IR	1,4
	2	NO ₂ a-stretch	1728.3vs	gas	IR	1,3,7
	3	OH bend	1396.9wm	gas	IR	1,3,4,7
	4	NO ₂ s-stretch	1304.2s	gas	IR	1–4,7
			941.0w	gas	IR	1,3
			922.1w	gas	IR	1,3
			919.2w	gas	IR	1,3
	6	N–O stretch	802.7m	gas	IR	1–4,7,9
	12	NO ₂ torsion	145(6)	gas	MW	8

A₀ = 0.400; B₀ = 0.156; C₀ = 0.113 gas MW⁸

References

¹H. Niki, P. D. Maker, C. M. Savage, and L. P. Breitenbach, *Chem. Phys. Lett.* **45**, 564 (1977).

²S. 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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⁴R. A. Graham, A. M. Winer, and J. N. Pitts, Jr., *Geophys. Res. Lett.* **5**, 909 (1978).

⁵R. A. Cox and K. Patrick, *Int. J. Chem. Kinet.* **11**, 635 (1979).

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⁹R. D. May, L. T. Molina, and C. R. Webster, *J. Phys. Chem.* **92**, 4667 (1988).

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CF₃O₂

In the gas phase, an absorption maximum at 255 nm, produced by the pulse radiolysis of CF₃Cl or CF₃Br in the presence of O₂, has been attributed³ to CF₃O₂.

$\tilde{\chi}$	C _s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	1	CF ₃ a-stretch	1303.9vs	Ar	IR	2,4,5
	2	C—O stretch	1173.8s	Ar	IR	1,2,4,5
	3	O—O stretch	1092.3m	Ar	IR	1,2,4,5
	4	CF ₃ s-stretch	870w	Ar	IR	2
	5	CF ₃ s-deform.	692.8m	Ar	IR	2,4,5
	6	CF ₃ a-deform.	580w	Ar	IR	2
	7	CF ₃ rock	448vw	Ar	IR	2
	8	COO bend	286vw	Ar	IR	2
<i>a''</i>	9	CF ₃ a-stretch	1263.2vs	Ar	IR	2,4,5
	10	CF ₃ a-deform.	597.2w	Ar	IR	2,5

References

- ¹R. R. Smardzewski, R. A. DeMarco, and W. B. Fox, *J. Chem. Phys.* **63**, 1083 (1975).
²R. Butler and A. Snelson, *J. Phys. Chem.* **83**, 3243 (1979).
³R. Cooper, J. B. Cumming, S. Gordon, and W. A. Mulac, *Radiat. Phys. Chem.* **16**, 169 (1980).
⁴K. C. Clemitshaw and J. R. Sodeau, *J. Phys. Chem.* **91**, 3650 (1987).
⁵K. C. Clemitshaw and J. R. Sodeau, *J. Phys. Chem.* **93**, 3552 (1989).

CCl₃O₂

In the gas phase, a broad, unstructured absorption maximum near 255 nm, produced by the pulse radiolysis of CCl₄ in the presence of O₂, has been attributed¹ to CCl₃O₂.

References

- ¹R. Cooper, J. B. Cumming, S. Gordon, and W. A. Mulac, *Radiat. Phys. Chem.* **16**, 169 (1980).

N₂O₄

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

$\tilde{\chi}$	V _h	Structure:	ED ¹			
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a_g</i>	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
			265(3)	Ne	Ra	8
	3		262	Ar	Ra	5
			257(3)	Xe	Ra	8
			79	gas	IR ^a	6
<i>a_u</i>	4		1718(3)	Xe	Ra	8
<i>b_{1g}</i>	5		498(3)	Ne	Ra	8
	6		485(3)	Xe	Ra	8
<i>b_{1u}</i>	7		425	gas	IR	6
<i>b_{2g}</i>	8		657(3)	Xe	Ra	8
<i>b_{2u}</i>	9		1758	gas	IR	6
			1749.2s	Ar	IR	2,3,9
			1735s			
	11		1761	N ₂	IR	4
			1737			
			1750	O ₂	IR	3
			1735			
			1264	gas	IR	2,6
			1257.0s	Ar	IR	2,3,9
			1261	N ₂	IR	4
	12		1261	O ₂	IR	3
			751	gas	IR	6
			755sh	Ar	IR	3
			745.8			
			751	N ₂	IR	4
			755	O ₂	IR	3
			746			

^aFrom analysis of sequence bands near 540 cm⁻¹.

References

- ¹D. W. Smith and K. Hedberg, *J. Chem. Phys.* **25**, 1282 (1956).
²W. G. Fateley, H. A. Bent, and B. Crawford, Jr., *J. Chem. Phys.* **31**, 204 (1959).
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⁸F. Bolduan and H. J. Jodl, *Chem. Phys. Lett.* **85**, 283 (1982).
⁹H. Bandow, H. Akimoto, S. Akiyama, and T. Tezuka, *Chem. Phys. Lett.* **111**, 496 (1984).

ONO—NO₂

In an argon matrix, photolysis is observed⁶ at 436 nm, but not at wavelengths longer than 510 nm. The major product is N₂O₄ (V_h), but infrared absorptions of NO, *c*-(NO)₂, O₂N—NO, and N₂O₅ also grow in intensity.

$\tilde{\chi}$ (Structure D)

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		N=O stretch	1806(3)	Ne	Ra	5
			1828	Ar	IR	1,2,6
			1861	N ₂	IR	3
			1829	O ₂	IR	1,2,4

$\bar{X}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		NO ₂ a-stretch	1635(3)	Ne	Ra	5
			1644	Ar	IR	1,2,6
			1646(3)	Xe	Ra	5
			1628	N ₂	IR	3
			1645	O ₂	IR	1,2,4
		NO ₂ s-stretch	1295(3)	Ne	Ra	5
			1290	Ar	IR	1,2,6
			1299(3)	Xe	Ra	5
			1279	N ₂	IR	3
			1291	O ₂	IR	1,2,4
		N—O stretch	903	Ar	IR	6
			905	O ₂	IR	2
		NO ₂ bend	783(3)	Ne	Ra	5
			787	Ar	IR	1,2,6
			788(3)	Xe	Ra	5
			792	N ₂	IR	3
			783	O ₂	IR	1,2,4
		O=N—O bend	622(3)	Ne	Ra	5
			626(3)	Xe	Ra	5
			647	N ₂	IR	3
			642	O ₂	IR	2,4
		NO ₂ rock or wag	488	O ₂	IR	2,4
			304	O ₂	IR	4

References

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⁶H. Bandow, H. Akimoto, S. Akiyama, and T. Tezuka, Chem. Phys. Lett. **111**, 496 (1984).

(SiO)₃

$\bar{X}$	D_{3h}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_2''	4	Deformation	74 ^a	Ar	IR	2
e'	5	SiO stretch	971.9s	Ar	IR	1,2
			972.6	N ₂	IR	1
	6	SiO stretch	629.0w	Ar	IR	1,2
			631.5	N ₂	IR	1
			311.5w	Ar	IR	1,2
	7	Deformation	312.0	N ₂	IR	1

^aTentative assignment.

References

- ¹J. S. Anderson and J. S. Ogden, J. Chem. Phys. **51**, 4189 (1969).
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(GeO)₃

$\bar{X}$	D_{3h}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
e'	5	GeO stretch	824s	Ar	IR	1
			824	N ₂	IR	1
	6	GeO stretch	438w	Ar	IR	1
			440	N ₂	IR	1

References

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

(PN)₃

$\bar{X}$	D_{3h}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
e'	5	PN stretch	1141	Ar	IR	2
			1137s	Kr	IR	1
	6	PN stretch	718w	Kr	IR	1

References

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F₂C=C=C=O

The gas-phase ultraviolet absorption spectrum¹ shows maxima at 375 and 240 nm.

$\bar{X}$	C_s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'			2169.1vs	gas	IR	1
			1763.6m	gas	IR	1
			1248.4wm	gas	IR	1
			1194.4wm	gas	IR	1
			821.9w	gas	IR	1
			611.2w	gas	IR	1
			522.9w	gas	IR	1
a''			486.3w	Ar	IR	1
			656.7w	gas	IR	1

References

- ¹J. C. Brahms and W. P. Dailey, J. Am. Chem. Soc. **111**, 3071 (1989).

F₂C=C=N=N $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			2104.7	N ₂	IR	1
			2085.2	N ₂	IR	1
			1672.7	N ₂	IR	1
			1650.7	N ₂	IR	1
			1262.8	N ₂	IR	1
			1143.9	N ₂	IR	1
			834.9	N ₂	IR	1

References¹J. C. Brahms and W. P. Dailey, *J. Am. Chem. Soc.* **112**, 4046 (1990).**cyc-(CF=CFC)=O** $\bar{\chi}$

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

References¹J. C. Brahms and W. P. Dailey, *J. Am. Chem. Soc.* **111**, 8940 (1989).**OPCl₂OCl** $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		P=O stretch	1284	Ar	IR	1
		POCl a-stretch	885	Ar	IR	1
		POCl s-stretch	671	Ar	IR	1
		PCl ₂ a-stretch	544	Ar	IR	1

References¹B. W. Moores and L. Andrews, *J. Phys. Chem.* **93**, 1902 (1989).**PF₃=PF** $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			967m	Ar	IR	1
			924vs	Ar	IR	1
			898m	Ar	IR	1
			811wm	Ar	IR	1

 $\bar{\chi}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			751m	Ar	IR	1
			580wm	Ar	IR	1
			408vw	Ar	IR	1
			399w	Ar	IR	1

References¹J. K. Burdett, L. Hodges, V. Dunning, and J. H. Current, *J. Phys. Chem.* **74**, 4053 (1970).**ClOClO₃**An unstructured gas-phase absorption with maximum at 42740 (234 nm) has been assigned⁴ to ClOClO₃. $\bar{\chi}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	ClO ₂ s-stretch	1283vs	gas	IR	1-3,5
			1287vs	Ar	IR	2
2		Cl=O stretch	1040s	gas	IR	1,2
			1039s	Ar	IR	2
3		O-Cl stretch	749wm	gas	IR	1,2
			746m	Ar	IR	2
4		Cl-O stretch	646vs	gas	IR	1,2
			647vs	Ar	IR	2
5		O=Cl=O bend	580sh	gas	IR	2
			582m	Ar	IR	2
6		ClO ₃ deform.	511wm	gas	IR	2
			513m	Ar	IR	2
7		O=Cl-O bend	355vw	Ar	IR	2
a''	9	ClO ₂ a-stretch	1283vs	gas	IR	1-3,5
			1271vs	Ar	IR	2
10		O=Cl=O bend	561m	gas	IR	2
			561ms	Ar	IR	2
11		O=Cl-O bend	382w	Ar	IR	2

References¹C. J. Schack and D. Pilipovich, *Inorg. Chem.* **9**, 1387 (1970).²K. O. Christe, C. J. Schack, and E. C. Curtis, *Inorg. Chem.* **10**, 1589 (1971).³A. J. Schell-Sorokin, D. S. Bethune, J. R. Lankard, M. M. T. Loy, and P. P. Sorokin, *J. Phys. Chem.* **86**, 4653 (1982).⁴M. I. Lopez and J. E. Sicre, *J. Phys. Chem.* **91**, 564 (1988).⁵J. B. Burkholder, J. J. Orlando, and C. J. Howard, *J. Phys. Chem.* **94**, 687 (1990).**CF₃IO** $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CF stretch	1214	Ar	IR	1
		CF stretch	1202	Ar	IR	1
		IO stretch + CF ₃ deform.	732	Ar	IR	1

References

- ¹L. Andrews, M. Hawkins, and R. Withnall, *Inorg. Chem.* **24**, 4234 (1985).

CF₃OI $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CF stretch	1241s ^a	Ar	IR	1,2
		CF stretch	1203s	Ar	IR	1,2
		CO stretch	913	Ar	IR	1,2
		COI bend	320	Ar	IR	1

^aModerately intense satellite at 1235 cm⁻¹ assigned to 913 + 320 combination band.

References

- ¹L. Andrews, M. Hawkins, and R. Withnall, *Inorg. Chem.* **24**, 4234 (1985).
²K. C. Clemitshaw and J. R. Sodeau, *J. Phys. Chem.* **93**, 3552 (1989).

6.13. Seven-Atomic Molecules

B₂H₅⁺ $\tilde{X}$ D_{3h} ?

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			~1290	gas	PI	1

References

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

C₂H₅⁺ $\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a ₁			400(30) ^a	gas	PE,PI	1-3

^aThe photoionization studies of Ref. 3 suggest that the measured vibrational spacings arise from transitions to higher vibrational states of the bridged ion structure and that $\Delta G(\frac{1}{2})$ may be as great as 730(90).

References

- ¹J. M. Dyke, N. Jonathan, and A. Morris, *Int. Rev. Phys. Chem.* **2**, 3 (1982).
²J. M. Dyke, A. R. Ellis, N. Keddar, and A. Morris, *J. Phys. Chem.* **88**, 2565 (1984).
³B. Ruscic, J. Berkowitz, L. A. Curtiss, and J. A. Pople, *J. Chem. Phys.* **91**, 114 (1989).

C₂H₅**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 C₂H₅. The detection of this band in MPI studies⁹ 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 C₂H₅.

 $\tilde{X}$ C_s Structure: MO⁴

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'		CH ₂ s-stretch	3033m	Ar	IR	2,4,5,8
		CH ₃ s-stretch	2920m	Ar	IR	4,5
		2-CH stretch	2842s	Ar	IR	2,4,5,8
		CH ₂ deform.	1440m	Ar	IR	2,4,5,8
			1383	Ar	IR	8
a''		CH ₃ deform.	1366m	Ar	IR	2,4,5,8
		CC stretch	1138w	Ar	IR	4,5,8
			1025	Ar	IR	8
		CCH ₂ umbrella	540vs	Ar	IR	2,4,5,8
		CH ₂ a-stretch	3112s	Ar	IR	2,4,5,8
		CH ₃ a-stretch	2987s	Ar	IR	2,4,5
		CH ₃ deform.	1440m	Ar	IR	2,4,5,8
		H deform.	1175m	Ar	IR	4,5,8

C₂D₅ $\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'		CD ₂ s-stretch	2199m	Ar	IR	4,5
		CD ₃ s-stretch	2094m	Ar	IR	4,5
		2-CD stretch	2048m	Ar	IR	4,5
		CD ₃ deform.	1070m	Ar	IR	4,5
		CD ₂ deform.	1035m	Ar	IR	4,5
a''		CCD ₂ umbrella	398vs	Ar	IR	4,5
		CD ₂ a-stretch	2249m	Ar	IR	4,5
		CD ₃ a-stretch	2170s	Ar	IR	4,5
		CD ₃ deform.	1041m	Ar	IR	4,5

References

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

C₂H₄Li $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CH stretch	3055vw	Ar	IR	1
		CH ₂ scissors	1428w	Ar	IR	1
		CC stretch	1176.5s	Ar	IR	1
			704vw	Ar	IR	1
		LiC stretch	369s	Ar	IR	1

C₂D₄Li $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CD stretch	2223vw	Ar	IR	1
		CC stretch	1312s	Ar	IR	1
		CD ₂ scissors	931m	Ar	IR	1
		LiC stretch	360s	Ar	IR	1

References¹L. Manceron and L. Andrews, J. Phys. Chem. **90**, 4514 (1986).**H₅O₂[±]** $\bar{\chi}$ C₂

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		H ₂ O a-stretch	3684.4	gas	PF	1
		H ₂ O s-stretch	3608.8	gas	PF	1

References¹L. I. Yeh, M. Okumura, J. D. Myers, J. M. Price, and Y. T. Lee, J. Chem. Phys. **91**, 7319 (1989).**HFeC₂H₃** $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CH ₂ a-stretch	2999.5	Ar	IR	1
		CH stretch	2923.1	Ar	IR	1
			2913.0	Kr	IR	1
		CH ₂ s-stretch	2901.6	Ar	IR	1
		FeH stretch	1696.6	Ar	IR	1
			1683.8	Kr	IR	1
		C=C stretch	1556.3	Ar	IR	1
			1563.0	Kr	IR	1
		CH ₂ scissors	1399.1	Ar	IR	1
			1408.3	Kr	IR	1
		CH ₂ rock	1019.0	Ar	IR	1
			1020.9	Kr	IR	1
		HCFe bend	972.9	Ar	IR	1
			980.2	Kr	IR	1

 $\bar{\chi}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CH ₂ wag	944.2	Ar	IR	1
			944.7	Kr	IR	1
		CFe stretch	507.2	Ar	IR	1

DFeC₂D₃ $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CD ₂ a-stretch	2264.5	Ar	IR	1
		CD stretch	2175.3	Ar	IR	1
		CD ₂ s-stretch	2150.5	Ar	IR	1
		C=C stretch	1477.4	Ar	IR	1
		FeD stretch	1220.5	Ar	IR	1
		CD ₂ scissors	1063.1	Ar	IR	1
		CD ₂ wag	737.4	Ar	IR	1
		CD ₂ rock	713.5	Ar	IR	1
		CFe stretch	491.0	Ar	IR	1

References¹Z. H. Kafafi, R. H. Hauge, and J. L. Margrave, J. Am. Chem. Soc. **107**, 7550 (1985).**AlC₂H₄** $\bar{\chi}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CH stretch	~3094	Ar	IR	1
		CH stretch	~2980	Ar	IR	1
		CH ₂ deform.	1381ms	Ar	IR	1
		CC stretch	1193s	Ar	IR	1
			781vs	Ar	IR	1
			686m	Ar	IR	1
		AlC s-stretch	352ms	Ar	IR	1
		AlC a-stretch	224m	Ar	IR	1

AlC₂D₄ $\bar{\chi}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CD stretch	~2337	Ar	IR	1
		CD stretch	~2194	Ar	IR	1
		CD stretch	~2175	Ar	IR	1
		CC stretch	1289ms	Ar	IR	1
		CD ₂ deform.	1041wm	Ar	IR	1
		CD ₂ deform.	941wm	Ar	IR	1
			596s	Ar	IR	1
			536w	Ar	IR	1
		AlC s-stretch	337ms	Ar	IR	1
		AlC a-stretch	212m	Ar	IR	1

References

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

HNIOCH₃ $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		NiH stretch	1868.9	Ar	IR	1
		NiO stretch	569.9	Ar	IR	1

DNIOCD₃ $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		NiD stretch	1347.3	Ar	IR	1
		NiO stretch	546.2	Ar	IR	1

References

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

CH₃NiOH $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OH stretch	3717.6	Ar	IR	1
		NiO stretch	715.0	Ar	IR	1

CD₃NiOD $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OD stretch	2738.7	Ar	IR	1
		NiO stretch	686.5 682.9	Ar	IR	1

References

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

CH₃CNH⁺ $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
	1	NH stretch	3527.29	gas	LD	1

$B_0 = 0.287 \text{ LD}^1$

References

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

HCH₃SiO $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		Si=O stretch	1207.6	Ar	IR	1,2

References

¹R. Withnall and L. Andrews, J. Am. Chem. Soc. **108**, 8118 (1986).

²R. Withnall and L. Andrews, J. Phys. Chem. **92**, 594 (1988).

NH₂NHOH $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OH stretch	3198s	Ar	IR	1
		HNOH wag	1329	Ar	IR	1
		NNH deform.	1282	Ar	IR	1
			734s	Ar	IR	1

References

¹R. Lascola, R. Withnall, and L. Andrews, Inorg. Chem. **27**, 642 (1988).

CH₃C≡CCI⁺ $\tilde{B}^2A_1, C_{3v}$

$T_0 = 36790(560) \text{ gas PE}^1$

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

$T_0 = 28334(3) \text{ gas EF}^1\text{LF}^3 \quad \tilde{A}-\tilde{X} \text{ 335-425 nm}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	3	CH ₃ deform.	1196(3)	gas	LF	3
	5	CCI stretch	479(3)	gas	EF,LF	3
e	9	Skel. bend	284 ^a	gas	LF	3
	10	CCI bend	184 ^a	gas	LF	3

$\tau_1 = 19(3) \text{ ns gas EF}^2$

$\tau_2 = 600(200) \text{ ns gas EF}^2$

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	2	C≡C stretch	2117(3)	gas	EF	3
	3	CH ₃ deform.	1260(3)	gas	EF	3
	5	CCl stretch	601(3)	gas	EF	3
e	9	Skel. bend	318 ^b	gas	EF	3
	10	CCl bend	271 ^a	gas	EF	3

 $CD_3C\equiv CCl^+$ $\tilde{A}^2E_{3/2}$ C_{3v}

$T_0 = 28314(3)$ gas EF³LF³ $\tilde{A}-\tilde{X}$ 335–385 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	3	CD ₃ deform.	963(3)	gas	LF	3
	5	CCl stretch	464(3)	gas	LF,EF	3
e	9	Skel. bend	263 ^a	gas	LF	3
	10	CCl bend	155 ^a	gas	LF	3

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	3	CD ₃ deform.	995(3)	gas	EF	3
	5	CCl stretch	566(3)	gas	EF	3
e	9	Skel. bend	311 ^b	gas	EF	3
	10	CCl bend	222 ^b	gas	EF	3

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

^b Tentative assignment.

References

- ¹G. Bieri, E. Heilbronner, V. Hornung, E. Kloster-Jensen, J. P. Maier, F. Thommen, and W. Von Niessen, Chem. Phys. **36**, 1 (1979).
- ²J. P. Maier, O. Marthaler, and E. Kloster-Jensen, J. Electron Spectrosc. Relat. Phenom. **18**, 251 (1980).
- ³D. Klapstein, R. Kuhn, J. P. Maier, M. Ochsner, and T. Wyttenbach, Chem. Phys. **101**, 133 (1986).

 $CH_3C\equiv CBr^+$ B^2A_1 C_{3v}

$T_0 = 35820(560)$ gas PE¹

 $\tilde{A}^2E_{3/2}$ C_{3v}

$T_0 = 21849$ gas EF³LF³ $\tilde{A}-\tilde{X}$ 410–580 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	3	CH ₃ deform.	1399(2)	gas	LF	3
	5	CBr stretch	392(2)	gas	EF,LF	3
e	10	CBr bend	207 ^a	gas	EF,LF	3

$\tau_1 = 13(3)$ ns gas EF²

$\tau_2 = 600(200)$ ns gas EF²

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	2	C≡C stretch	2030(2)	gas	EF	3
	3	CH ₃ deform.	1187(2)	gas	EF	3
	5	CBr stretch	486(2)	gas	EF	3
e	9	Skel. bend	335 ^b	gas	EF	3
	10	CBr bend	259 ^a	gas	EF	3

 $CD_3C\equiv CBr^+$ $\tilde{A}^2E_{3/2}$ C_{3v}

$T_0 = 21824$ gas EF³LF³ $\tilde{A}-\tilde{X}$ 440–525 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	5	CBr stretch	373(2)	gas	EF,LF	3
e	10	CBr bend	195 ^a	gas	EF,LF	3

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	2	C≡C stretch	2011(2)	gas	EF	3
	5	CBr stretch	462(2)	gas	EF	3
e	10	CBr bend	243 ^a	gas	EF	3

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

^b Tentative assignment.

References

- ¹G. Bieri, E. Heilbronner, V. Hornung, E. Kloster-Jensen, J. P. Maier, F. Thommen, and W. Von Niessen, Chem. Phys. **36**, 1 (1979).
- ²J. P. Maier, O. Marthaler, and E. Kloster-Jensen, J. Electron Spectrosc. Relat. Phenom. **18**, 251 (1980).
- ³D. Klapstein, R. Kuhn, J. P. Maier, M. Ochsner, and T. Wyttenbach, Chem. Phys. **101**, 133 (1986).

 CH_3CNO $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CN stretch	2309	Ar	IR	1
		CH ₃ deform.	1381	Ar	IR	1
		NO stretch	1332	Ar	IR	1
		CC stretch	780	Ar	IR	1

 CD_3CNO $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CN stretch	2297	Ar	IR	1
		NO stretch	1341	Ar	IR	1

References

¹Z. Mielke, M. Hawkins, and L. Andrews, J. Phys. Chem. **93**, 558 (1989).

HOCH₂CN $\tilde{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OH stretch	3641	Ar	IR	1
		CN stretch	2291	Ar	IR	1
			2262			
			1274	Ar	IR	1
		OH bend	1209m	Ar	IR	1
		CO stretch	1061s	Ar	IR	1
		CH ₂ rock	971m	Ar	IR	1
			901	Ar	IR	1
		CC stretch	888	Ar	IR	1
		CCN deform.	355	Ar	IR	1
		OH torsion	256s	Ar	IR	1

DOCH₂CN $\tilde{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OD stretch	2688	Ar	IR	1
		CN stretch	2248	Ar	IR	1
			1274	Ar	IR	1
		CD ₂ wag	1134	Ar	IR	1
		CO stretch	980	Ar	IR	1
		OD bend	897	Ar	IR	1
		CC stretch	772	Ar	IR	1
		CD ₂ rock	724	Ar	IR	1

References

¹Z. Mielke, M. Hawkins, and L. Andrews, J. Phys. Chem. **93**, 558 (1989).

CH₃OCCL^a $\tilde{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CH stretch	2963	Ar	IR	1
			2975	N ₂	IR	2
			1475m	N ₂	IR	2
			1465m	N ₂	IR	2
			1449m	Ar	IR	1
			1445m	N ₂	IR	2
			1439m	N ₂	IR	2
		COC a-stretch	1300s	Ar	IR	1
			1309vs	N ₂	IR	2
		COC a-stretch	1286m	Ar	IR	1
			1280sh	Ar	IR	1
			1299m	N ₂	IR	2
			1135vs	Ar	IR	1
			1140s	N ₂	IR	2

 $\tilde{\chi}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		COC s-stretch	950s	Ar	IR	1
			947s	N ₂	IR	2
			842wm	Ar	IR	1
			840m	N ₂	IR	2
			810w	N ₂	IR	2
		CCl stretch	777s	Ar	IR	1
			773vs	N ₂	IR	2
		CCl stretch	698s	Ar	IR	1
			690m	N ₂	IR	2
			451m	Ar	IR	1
			402m	Ar	IR	1
			400m	N ₂	IR	2
			394m	N ₂	IR	2

CD₃OCCL^a $\tilde{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CD stretch	2178	Ar	IR	1
			2180w	N ₂	IR	2
			1370w	Ar	IR	1
			1362m	N ₂	IR	2
		COC a-stretch	1330	Ar	IR	1
			1329vs	N ₂	IR	2
			1324	Ar	IR	1
			1305vw	N ₂	IR	2
			1073	Ar	IR	1
			1071m	N ₂	IR	2
			1053	Ar	IR	1
			1050m	N ₂	IR	2
			950s	N ₂	IR	2
			926	Ar	IR	1
			925w	N ₂	IR	2
			807	Ar	IR	1
			805m	N ₂	IR	2
			794vw	N ₂	IR	2
			777w	N ₂	IR	2
			769w	N ₂	IR	2
		CCl stretch	755	Ar	IR	1
			749s	N ₂	IR	2
		CCl stretch	680	Ar	IR	1
			669m	N ₂	IR	2
			434m	N ₂	IR	2
			386	Ar	IR	1
			383m	N ₂	IR	2
			377w	N ₂	IR	2

^aIt has been suggested² that *cis*- and *trans*- stereoisomers contribute to the observed spectrum.

References

¹R. S. Sheridan and M. A. Kesselmayer, J. Am. Chem. Soc. **106**, 436 (1984).

²M. A. Kesselmayer and R. S. Sheridan, J. Am. Chem. Soc. **108**, 99 (1986).

(HO)₂HPO $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OH stretch	3634.8	Ar	IR	1
		PH stretch	2487.5	Ar	IR	1
		P=O stretch	1298.6	Ar	IR	1
		PO ₂ a-stretch	902.0	Ar	IR	1
		PO ₂ s-stretch	872.6	Ar	IR	1

References¹R. Withnall and L. Andrews, *J. Phys. Chem.* **91**, 784 (1987).**H(C≡C)₂CN⁺** $\tilde{C}^2\Pi$ $C_{\infty v}$ $T_0 = 27350(160)$ gas PE¹ $B^2\Sigma^+ C_{\infty v}$ $T_0 = 21860(160)$ gas PE¹ $A^2\Pi C_{\infty v}$ $T_0 = 17190(5)$ gas EF¹ $\tilde{A}-\tilde{X}$ 580–670 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type	Refs. meas.
Σ^+		C≡C stretch	1870(160)	gas	EF	1
	6	C–C stretch	600(160)	gas	EF	1

 $\tau_0 = 15(2)$ ns gas EF¹ $\tilde{X}^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ^+	2	C≡N,C≡C str.	2190(10)	gas	EF	1
	3	C≡N,C≡C str.	2070(10)	gas	EF	1
	5	C–C stretch	1220(10)	gas	EF	1
	6	C–C stretch	630(10)	gas	EF	1

References¹G. Bieri, E. Kloster-Jensen, S. Kvisle, J. P. Maier, and O. Marthaler, *J. Chem. Soc., Faraday Trans. 2* **76**, 676 (1980).**C₅O₂**In an argon matrix, photodissociates into C₄O + CO on irradiation at 230 nm, the position of a prominent absorption maximum observed in cyclohexane.¹ $\tilde{X}$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ_u^+	4		2242.01	gas	IR	2
			2213.0vs	Ar	IR	1
	5		2065	gas	IR	2
			2058.7m	Ar	IR	1
	6		1152	gas	IR	2
			1144.1w	Ar	IR	1
Π_u	9		542	gas	IR	2
			539.0w	Ar	IR	1
	10		474	gas	IR	2
			470.0vw	Ar	IR	1

 $B_0 = 0.027$ IR²**References**¹G. Maier, H. P. Reisenauer, U. Schäfer, and H. Balli, *Angew. Chem.* **100**, 590 (1988); *Angew. Chem. Int. Ed. Engl.* **27**, 566 (1988).²F. Holland, M. Winnewisser, G. Maier, H. P. Reisenauer, and A. Ulrich, *J. Mol. Spectrosc.* **130**, 470 (2988).**O₂N–O–NO₂** $\tilde{X}$ C_{2v} (C_2 ?)^a Structure: ED⁶

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	1	NO ₂ a-stretch	1720vs	gas	IR	1,2,5,8
			1745	N ₂	IR	3
			1752	CO ₂	IR	1
	2	NO ₂ s-stretch	1338m	gas	IR	2,8
			1305	N ₂	IR	3
			1300	O ₂	IR	4
			1316	CO ₂	IR	1
	3	NO ₂ bend	743.4s	gas	IR	2
			737	Ar	IR	7
			739	N ₂	IR	3
			736	O ₂	IR	4
			737	CO ₂	IR	1
	4	NO ₂ rock	~614m	gas	IR	2
	5	NON s-stretch	~353vs	gas	IR	2
b_1	9	NO ₂ wag	557s	gas	IR	2,5
	10	NO ₂ twist	~50w,br	gas	IR	9
b_2	11	NO ₂ a-stretch	1720vs	gas	IR	1,2,5,8
			1704	Ar	IR	7
			1704	N ₂	IR	3
			1704	O ₂	IR	4
			1700	CO ₂	IR	1
	12	NO ₂ s-stretch	1245.9s	gas	IR	1,2,5,8
			1245	Ar	IR	7
			1247	N ₂	IR	3
			1241	O ₂	IR	4
			1248	CO ₂	IR	1
	13	NON a-stretch	860m	gas	IR	2,8
	14	NO ₂ bend	743.4s	gas	IR	1,2,5,8
			737	Ar	IR	7
			739	N ₂	IR	3
			736	O ₂	IR	4
			719	CO ₂	IR	1
	15	NO ₂ rock	~353vs	gas	IR	2,9

^aRef. 2 analyzed the spectrum in terms of a C_{2v} structure. No evidence has since been obtained for the appearance of the two infrared-inactive fundamentals expected for that point group. The electron diffraction measurements of Ref. 6, analyzed using a dynamical model, suggest instead a C_2 structure.

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P₂O₅

$\tilde{X}$	C_{2v}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		PO ₂ a-stretch	1473.2	Ar	IR	1,2
		PO ₂ s-stretch	1158.2	Ar	IR	1,2
		POP s-stretch	735.1	Ar	IR	1,2
		PO ₂ deform.	479.5	Ar	IR	1

References

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6.14. Eight-Atomic Molecules**Ga₂H₆**

$\tilde{X}$	D_{2h}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
b_{1u}	8	GaH _i stretch	1998m	gas	IR	1
			2015m	Ar	IR	1
	9	GaH ₂ rock?	1996m			
			2000m	N ₂	IR	1
			659m	Ar	IR	1
b_{2u}	13	GaH ₆ stretch	655m			
			653m			
			648m			
			655s	N ₂	IR	1
			647w			
	14	GaH ₂ rock	1267s	gas	IR	1
			1283s	Ar	IR	1
			1278m			
			1253m			
			1282m	N ₂	IR	1
			760w	gas	IR	1
			773m	Ar	IR	1
			761m			
			770m	N ₂	IR	1

 $\tilde{X}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
b_{3u}	16	GaH _i stretch	~1976	gas	IR	1
			1985s	Ar	IR	1
			1968m			
			1985m	N ₂	IR	1
	17	GaH ₆ stretch	~1200m	gas	IR	1
			1213m	Ar	IR	1
			1208m			
			1195m			
			1220s	N ₂	IR	1
	18	GaH ₂ bend	~671vs	gas	IR	1
			676vs	Ar	IR	1
			666s			
			673vs	N ₂	IR	1

Ga₂D₆

$\tilde{X}$	D_{2h}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
b_{1u}	8	GaD _i stretch	1446m	gas	IR	1
			1434m,sh			
b_{2u}	9	GaD ₂ rock	439wm	gas	IR	1
	13	GaD ₆ stretch	914s	gas	IR	1
	14	GaD ₂ rock	545m	gas	IR	1
b_{3u}	16	GaD _i stretch	~1416m	gas	IR	1
	17	GaD ₆ stretch	~860m	gas	IR	1
	18	GaD ₂ bend	~484vs	gas	IR	1

References

- ¹A. J. Downs, M. J. Goode, and C. R. Pulham, *J. Am. Chem. Soc.* **111**, 1936 (1989).

cyc-C₃H₅

$\tilde{X}$	C_{2v}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1		α -CH bend	1000(70)	gas	PE	1

References

- ¹J. Dyke, A. Ellis, N. Jonathan, and A. Morris, *J. Chem. Soc., Faraday Trans. 2* **81**, 1573 (1985).

CH₂CHCH₂

$\tilde{B}^2B_1$	C_{2v}					
gas	AB ²					
						$\tilde{B}-\tilde{X}$ 220–250 nm
In an argon matrix, a very prominent absorption maximum at 213 nm, with a shoulder at 220 nm, has been assigned ⁵ to this transition of CH ₂ CHCH ₂ .						

3s²A₁ C_{2v}T₀ = 40056.8(2.0) gas MPI^{7,8}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a ₁		C ₃ bend	394(3)	gas	MPI	7,8
a ₂		CH ₂ a-twist	529(3)	gas	MPI	8
b ₁		CH ₂ s-twist	491(7)	gas	MPI	8

 $\bar{A}^2B_1$ C_{2v}T₀ = 24485 gas AB¹
24480 Ar AB⁵

Diffuse bands.

 $\bar{A}-\bar{X}$ 370–410 nm
 $\bar{A}-\bar{X}$ 360–410 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a ₁			1241	gas	AB	1
			1005	gas	AB	1
			908	gas	AB	1
			359	gas	AB	1

 $\bar{X}^2A_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CH stretch	3107m	Ar	IR	4,5
		CH stretch	3051w	Ar	IR	4,5
		CH stretch	3040w	Ar	IR	4
		CH stretch	3019m	Ar	IR	4,5
			1602m	Ar	IR	4
			1477m	Ar	IR	4,5
			1463m	Ar	IR	4,5
			1403vw	Ar	IR	5
			1388s	Ar	IR	4,5
			1317vw	Ar	IR	4
			1283w	Ar	IR	4,5
			1242w	Ar	IR	4,5
			1182w	Ar	IR	4
			983.6s	Ar	IR	4,5,9
			972m	Ar	IR	4
			810w	Ar	IR	5
a ₁		C ₃ bend	427(5)	gas	MPI	7,8
a ₂		CH ₂ a-twist	547(15)	gas	MPI	8
b ₁			801.1vs	Ar	IR	3–5,9
		CH ₂ s-twist	508(12)	gas	MPI	7,8
			510.1s	Ar	IR	4,5,9

CD₂CD₂CD₂**3s²A₁** C_{2v}T₀ = 40125(30) gas MPI⁷

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a ₁		C ₃ bend	342(60)	gas	MPI	7

 $\bar{A}^2B_1$ C_{2v}T₀ = 24745 gas AB¹

Diffuse bands.

 $\bar{A}-\bar{X}$ 360–405 nm

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

 $\bar{X}^2A_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a ₁		C ₃ bend	380(225)	gas	PE	6
b ₁			646.5	Ar	IR	9

References

- ¹C. L. Currie and D. A. Ramsay, J. Chem. Phys. **45**, 488 (1966).
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- ⁹J. W. Huang and W. R. M. Graham, J. Chem. Phys. **93**, 1583 (1990).

***t*-CH₃CH=NH**

$\bar{X}$	C _s	Structure:	MW ²			
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	NH stretch	3264vvw	Ar	IR	1
	2	CH ₃ a-stretch	3018m	Ar	IR	1
	3	CH stretch	2954ms	Ar	IR	1
	4	CH ₃ s-stretch	2886	gas	IR	3
			2885m	Ar	IR	1
	5	C=N stretch	1651	gas	IR	3
			1659sh	Ar	IR	1
	7	CH ₃ s-deform.	1398wm	Ar	IR	1
			1392m			
	8	Mixed	~1359	gas	IR	3
			1358s	Ar	IR	1
	9	CH deform.	1102	gas	IR	3
			1106s	Ar	IR	1
	10	CNH deform.	1040	gas	IR	3
			1040s	Ar	IR	1
	11	CC stretch	920wm	Ar	IR	1
	12	CCN bend	498wm	Ar	IR	1
a''	13	CH ₃ a-stretch	2990m	Ar	IR	1
	14	CH ₃ a-deform.	1454	gas	IR	3
			1435s	Ar	IR	1
			1433s			
	15	C=N torsion	1160vw	Ar	IR	1
	16	CH ₃ wag	1040s	Ar	IR	1
	17	CH wag	654	gas	IR	3
			668s	Ar	IR	1

A₀ = 1.666; B₀ = 0.328; C₀ = 0.289 MW²

***t*-CD₃CD=ND**

$\tilde{X}$	C _s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	1	ND stretch	2452vww	Ar	IR	1
	2	CD ₃ a-deform.	2243wm	Ar	IR	1
	3	CD stretch	2209wm	Ar	IR	1
	4	CD ₃ s-stretch	2058w	Ar	IR	1
	5	C=N stretch	1613m	Ar	IR	1
	6	CC stretch	1200m	Ar	IR	1
	7	CD ₃ s-deform.	1065m	Ar	IR	1
	8	CD ₃ a-deform.	1042m	Ar	IR	1
	9	CD deform.	848ms	Ar	IR	1
	10	Mixed	804s	Ar	IR	1
	11	CND deform.	736m	Ar	IR	1
	12	CCN bend	411s	Ar	IR	1
<i>a''</i>	13	CD ₃ a-stretch	2243wm	Ar	IR	1
	14	CD ₃ a-deform.	1046m	Ar	IR	1
	15	C=N torsion	986m	Ar	IR	1
	16	CD ₃ wag	799wm	Ar	IR	1
	17	CD wag	495vs	Ar	IR	1

References

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***c*-CH₃CH=NH**

$\tilde{X}$	C _s	Structure:	MW ²			
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	1	NH stretch	3247vww	Ar	IR	1
	2	CH ₃ a-stretch	3018m	Ar	IR	1
	3	CH stretch	2916	gas	IR	3
			2925ms	Ar	IR	1
			2920m			
	4	CH ₃ s-stretch	2886	gas	IR	3
			2885m	Ar	IR	1
	5	C=N stretch	1655	gas	IR	3
			1652vs	Ar	IR	1
	6	CH ₃ a-deform.	1438ms	Ar	IR	1
	7	CH ₃ s-deform.	1412m	Ar	IR	1
	8	Mixed	1250	gas	IR	3
			1252vs	Ar	IR	1
	9	CH deform.	1107	gas	IR	3
			1114ms	Ar	IR	1
	10	CNH deform.	1052wm	Ar	IR	1
	11	CH ₃ rock	950w	Ar	IR	1
	12	CCN deform.	485s	Ar	IR	1
<i>a''</i>	13	CH ₃ a-stretch	2988	gas	IR	3
			2990m	Ar	IR	1
	14	CH ₃ a-deform.	1454	gas	IR	3
			1435s	Ar	IR	1
			1433s			
	15	C=N torsion	1132vw	Ar	IR	1
	16	CH ₃ wag	1045	gas	IR	3
			1045vs	Ar	IR	1
	17	CH wag	678	gas	IR	3
			674w	Ar	IR	1

$$A_0 = 1.772; \quad B_0 = 0.326; \quad C_0 = 0.290 \quad \text{MW}^2$$

***c*-CH₃CD=ND**

$\tilde{X}$	C _s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	1	ND stretch	2425vww	Ar	IR	1
	2	CD ₃ a-stretch	2256wm	Ar	IR	1
	3	CD stretch	2191m	Ar	IR	1
	4	CD ₃ s-stretch	2062w	Ar	IR	1
	5	C=N stretch	1631s	Ar	IR	1
			1628vs			
	6	Mixed	1159ms	Ar	IR	1
	7	Mixed	1072m	Ar	IR	1
	8	CD ₃ a-deform.	1032wm	Ar	IR	1
	9	Mixed	850w	Ar	IR	1
<i>a''</i>	10	CD rock	796s	Ar	IR	1
	11	CD ₃ rock	736m	Ar	IR	1
	12	CCN bend	405m	Ar	IR	1
	13	CD ₃ a-stretch	2216wm	Ar	IR	1
	14	CD ₃ a-deform.	1039s	Ar	IR	1
	15	CD ₃ wag	848ms	Ar	IR	1
	16	C=N torsion	811s	Ar	IR	1
	17	CD wag	527m	Ar	IR	1

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²F. J. Lovas, R. D. Suenram, D. R. Johnson, F. O. Clark, and E. Tiemann, J. Chem. Phys. **72**, 4964 (1980).
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C₂H₃NH₂

$\tilde{X}$	C ₁ ^a					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
	5	CH stretch	2987	gas	IR	2
			2976			
	6	C=C stretch	1672	gas	IR	2
			1668			
	7	NH ₂ scissors	~1625	gas	IR	2
	8	CH ₂ scissors	1454	gas	IR	2
	10	NH ₂ twist	1260	gas	IR	2
			1248			
	11	C-N stretch	1084	gas	IR	2
			1078			
	12	CH wag	1046	gas	IR	2
			1039			
	14	CH ₂ wag	812s	gas	IR	2
			805s			
	15	NH ₂ wag	615 ^b	gas	IR	2,4
			570 ^c	gas	IR	2,4
			470 ^d	gas	IR	4
			425 ^e	gas	IR	4
	16	C=C torsion	379 ^b	gas	IR	4
			~334 ^c	gas	IR	4
			~332 ^d	gas	IR	4
			287 ^e	gas	IR	4

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

^aThe barrier to inversion about the N atom is estimated to be between 400 and 800 cm⁻¹,^{3,4} leading to splittings in a number of the vibrational band centers.

^b1⁻ - 0⁺.

^c1⁻ - 0⁻.

^d1⁺ - 0⁺.

^e1⁺ - 0⁻.

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⁴Y. Hamada, N. Sato, and M. Tsuboi, *J. Mol. Spectrosc.* **124**, 172 (1987).

H₂C=NCH₃

$\tilde{X}$	C _s	Structure:	MW ¹			
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	1	CH ₂ a-stretch	3024s	gas	IR	3
			3012s	Ar	IR	2-4
	2	CH ₃ a-stretch	2962s	gas	IR	3
			2953s	Ar	IR	3
	3	CH ₂ s-stretch	2897w	gas	IR	3
			2900s	Ar	IR	2-4
	4	CH ₃ s-stretch	2854s	Ar	IR	3,4
			2849s			
	5	C=N stretch	1661s	gas	IR	3
			1659m	Ar	IR	2,3
	6	CH ₂ scissors	1475vs	gas	IR	3
			1470vvs	Ar	IR	2,3
	7	CH ₃ a-deform.	1425w ^a	gas	IR	3
	8	CH ₃ s-deform.	1405vw	gas	IR	3
			1402m	Ar	IR	2,3
	9	CH ₃ rock	1220s	gas	IR	3
			1221s	Ar	IR	2-4
			1221	N ₂	IR	4
	10	C-N stretch	952m	gas	IR	3
<i>a''</i>			950ms	Ar	IR	2-4
			949	N ₂	IR	4
	12	CNC bend	484ms	gas	IR	3
			479ms	Ar	IR	2-4
			484	N ₂	IR	4
	13	CH ₃ a-stretch	2975s	gas	IR	3
			2962ms	Ar	IR	2-4
	14	CH ₃ a-deform.	1444s	gas	IR	3
			1441m	Ar	IR	2,3
	15	CH ₃ wag	1100vw	Ar	IR	2,3
	16	CH ₂ OPLA	1026vs	gas	IR	3
			1026vvs	Ar	IR	2-4
			1030	N ₂	IR	4
	17	C=N torsion	686w	gas	IR	3
	18	CH ₃ twist	220w ^a	Ar	IR	3

$A_0 = 1.752$; $B_0 = 0.356$; $C_0 = 0.313$ MW¹

^aTentative assignment.

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C₂H₅O

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

$T_0 = 29204$ gas EM^{1,2,4}LF^{3,5}

$\tilde{A}-\tilde{X}$ 310-500 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>		CO stretch	596	gas	LF	5

$\tau_0 = 1.7(2)$ μ s gas LF³EM⁴

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CH ₂ wag	1370	gas	LF	3
		C-O stretch	1067	gas	LF,EM	3-5
		C-C stretch	875 ^a	gas	LF	3
		CCO bend	442	gas	LF	3

^aAssignment to overtone of CCO bend cannot be excluded.

References

- ¹D. W. G. Style and J. C. Ward, *Trans. Faraday Soc.* **49**, 999 (1953).
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³G. Inoue, M. Okuda, and H. Akimoto, *J. Chem. Phys.* **75**, 2060 (1981).
⁴T. Ebata, H. Yanagishita, K. Obi, and I. Tanaka, *Chem. Phys.* **69**, 27 (1982).
⁵S. C. Foster, Y.-C. Hsu, C. P. Damo, X. Liu, C.-Y. Kung, and T. A. Miller, *J. Phys. Chem.* **90**, 6766 (1986).

C₂H₅S

$\tilde{A}$ C_s

$T_0 = 22720$ gas LF¹

$\tilde{A}-\tilde{X}$ 390-600 nm

Predissociation occurs.

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CS stretch	408(8)	gas	LF	1

$\tau = 75$ ns gas LF¹

$\tilde{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CS stretch	681(15)	gas	LF	1

References

- ¹G. Black and L. E. Jusinski, *Chem. Phys. Lett.* **136**, 241 (1987).

1,2-C₂H₄Li₂ $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CH stretch	3036w	Ar	IR	1
		CH stretch	2964vw	Ar	IR	1
			1240vw	Ar	IR	1
		CC stretch	1162w	Ar	IR	1
			695.5s	Ar	IR	1
			583m	Ar	IR	1
		LiC s-stretch	551w	Ar	IR	1
		LiC a-stretch	364w	Ar	IR	1
			360.5m	Ar	IR	1

1,2-C₂D₄Li₂ $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CD stretch	2288w	Ar	IR	1
		CD stretch	2154w	Ar	IR	1
			915w	Ar	IR	1
		LiC s-stretch	595s	Ar	IR	1
			487	Ar	IR	1
			477m	Ar	IR	1
			351w	Ar	IR	1
			279m	Ar	IR	1

References¹L. Manceron and L. Andrews, J. Phys. Chem. **90**, 4514 (1986).**CH₃CCHLi** $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CH stretch	2893	Ar	IR	1
		C=C stretch	1738	Ar	IR	1
		H deform.	722	Ar	IR	1
		OPLA deform.	458	Ar	IR	1

References¹L. Manceron and L. Andrews, J. Am. Chem. Soc. **107**, 563 (1985).**H₂C=(cyc-C₃H₂)** $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			1770vs	Ar	IR	1,2
			1519m	Ar	IR	1,2
			754s	Ar	IR	1,2
			664m	Ar	IR	1,2

References¹W. E. Billups, L.-J. Lin, and E. W. Casserly, J. Am. Chem. Soc. **106**, 3698 (1984).²G. Maier, M. Hoppe, K. Lanz, and H. P. Reisenauer, Tetrahedron Lett. **25**, 5645 (1984).**cyc-C₄H₄** $\bar{X}$ D_{2h}Structure: IR³⁻⁵

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
b _{1u}		CH stretch	3105wm	Ar	IR	5
		C=C stretch	1526w	Ar	IR	4,5
		CH deform.	1028vw	Ar	IR	5
b _{2u}		CH stretch	3073w	Ar	IR	5
		CH deform.	1242s	Ar	IR	1-5
		Ring deform.	719wm	Ar	IR	4,5
b _{3u}		CH OPLA	569vs	Ar	IR	1-5

cyc-C₄D₄ $\bar{X}$ 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

References¹O. L. Chapman, C. L. McIntosh, and J. Pacansky, J. Am. Chem. Soc. **95**, 614 (1973).²C. Y. Lin and A. Krantz, J. Chem. Soc., Chem. Commun. 1111 (1972).³G. Maier, H.-G. Hartan, and T. Sayrac, Angew. Chem. **88**, 252 (1976); Angew. Chem., Int. Ed. Engl. **15**, 226 (1976).⁴S. Masamune, F. A. Souto-Bachiller, T. Machiguchi, and J. E. Bertie, J. Am. Chem. Soc. **100**, 4889 (1978).⁵G. Maier, Angew. Chem. **100**, 317 (1988); Angew. Chem. Int. Ed. Engl. **27**, 309 (1988).**cyc-C₂H₄OFe** $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			1457.9	Ar	IR	1
			1259.5	Ar	IR	1
			1138.0	Ar	IR	1
			1134.9			
			836.0	Ar	IR	1
			756.0	Ar	IR	1

cyc-C₂D₄OFe $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			1076.1	Ar	IR	1
			1003.1	Ar	IR	1
			924.5	Ar	IR	1
			749.5	Ar	IR	1
			747.5			

References

¹Z. H. Kafafi, R. H. Hauge, W. E. Billups, and J. L. Margrave, *J. Am. Chem. Soc.* **109**, 4775 (1987).

CH₂=CHFeOH $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OH stretch	3749.7	Ar	IR	1
		CH stretch	2917.1	Ar	IR	1
		C=C stretch	1556.3	Ar	IR	1
		CH ₂ rock	1019.0	Ar	IR	1
		CH ₂ wag	944.2	Ar	IR	1
		Fe—O stretch	699.6	Ar	IR	1
		Fe—C stretch	541.7	Ar	IR	1

CD₂=CDFeOD $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OD stretch	2762.3	Ar	IR	1
		C=C stretch	1484.9	Ar	IR	1
		CD ₂ wag	737.6	Ar	IR	1
		Fe—O stretch	681.5	Ar	IR	1
		Fe—C stretch	527.9	Ar	IR	1

References

¹Z. H. Kafafi, R. H. Hauge, W. E. Billups, and J. L. Margrave, *J. Am. Chem. Soc.* **109**, 4775 (1987).

cyc-(H₂COC)=CH₂ $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		C=C stretch	1823.4s	Ar	IR	1
			1820.4	Kr	IR	1
		CO stretch + CH ₂ deform.	1109.2wm	Ar	IR	1
			1107.3	Kr	IR	1
			1107	Xe	IR	1

 $\bar{\chi}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		Ring breathing	881.1wm	Ar	IR	1
			879.4	Kr	IR	1
			880.6	Xe	IR	1
		=CH ₂ deform.	793.8wm	Ar	IR	1
			793.6	Kr	IR	1
			790.1	Xe	IR	1

cyc-(D₂COC)=CD₂ $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		C=C stretch	1765.2	Ar	IR	1
			1760.9	Xe	IR	1
		CO stretch + CD ₂ deform.	919.9	Ar	IR	1
		Ring breathing	748.0	Ar	IR	1
		=CD ₂ deform.	629.2 ^a	Ar	IR	1
			626.0	Xe	IR	1

^aTentative assignment.

References

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

HO₂CH₂OH $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OH stretch	3648	gas	IR	2
		OH stretch	3598	gas	IR	2
		CH stretch	~2900	gas	IR	1
		OOH bend	~1350	gas	IR	1
		CO stretch	1050	gas	IR	1
		OO stretch	~820	gas	IR	1

References

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

²H. Niki, P. D. Maker, C. M. Savage, and L. P. Breitenbach, *Chem. Phys. Lett.* **75**, 533 (1980).

CH₃ONCO $\bar{\chi}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		NCO a-stretch	2204vs	Ar	IR	1
			2152wm			
			1049m	Ar	IR	1
			828wm	Ar	IR	1

$\tilde{X}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			657wm	Ar	IR	1
			510wm	Ar	IR	1
			425wm	Ar	IR	1

References

¹J. H. Teles and G. Maier, Chem. Ber. **122**, 745 (1989).**CH₃COO₂**

A prominent gas-phase absorption with maximum near 207 nm has been attributed^{3,4} to CH₃COO₂.

A weaker, broad gas-phase absorption with maximum near 245 nm has been attributed²⁻⁴ to CH₃COO₂.

 $\tilde{A}$ $T_0 = 5562(3)$ gas AB¹ $\tilde{A}-\tilde{X}$ 1348-1798 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OO stretch	932(5)	gas	AB	1
			530	gas	AB	1

References

¹H. E. Hunziker and H. R. Wendt, J. Chem. Phys. **64**, 3488 (1976).²M. C. Addison, J. P. Burrows, R. A. Cox, and R. Patrick, Chem. Phys. Lett. **73**, 283 (1980).³N. Basco and S. S. Parmar, Int. J. Chem. Kinet. **17**, 891 (1985).⁴G. Moortgat, B. Veyret, and R. Lesclaux, J. Phys. Chem. **93**, 2362 (1989).**C₆H_{1/2}** $B^2\Pi_u$ D_{∞h} $T_0 = 27350(160)$ gas PE¹

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			650(80)	gas	PE	1

 $\tilde{A}^2\Pi_g$ D_{∞h} $T_0 = 16658$ gas EF^{2,3}LF³ $\tilde{A}-\tilde{X}$ 485-725 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ_g^+	1	CH stretch	3243(2) ^a	gas	LF	3
	2	C=C stretch	2053(2)	gas	LF	3
	3	C=C stretch	1880(2)	gas	LF	3
	4	C-C stretch	617(2)	gas	LF,EF	2,3
Π_g	10	Skel. bend	244 ^a	gas	LF	3

 $\tau_0 = 17(2)$ ns gas EF² $\tilde{X}^2\Pi_u$ D_{∞h}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ_g^+	2	C=C stretch	2182(2)	gas	EF	2,3
	3	C=C stretch	1903(2)	gas	EF	2,3
	4	C-C stretch	632(2)	gas	EF	2,3
Π_g	10	Skel. bend	228(2) ^a	gas	LF	3

^aTentative assignment.

References

¹F. Brogli, E. Heilbronner, V. Hornung, and E. Kloster-Jensen, Helv. Chim. Acta **56**, 2171 (1973).²M. Allan, E. Kloster-Jensen, and J. P. Maier, Chem. Phys. **17**, 11 (1976).³D. Klapstein, R. Kuhn, J. P. Maier, M. Ochsner, and W. Zambach, J. Phys. Chem. **88**, 5176 (1984).**HON=CHCNO** $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OH stretch	3621vs	Ar	IR	1
		CNO a-stretch	2301vs	Ar	IR	1
		CNO s-stretch	1453m	Ar	IR	1
			1346w	Ar	IR	1
			1258m	Ar	IR	1
			1241wm	Ar	IR	1
			989ms	Ar	IR	1
			940wm	Ar	IR	1
			914wm	Ar	IR	1
			425s	Ar	IR	1
			423m			

References

¹G. Maier and J. H. Teles, Angew. Chem. **99**, 152 (1987); Angew. Chem. Int. Ed. Engl. **26**, 155 (1987).**HON=CHNCO** $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OH stretch	3638	Ar	IR	1
		NCO a-stretch	2276	Ar	IR	1
			1646	Ar	IR	1
			976	Ar	IR	1

References

¹G. Maier and J. H. Teles, Angew. Chem. **99**, 152 (1987); Angew. Chem. Int. Ed. Engl. **26**, 155 (1987).

CF₂=PCF₃

$\bar{\chi}$	C _s	Structure: ED ²				
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	C=P stretch	1365.3vs	gas	IR	1,3
	2	CF ₂ a-stretch	1248.9s	gas	IR	1,3
	3	CF ₃ a-stretch	1149.1vs	gas	IR	1,3
	4	CF ₃ s-stretch	1095w	gas	IR	3
	5	CF ₂ s-stretch	746vw	gas	IR	1,3
	6	Mixed	737w	gas	IR	1,3
	7	Mixed	484vw	gas	IR	3
	8	CF ₃ a-deform.	470w	gas	IR	1,3
	9	CF ₂ scissors	432vw	gas	IR	3
a''	13	CF ₃ a-stretch	1134.5m	gas	IR	1,3
	14	CF ₂ wag	551vw	gas	IR	1,3
	15	CF ₃ a-deform.	475w	gas	IR	1,3

References

- ¹A. B. Burg, *Inorg. Chem.* **22**, 2573 (1983).
²B. Steger, H. Oberhammer, J. Grobe, and D. Le Van, *Inorg. Chem.* **25**, 3177 (1986).
³K. Ohno, E. Kurita, M. Kawamura, and H. Matsuura, *J. Am. Chem. Soc.* **109**, 5614 (1987).

CF₃ONO₂

$\bar{\chi}$	C _s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		NO ₂ a-stretch	1735.5	Ar	IR	1
			1345.2	Ar	IR	1
		NO ₂ s-stretch	1327.1	Ar	IR	1
		CF ₃ stretch	1260.8s	Ar	IR	1
		CF ₃ stretch	1249.5vs	Ar	IR	1
			1142.5vs	Ar	IR	1
		C—O stretch	924.1w	Ar	IR	1
		NO ₂ scissors	785.2	Ar	IR	1
		ONO ₂ OPLA	752.9	Ar	IR	1
			519.0	Ar	IR	1

References

- ¹K. C. Clemitshaw and J. R. Sodeau, *J. Phys. Chem.* **91**, 3650 (1987).

6.15. Hydrocarbons with More Than Eight Atoms**C₂H₇⁺**

$\bar{\chi}$	C _s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	HH stretch	3964.0	gas	PF	1
		CH stretch	2683	gas	PF	1
		CH stretch	2601	gas	PF	1
		CH stretch	2521	gas	PF	1

References

- ¹L. I. Yeh, J. M. Price, and Y. T. Lee, *J. Am. Chem. Soc.* **111**, 5597 (1989).

br-C₂H₇⁺

$\bar{\chi}$	C ₂					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a		CH stretch	3128	gas	PF	1
b		CH stretch	3082	gas	PF	1
		CH stretch	2945.4	gas	PF	1

References

- ¹L. I. Yeh, J. M. Price, and Y. T. Lee, *J. Am. Chem. Soc.* **111**, 5597 (1989).

1-C₃H₇⁺

$\bar{\chi}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		Skel. bend	700(30)	gas	PE	1,2

References

- ¹J. C. Schultz, F. A. Houle, and J. L. Beauchamp, *J. Am. Chem. Soc.* **106**, 3917 (1984).
²J. Dyke, A. Ellis, N. Jonathan, and A. Morris, *J. Chem. Soc., Faraday Trans. 2* **81**, 1573 (1985).

2-C₃H₇⁺

$\bar{\chi}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a ₁		Skel. bend	600(30)	gas	PE	1

References

- ¹J. Dyke, A. Ellis, N. Jonathan, and A. Morris, *J. Chem. Soc., Faraday Trans. 2* **81**, 1573 (1985).

(CH₃)₂CH**3d Rydberg state**

A gas-phase absorption maximum at 207 nm has been assigned³ to the 3d- $\bar{\chi}$ transition of (CH₃)₂CH.

3p Rydberg state

An unstructured gas-phase absorption between 225 and 260 nm, with maximum at 236 nm, has been assigned^{1,3} to the 3p- $\bar{\chi}$ transition of (CH₃)₂CH.

3s Rydberg state

In gas-phase absorption studies, a shoulder at 270 nm has been tentatively assigned³ to the 3s- $\tilde{X}$ transition of (CH₃)₂CH.

 $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CH stretch	3052	Ar	IR	2,4
		CH ₃ stretch	2920	Ar	IR	2
		CH ₃ stretch	2850	Ar	IR	2
		CH ₃ stretch	2830	Ar	IR	2
		CH ₃ deform.	1468	Ar	IR	2
		CH ₃ deform.	1440	Ar	IR	2
		CH ₃ deform.	1388	Ar	IR	2
		CH ₃ deform.	1378	Ar	IR	2
		CH ₃ rock	1165	Ar	IR	4
		CC stretch	879	Ar	IR	4
		HC(CH ₃) ₂ OPLA	364s	Ar	IR	2,4

References

- ¹D. A. Parkes and C. P. Quinn, J. Chem. Soc., Faraday Trans. 1 **72**, 1952 (1976).
²J. Pacansky and H. Coufal, J. Chem. Phys. **62**, 3298 (1980).
³H. R. Wendt and H. E. Hunziker, J. Chem. Phys. **81**, 717 (1984).
⁴G. Chettur and A. Snelson, J. Phys. Chem. **91**, 913 (1987).

t*-C₄H₉*3d Rydberg state**

In the gas phase, an absorption with maximum at 233 nm has been assigned^{1,2,5} to the 3d- $\tilde{X}$ transition of *t*-C₄H₉.

3p Rydberg state

In the gas phase, an absorption with maximum at 253 nm has been assigned^{2,5} to the 3p- $\tilde{X}$ transition of *t*-C₄H₉.

3s Rydberg state

In the gas phase, a broad absorption with maximum at 333 nm has been assigned⁵ to the 3s- $\tilde{X}$ transition of *t*-C₄H₉.

 $\tilde{X}$ C_{3v} Structure: IR^{3,6}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₁		CH stretch	2931	Ar	IR	3,6
		CH stretch	2833 ^b	gas	IR	4
			2825 ^{vs}	Ar	IR	3,6
		CH ₃ deform.	1455	Ar	IR	3,6
		CH ₃ deform.	1367	Ar	IR	3,6
		CH ₃ rock	992	Ar	IR	3,6
<i>e</i>		CC stretch	733	Ar	IR	3,6
		CH stretch	2931	Ar	IR	3,6
		CH stretch	2825 ^{vs}	Ar	IR	3,6
		CH ₃ deform.	1455	Ar	IR	3,6
		CH ₃ deform.	1371	Ar	IR	3,6
		CC stretch	1279	Ar	IR	3,6
		CH ₃ rock	811	Ar	IR	3,6
		C ₃ bend	541	Ar	IR	3,6

^aUnassigned absorptions, attributed to combination bands or impurities, were also observed at 1252, 1205, 1184, and 1129 cm⁻¹.

^bTime-resolved infrared spectral photography (TRISP); resolution 3 cm⁻¹.

References

- ¹D. A. Parkes and C. P. Quinn, Chem. Phys. Lett. **33**, 483 (1975).
²D. A. Parkes and C. P. Quinn, J. Chem. Soc., Faraday Trans. 1 **72**, 1952 (1976).
³J. Pacansky and J. S. Chang, J. Chem. Phys. **74**, 5539 (1981).
⁴D. S. Bethune, J. R. Lankard, P. P. Sorokin, A. J. Schell-Sorokin, R. M. Plecenik, and Ph. Avouris, J. Chem. Phys. **75**, 2231 (1981).
⁵H. R. Wendt and H. E. Hunziker, J. Chem. Phys. **81**, 717 (1984).
⁶B. Schrader, J. Pacansky, and U. Pfeiffer, J. Phys. Chem. **88**, 4069 (1984).

CH₃(C≡C)₂H⁺ $\tilde{A}^2E$ C_{3v}

*T*₀ = 20374.5(5) gas EF^{1,4}LF² $\tilde{A}$ - $\tilde{X}$ 450-630 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₁	3	C≡C stretch	2135(10)	gas	LF	2
	4	C≡C stretch	2000(10)	gas	LF	2
	5	CH ₃ deform.	1272(10)	gas	LF	2
	6	C-C a-stretch	1130	gas	EF,LF	1,2,4
	7	C-C s-stretch	664 ^a	gas	EF,LF	1,2,4
<i>e</i>	13	Skel. deform.	303 ^{ab}	gas	EF,LF	1,2,4
			306			

*T*₀ = 50(3) ns gas EF¹PEPICO³

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₁	3	C≡C stretch	2212	gas	EF	1,4
	4	C≡C stretch	1921	gas	EF	4
	6	C-C a-stretch	1203	gas	EF	1,4
	7	C-C s-stretch	685 ^a	gas	EF	1,4
			691			
<i>e</i>	13	Skel. deform.	313 ^{ab}	gas	EF	4
			324			

CD₃(C≡C)₂D⁺ $\tilde{A}^2E$ C_{3v}

*T*₀ = 20374.7(5) gas EF^{1,4} $\tilde{A}$ - $\tilde{X}$ 460-570 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₁	5	C-C a-stretch	1157	gas	EF	4
	6	CD ₃ deform.	1019 ^a	gas	EF	4
	7	C-C s-stretch	617 ^a	gas	EF	1,4
<i>e</i>	13	Skel. bend	284 ^{ab}	gas	EF	4

*T*₀ = 53(3) ns gas EF¹PEPICO³

$\bar{A}^2B_1$ C_{2v}

$T_0 = 18908$ gas AB^1 $\bar{A}-\bar{X}$ 440–530 nm
 18716 Ar AB^4 $\bar{A}-\bar{X}$ 530–535 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			896	gas	AB	1
			722	gas	AB	1
			571	gas	AB	1

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		C ₆ deform.	707s	Ar	IR	2–5

C₆D₅

A prominent absorption at 286 nm in argon-matrix studies of photolyzed benzene samples has been attributed⁴ to C₆D₅.

 $\bar{A}^2B_1$ C_{2v}

$T_0 = 18840$ Ar AB^4 $\bar{A}-\bar{X}$ 530–535 nm

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		C ₆ deform.	519s	Ar	IR	2,5

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C₆H₆⁺ **$\bar{G}^2A_{1g}$** D_{6h}

$T^a = 61290(100)$ gas PE^{1,5}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_{1g}	1 ^b (2)	CH stretch	2790(100)	gas	PE	1
	2 (1)	Ring stretch	930(100)	gas	PE	1

 $\bar{F}^2B_{1u}$ D_{6h}

$T^a = 50160(100)$ gas PE^{1,5}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_{1g}	1 ^b (2)	CH stretch	2340(100)	gas	PE	1

 $\bar{E}^2B_{2u}$ D_{6h}

$T^a = 45320(100)$ gas PE⁵

 $\bar{D}^2E_{1u}$ D_{6h}

$T^a = 38220(100)$ gas PE⁵

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

$T^a = 25310(100)$ gas PE⁵

In the gas phase, the mass-selected ion-dip spectrum of C₆H₆⁺ 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 $\bar{C}-\bar{X}$ transition of C₆H₆⁺ produced by vacuum-ultraviolet photolysis of benzene isolated in a neon matrix.²

$T_0 \sim 19840^c$ Ar LF³AB⁴ $\bar{C}-\bar{X}$ 420–547 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
e_{2g}	18 ^b (6)	Ring deform.	600(30) ^c	Ar	AB	4

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

$T_0 = 18113$ gas PF⁹

In an argon matrix, a weak, sharp absorption at 18100 has been attributed³ to a vibronically allowed transition in the excitation of C₆H₆⁺ to the $\bar{B}$ state.

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_{1g}	1 ^b (2)	CH stretch	2850(100)	gas	PE	1
	2 (1)	Ring stretch	990 ^d	gas	PF	9
e_{2g}	16 (8)	Ring stretch	1520(100) ^c	gas	PE	1
	17 (9)	CH bend	1140 ^d	gas	PF	9
	18 (6)	Ring deform.	645(100) ^c	gas	PE	1
e_{2u}	19 (17)	CH bend	574	gas	PF	9
	20 (16)	Ring deform.	224	gas	PF	9

$\tilde{X}^2E_{1g}$ D_{6h}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_{1g}	1 ^b (2)	CH stretch	2960(100) ^c	gas	PE	1
	2 (1)	Ring stretch	975(15)	gas	PE,MPI	1,6,8
b_{2g}	8 (4)	Ring deform.	415(20)	gas	PE	6
e_{1g}	11 (10)	CH bend	835(15)	gas	MPI	8
e_{2g}	16 (8)	Ring stretch	1561(20) ^c	gas	PE	1,6
			1480(10) ^c	Ar	LF	3
	17 (9)	CH bend	1230(15) ^c	gas	PE,MPI	1,6,8
	18 (6)	Ring deform.	660(15) ^c	gas	PE,MPI	1,6,8
			630(10) ^c	Ar	LF	3
			340(10) ^f	gas	PE	6
e_{2u}	20 (16)	Ring deform.	295(5)	gas	PE,MPI	6,8

 $B_0 \sim 0.2$ gas PE⁷ $C_6D_6^+$ $\tilde{G}^2A_{1g}$ D_{6h} $T^a \sim 62000$ gas PE¹

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_{1g}	1 ^b (2)	CD stretch	2240(100)	gas	PE	1
	2 (1)	Ring stretch	920(100)	gas	PE	1

 $\tilde{F}^2B_{1u}$ D_{6h} $T^a \sim 50000$ gas PE¹

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

 $\tilde{C}^2A_{2u}$ D_{6h} $T_0 \sim 19930^c$ Ar LF³AB⁴ $\tilde{C}-\tilde{X}$ 470–545 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
e_{2g}	18 ^b (6)	Ring deform.	590(60) ^c	Ar	AB	4

 $\tilde{B}^2E_{2g}$ D_{6h} $T^a \sim 18600$ gas PE¹

In an argon matrix, a weak, sharp absorption at 18215 has been attributed³ to a vibronically allowed transition in the excitation of $C_6D_6^+$ to the $\tilde{B}$ state.

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_{1g}	1 ^b (2)	CD stretch	2140(100)	gas	PE	1
e_{2g}	16 (8)	Ring stretch	1450(100)	gas	PE	1
	17 (9)	CD bend	870(100)	gas	PE	1
	18 (6)	Ring deform.	600(100)	gas	PE	1

 $\tilde{X}^2E_{1g}$ D_{6h}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_{1g}	1 ^b (2)	CD stretch	2330(100)	gas	PE	1
	2 (1)	Ring stretch	928(20)	gas	PE	1,6
b_{2g}	8 (4)	Ring deform.	351(20)	gas	PE	6
e_{2g}	16 (8)	Ring stretch	1565(100)	gas	PE	1
			1460(10) ^c	Ar	LF	3
	18 (6)	Ring deform.	637(20) ^c	gas	PE	1,6
			590(10) ^c	Ar	LF	3
			343(20) ^f	gas	PE	6
e_{2u}	20 (12)	Ring deform.	278(20)	gas	PE	6

^aFrom vertical ionization potentials. The first ionization potential of benzene is taken to equal 74555.0(4), or 9.2405 eV, from Ref. 7.

^bIn 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.

^cTentative assignment.

^dFrom analysis of combination bands.

^e $j = 1/2$.

^f $j = 3/2$.

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CH₃(C≡C)₂CH[‡]

$\tilde{A}^2E_u$ D_{3d}

$T_0 = 20556$ gas EF^{1,4,7}LF^{3,5}

$\tilde{A}-\tilde{X}$ 425–625 nm

20499 Ne LF²

$\tilde{A}-\tilde{X}$ 425–555 nm

~20190 Ar

LF²

The emission spectrum in an argon matrix is highly perturbed.

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_{1g}	2	C≡C stretch	2126(2)	gas	LF	3,5
			2137	Ne	LF	2
			2118(10)	Ar	LF	2
	4	C—C stretch	1219	gas	LF,EF	3,5,7
			1231	Ne	LF	2
			1220	Ar	LF	2
			524	gas	LF,EF	3–5,7
	5	C—C stretch	531	Ne	LF	2
			518	Ar	LF	2
			248 ^a	gas	EF	7
e_g	20	Skel. bend	248 ^a	gas	EF	7

$\tau_0 = 25(3)$ ns gas EF^{1,4}PEPICO⁶

$\tilde{X}^2E_g$ D_{3d}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_{1g}	2	C≡C stretch	2247	gas	EF	1,4,7
			2246	Ne	LF	2
			1323	gas	EF	1,7
	4	C—C stretch	1322	Ne	LF	2
			555	gas	EF,LF	1,3,4,7
			558	Ne	LF	2
e_u	14	Skel. deform.	327 ^a	gas	EF	7
e_g	20	Skel. deform.	237 ^a	gas	EF	7

CD₃(C≡C)₂CD[‡]

$\tilde{A}^2E_u$ D_{3d}

$T_0 = 20575$ gas EF^{4,7}LF⁵

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_{1g}		C≡C stretch	2137(10)	gas	LF	5
			1236	gas	LF,EF	5,7
			483	gas	EF,LF	4,5,7
e_g	20	Skel. bend	230 ^a	gas	EF	7

$\tau_0 = 32(3)$ ns gas EF⁴PEPICO⁶

$\tilde{X}^2E_g$ D_{3d}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹ mode	Med.	Type	Refs. meas.
a_{1g}	2	C≡C stretch	2248	gas	EF	4,7
	4	C—C stretch	1335	gas	EF	4,7
	5	C—C stretch	509	gas	EF,LF	4,5,7
e_g	20	Skel. deform.	217 ^a	gas	EF	7

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

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C₆H₅CH

In an argon matrix, absorption maxima have been observed² at 240 and 245 nm.

In an argon matrix, structured absorption has been observed^{1,2} between 372 and 430 nm.

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			3078ms	Ar	IR	1,2
			1505(5)m	Ar	IR	1
			1460(5)m	Ar	IR	1
			1430(5)m	Ar	IR	1
			1390(5)m	Ar	IR	1
			1210(5)wm	Ar	IR	1
			1020(5)m	Ar	IR	1
			945(5)wm	Ar	IR	1
			885(5)m	Ar	IR	1
			740vs	Ar	IR	1,2
			670vs	Ar	IR	1,2
			550(5)wm	Ar	IR	1
			445s	Ar	IR	1,2

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cyc-C₇H₆

(1,2,4,6-Cycloheptatetraene)

In an argon matrix, the onset of absorption occurs near 390 nm, with increasing absorption out to the limit of the measurements, near 220 nm.²

$\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			3040s	Ar	IR	1,2
			3010s	Ar	IR	1,2
			1824m	Ar	IR	1-3
			1816w	Ar	IR	1-3
			1500(5)wm	Ar	IR	1
			1425(5)wm	Ar	IR	1
			1380vs	Ar	IR	1-3
			1365(5)wm	Ar	IR	1
			1270m	Ar	IR	1,2
			1190(5)m	Ar	IR	1
			965(5)m	Ar	IR	1
			912m	Ar	IR	1,2
			771vs	Ar	IR	1-3
			690s	Ar	IR	1-3
			679vs	Ar	IR	1,2
			582ms	Ar	IR	1,2
			410(5)m	Ar	IR	1

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cyc-C₇H₆:

(Cycloheptatrienylidene)

In an argon matrix, absorption maxima have been observed¹ between 460 and 530 nm, between 282 and 307 nm, and at 220 nm.

 $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			638	Ar	IR	1

References

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C₆H₅CH₂^a $\tilde{E}$

A gas-phase absorption maximum near 230 nm has been attributed⁹ to the first Rydberg transition of C₆H₅CH₂.

 $\tilde{D}$

A gas-phase absorption between 260 and 245 nm, with maximum near 255 nm, has been attributed⁹ to the $\tilde{D}-\tilde{X}$ transition of C₆H₅CH₂. This band may have been excited in the MPI studies of Ref. 15. In a neon matrix, the counterpart of this absorption maximum has been observed near 245 nm.⁶

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

$T_0 = 32760$ gas AB^{2,5,7} $\tilde{C}-\tilde{X}$ 291-309 nm
 32730 Ne AB⁶

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
b_2	6a	Ring deform.	432	gas	AB	7
	6b	Ring deform.	525	gas	AB	7
	18b	CH deform.	276	gas	AB	7

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

$T_0 = 22460(30)$ gas AB¹¹EM¹¹
 Vibronically coupled to modes of b_2 symmetry in the $\tilde{A}$ state.¹¹

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

$T_0 = 22001.5$ gas EM^{1,3,5,10}AB⁴LF¹² $\tilde{A}-\tilde{X}$ 429-455 nm
 22003 Ne AB⁶ $\tilde{A}-\tilde{X}$ 429-455 nm
 21862 Ar LF¹³ $\tilde{A}-\tilde{X}$ 430-510 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
6a	Ring deform.		910	Ar	LF	13
			798	Ar	LF	13
			433	gas	AB	11,17
			433	Ne	AB	6
			456	Ar	LF	13
			388	gas	AB	11,16,17
			402	Ne	AB	6
			328	gas	AB	11,16,17
			344	Ne	AB	6

$\tau_{6a} = 880(10)$ ns gas LF¹⁴
 $A_0 \sim 0.180^b$; $B_0 = 0.089^b$; $C_0 = 0.059^b$ EM^{10,16,18}

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

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	8a	Ring stretch	1603	gas	EM	5,8,17
	19a	Ring stretch	1431	gas	EM	5,8,17
			1423	Ar	LF	13
	7a	C-CH ₂ stretch	1258	gas	EM	5,7,17
	9a	CH deform.	1181	gas	EM	5,8
	18a	CH deform.	1046	gas	EM	17
a_2	1	Ring breathing	987.4	gas	EM	5,8,10
						17
			982	Ar	LF	13
	12a	Ring deform.	818	gas	EM	5,8,17
	6a	Ring deform.	524	gas	EM	5,8,10
			520	Ar	LF	13
	17a	CH deform.	963	gas	EM	17
	10a	CH deform.	860	gas	EM	8,17
	16a	Ring deform.	393	gas	EM	8
	16b	Ring deform.	430	gas	EM	8
b_2	8b	Ring stretch	1549	gas	EM	5,8,17
			1530	Ar	LF	13
	9b	CH deform.	1152	gas	EM	5,8,17
	15	CH deform.	1089	gas	EM	5,8

$\bar{X}$ — Continued

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

 $A^o \sim 0.185^b$; $B_0 = 0.090^b$; $C_0 = 0.060^b$ EM^{10,16,18}**C₆D₅CD₂** $\bar{B}^2B_1$, C_{2v} $T_0 = 22455(10)$ gas AB¹¹EM¹¹ $\bar{A}$, C_{2v} $T_0 = 22093.7$ gas EM^{5,10}
21962 Ar LF¹³ $\bar{A}-\bar{X}$ 434–502 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			844	Ar	LF	13
			731	Ar	LF	13
	6a	Ring deform.	404	Ar	LF	13

 $\tau \sim 1340$ ns gas LF¹⁴ $\bar{X}^2B_1$, C_{2v}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	8a	Ring stretch	1593	gas	EM	5,8
	19a	Ring stretch	1327	gas	EM	5,8
			1323	Ar	LF	13
	7a	C—CD ₂ stretch	1204	gas	EM	5,8
	1	Ring breathing	945.7	gas	EM	5,8,10
			945	Ar	LF	13
	9a	CD deform.	895	gas	EM	5,8
	18a	CD deform.	848	gas	EM	8
	12a	Ring stretch	791	gas	EM	5,8
	6a	Ring deform.	497.5	gas	EM	5,8,10
a_2			495	Ar	LF	13
	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

^aIn 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.

^bFrom analysis of rotational band contours.

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C₆H₅CH₂⁻ $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			945	gas	MPD	1

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p*-CH₃C₆H₄CH:(p*-Tolylmethylene)Ar AB^{1,2} 395–444 nm

Irradiation in this spectral region results in isomerization to 5-methylcycloheptatetraene.

 $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			3073w	Ar	IR	1,2
			3053vw	Ar	IR	1,2
			3021vw	Ar	IR	1,2
			2987w	Ar	IR	1,2
			2957w	Ar	IR	1,2
			2925w	Ar	IR	1,2
			2891vw	Ar	IR	1,2
			2871w	Ar	IR	1,2
			2847vw	Ar	IR	1,2
			2736vw	Ar	IR	1,2
			1881vw	Ar	IR	1,2
			1573m	Ar	IR	1,2
			1522w	Ar	IR	1,2
			1518w	Ar	IR	1,2
			1512w	Ar	IR	1,2
			1467m	Ar	IR	1,2

$\bar{\chi}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			1454w	Ar	IR	1,2
			1449m	Ar	IR	1,2
			1380w	Ar	IR	1,2
			1116w	Ar	IR	1,2
			1089w	Ar	IR	1,2
			1035w	Ar	IR	1,2
			1029w	Ar	IR	1,2
			1018w	Ar	IR	1,2
			1000w	Ar	IR	1,2
			992w	Ar	IR	1,2
			983w	Ar	IR	1,2
			953w	Ar	IR	1,2
			948w	Ar	IR	1,2
			798s	Ar	IR	1,2
			779w	Ar	IR	1,2
			494w	Ar	IR	1,2
			446s	Ar	IR	1,2

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m*-CH₃C₆H₄CH:(m-Tolylmethylene)*Ar AB^{1,2} 394–448 nm

Irradiation in this spectral region results in isomerization to 4- and 5-methylcycloheptatetraene.

 $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			3072w	Ar	IR	1,2
			3047w	Ar	IR	1,2
			3029w	Ar	IR	1,2
			2991w	Ar	IR	1,2
			2985w	Ar	IR	1,2
			2962w	Ar	IR	1,2
			2933w	Ar	IR	1,2
			2876w	Ar	IR	1,2
			1570m	Ar	IR	1,2
			1567m	Ar	IR	1,2
			1520w	Ar	IR	1,2
			1462m	Ar	IR	1,2
			1379w	Ar	IR	1,2
			927w	Ar	IR	1,2
			922w	Ar	IR	1,2
			873w	Ar	IR	1,2
			852w	Ar	IR	1,2
			786m	Ar	IR	1,2
			764s	Ar	IR	1,2
			761s	Ar	IR	1,2
			747w	Ar	IR	1,2
			697m	Ar	IR	1,2
			687m	Ar	IR	1,2
			669s	Ar	IR	1,2

 $\bar{\chi}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			540w	Ar	IR	1,2
			471w	Ar	IR	1,2
			463m	Ar	IR	1,2
			457m	Ar	IR	1,2
			421m	Ar	IR	1,2

References

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o*-CH₃C₆H₄CH:(o-Tolylmethylene)*

Ar AB^{1,2} 244–249 nm
 Ar AB^{1,2} 292–305 nm
 Ar AB^{1,2} 413–450 nm

 $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			742	Ar	IR	1

References

- ¹R. J. McMahon and O. L. Chapman, J. Am. Chem. Soc. **109**, 683 (1987).
²O. L. Chapman, J. W. Johnson, R. J. McMahon, and P. R. West, J. Am. Chem. Soc. **110**, 501 (1988).

o*-(CH₂)₂C₆H₄(o-Xylylene)*Ar AB¹⁻³ 326–403 nm $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			3105w	Ar	IR	1
			3070w	Ar	IR	1
			3045w	Ar	IR,Ra	1
			2950w	Ar	IR	1
			1741w	Ar	IR	1
			1576w	Ar	IR,Ra	1–3
			1552m	Ar	IR,Ra	1–3
			1542w	Ar	IR	1
			1529m	Ar	Ra	1
			1493m	Ar	IR	1–3
			1471w	Ar	IR	1–3
			1465w	Ar	IR	1
			1427w	Ar	IR	1
			1333w	Ar	IR	1

CH₃SiH=CH₂

In an argon matrix, an absorption maximum at 260 nm has been assigned^{1,3,4} to CH₃SiH=CH₂.

$\bar{\chi}$	C _s					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>		CH stretch	3018w	Ar	IR	5
		CH stretch	2976w	Ar	IR	5
	5	SiH stretch	2187s	Ar ^a	IR	1-5
	6	CH ₃ a-deform.	1394w	Ar ^a	IR	3,5
	7	CH ₂ scissors	1297w	Ar ^a	IR	1,3-5
	8	CH ₃ s-deform.	1255s	Ar ^a	IR	1-5
	9	Si=C stretch	989s	Ar ^a	IR	1-5
	10	Deform.	880s	Ar ^a	IR	1-3,5
	11	CH ₃ rock	811s	Ar ^a	IR	1-5
	12	Si-C stretch	729w	Ar ^a	IR	3,5
	13	Deform.	678m	Ar ^a	IR	3,5
	<i>a''</i>	CH ₃ a-deform.	1412w	Ar ^a	IR	3,5
		CH ₂ OPLA wag	830w	Ar ^a	IR	3,5
		CH ₃ rock	711m	Ar ^a	IR	1-5
		CH ₂ torsion	614m	Ar ^a	IR	1,3-5

^aObserved by Ref. 3 in both Ar and N₂; frequencies in these two matrices were not distinguished.

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- ¹T. J. Drahnak, J. Michl, and R. West, *J. Am. Chem. Soc.* **103**, 1845 (1981).
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- ³C. A. Arrington, K. A. Klingensmith, R. West, and J. Michl, *J. Am. Chem. Soc.* **106**, 525 (1984).
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- ⁵G. Raabe, H. Vancik, R. West, and J. Michl, *J. Am. Chem. Soc.* **108**, 671 (1986).

(CH₃)₂Ge

In an argon matrix, an absorption maximum has been observed^{1,2} at 420 nm.

$\bar{\chi}$						
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CH stretch	2987w	Ar	IR	2
		CH stretch	2974s	Ar	IR	2
		CH stretch	2957s	Ar	IR	2
		CH stretch	2897w	Ar	IR	2
		CH ₃ deform.	1234m	Ar	IR	2
		CH ₃ deform.	1217w	Ar	IR	2
		CH ₃ deform.	1205m	Ar	IR	2
		CH ₃ deform.	1195w	Ar	IR	2
		CH ₃ rock	882m	Ar	IR	2
		CH ₃ rock	817m	Ar	IR	2
		GeC stretch	541w	Ar	IR	2
		GeC stretch	527vs	Ar	IR	2

References

- ¹S. Tomoda, M. Shimoda, Y. Takeuchi, Y. Kajii, K. Obi, I. Tanaka, and K. Honda, *J. Chem. Soc., Chem. Commun.* 910 (1988).
- ²J. Barrau, D. L. Bean, K. M. Welsh, R. West, and J. Michl, *Organometallics* **8**, 2606 (1989).

(CH₃)₂Sn

$\bar{\chi}$	C _{2v}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CH ₃ stretch	2990	Ar	IR	1
		CH ₃ stretch	2924	Ar	IR	1
		CH ₃ deform.	1187	Ar	IR	1
			1182sh			
		CH ₃ rock	774	Ar	IR	1
			745sh			
			739	Ar	IR	1
		SnC a-stretch	518	Ar	IR	1
		SnC s-stretch	504	Ar	IR	1

(CD₃)₂Sn

$\bar{\chi}$	C _{2v}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CD ₃ stretch	2240	Ar	IR	1
		CD ₃ stretch	2123	Ar	IR	1
		CD ₃ deform.	1032	Ar	IR	1
		CD ₃ deform.	932	Ar	IR	1
			927sh			
		CD ₃ rock	596	Ar	IR	1
			569sh			
			565	Ar	IR	1
		SnC a-stretch	476	Ar	IR	1
		SnC s-stretch	462	Ar	IR	1

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(CH₃)₂Si=CH₂^a

$\bar{\chi}$		Structure:	ED ³			
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₁			1251	Ar	IR	1,4,5
			1260w			
			1004m	Ar	IR	1,2,4,5
		HCSi deform.	818w	Ar	IR	1,4,5
<i>b</i> ₁		Si-C stretch	643m	Ar	IR	1,2,4,5
		HCSi deform.	825m	Ar	IR	1,2,4,5

(CD₃)₂Si=CD₂ $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		Si=C stretch	1112	Ar	IR	6
			1028	Ar	IR	6
		CD ₃ deform.	1005	Ar	IR	6
			1002			
			866	Ar	IR	6
			732	Ar	IR	6
			651	Ar	IR	6
			502	Ar	IR	6

^aPeaks at 696, 932, and 992 cm⁻¹ have also been attributed to (CH₃)₂Si=CH₂ in an argon matrix in Ref. 5. However, Ref. 4, in which the product yield was higher and very dilute samples were used, presents evidence for the assignment of the peaks at 696 and 932 cm⁻¹ to the dimer and of the 992-cm⁻¹ peak to propylene.

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C₅SiH₆⁺**(Silabenzene Cation)** $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		Ring deform.	800(50)	gas	PE	1

References

- ¹H. Bock, P. Rosmus, B. Solouki, and G. Maier, J. Organomet. Chem. **271**, 145 (1984).

C₅SiH₆**(Silabenzene)** $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		SiH stretch	2244sh	Ar	IR	2
			2217s	Ar	IR	1,2
			1526m	Ar	IR	1,2
			1502s	Ar	IR	1,2
			1409wm	Ar	IR	2

 $\bar{X}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			1354vs	Ar	IR	1,2
			1259vs	Ar	IR	1,2
			1069wm	Ar	IR	2
			886m	Ar	IR	1,2
			720wm	Ar	IR	2
			716			
			700vs	Ar	IR	2
			698			
			568vs	Ar	IR	1,2
			565			
			419s	Ar	IR	1,2

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C₅SiH₆ (Dewar) $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		SiH stretch	2142vs	Ar	IR	1,2
			1890ms	Ar	IR	1,2
			1263ms	Ar	IR	1,2
			1084m	Ar	IR	1,2
			818vs	Ar	IR	1,2
			761vs	Ar	IR	1,2
			728ms	Ar	IR	1,2
			689s	Ar	IR	1,2
			591s	Ar	IR	1,2
			559s	Ar	IR	1,2

References

- ¹G. Maier, G. Mihm, and H. P. Reisenauer, Angew. Chem. **92**, 58 (1980); Angew. Chem. Int. Ed. Engl. **19**, 52 (1980).
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LiC₆H₆ $\bar{X}$ C_{6v}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CH stretch	3055w	Ar	IR	1
			1458w,br	Ar	IR	1
		C ₆ a-stretch	1325m	Ar	IR	1
			990vw	Ar	IR	1
		C ₆ s-stretch	924s	Ar	IR	1
			701w,sh	Ar	IR	1
		CH deform.	607s	Ar	IR	1
		Ax. LiC stretch	451s	Ar	IR	1

LiC₆D₆

$\tilde{\nu}$	C_{6v}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CD stretch	2234vw	Ar	IR	1
			1425w,br	Ar	IR	1
			1217w	Ar	IR	1
		C ₆ a-stretch	1134w	Ar	IR	1
			883s	Ar	IR	1
			757m	Ar	IR	1
		Ax. LiC stretch	478s	Ar	IR	1
		CD deform.	401vw	Ar	IR	1
			281w	Ar	IR	1

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CH₃(C≡C)₂Cl⁺

$\tilde{\nu}$	C_{3v}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
						$T_0 = 19820$ gas EF ^{2,3} LF ³ $\tilde{A}-\tilde{X}$ 445-650 nm
a_1	2	C≡C s-stretch	2123(2)	gas	LF	3
	4	CH ₃ s-deform.	1296(2)	gas	LF	3
	5	C—C a-stretch	1207(2)	gas	LF	3
	6	C—C s-stretch	888(2)	gas	LF	3
	7	CCl stretch	424(2)	gas	EF,LF	2,3
e	12	Skel. s-bend	319 ^b	gas	LF	3
	13	CCCl bend	235(2)	gas	LF	3
	14	Skel. bend	87 ^b	gas	LF	3

$\tau_0 = 22(2)$ ns gas EF²

$\tilde{\nu}$	C_{3v}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	2	C≡C s-stretch	2232(2)	gas	EF	2,3
	4	CH ₃ deform.	1334(2)	gas	EF	3
	5	C—C a-stretch	1320(2)	gas	EF	2,3
	7	C—Cl stretch	503(2)	gas	EF	3
e	13	C≡CCl bend	228(2)	gas	EF	3
	14	Skel. bend	92(2) ^b	gas	EF	2

^aFrom vertical ionization potential.

^bTentative assignment.

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CH₃(C≡C)₂Br⁺

$\tilde{\nu}$	C_{3v}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
						$T_0 = 18553$ gas EF ^{2,3} LF ³ $\tilde{A}-\tilde{X}$ 480-710 nm
a_1	2	C≡C s-stretch	2141 ^b	gas	LF	3
	5	C—C a-stretch	1151(2)	gas	LF,EF	3
	6	C—C s-stretch	780(2)	gas	LF	3
	7	CBr stretch	350(2)	gas	EF,LF	2,3
e	12	Skel. s-bend	306 ^b	gas	LF	3
	13	CCBr bend	203(2)	gas	LF	3
	14	Skel. bend	76(2)	gas	LF	3

$A = -720(80)$ gas PE¹EF³

$\tau_0 = 10(2)$ ns gas EF²

$\tilde{\nu}$	C_{3v}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a_1	2	C≡C s-stretch	2216(2)	gas	EF	2,3
	3	C≡C a-stretch	1989(2)	gas	EF	2,3
	5	C—C a-stretch	1276(2)	gas	EF	2,3
	6	C—C s-stretch	795(2)	gas	EF	3
	7	C—Br stretch	368(2)	gas	EF	2,3
e	13	C≡CBr bend	226(2)	gas	EF	3
	14	Skel. bend	101(2) ^b	gas	EF	3

$A = -400(80)$ gas PE¹EF³

^aFrom vertical ionization potential.

^bTentative assignment.

References

- ¹E. Heilbronner, V. Hornung, J. P. Maier, and E. Kloster-Jensen, J. Am. Chem. Soc. **96**, 4252 (1974).
²J. P. Maier, O. Marthaler, and E. Kloster-Jensen, J. Electron Spectrosc. Relat. Phenom. **18**, 251 (1980).
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1,3,5-C₆H₃F₃⁺

$\tilde{\nu}$	D_{3h}					
Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
						$T_0 = 21867.479$ gas EF ^{1,12} EM ⁵ LF ^{3,9,15,16} $\tilde{B}-\tilde{X}$ 457-571 nm
			21776	Ne	LF ⁷	$\tilde{B}-\tilde{X}$ 364-460 nm
a'_1	3		995	gas	EM,LF	5,9
			1005	Ne	LF	7
	4		569	gas	LF,EM	3,5,9
			571	Ne	LF	7
e'	9		1499	gas	LF	3,9
			1505	Ne	LF	7
	2		954	gas	LF	9
			959	Ne	LF	7

B — Continued

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
	13		489.99	gas	LF	3,8,9
			484	Ne	LF	16
	14		323.81	gas	LF	7,14
			327	Ne	LF	8,9,16
	17		198 ^a	gas	LF	7
			209 ^a	Ne	LF	9

$\tau_0 = 59(3)$ ns gas EF²PIFCO¹⁰PEFCO¹¹
 53(2) ns Ne LF¹³

$B_0 = 1.748(4)$; $C_0 = 0.874(2)$ LF¹⁶

X²E'' D_{3h}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₁ '	1		2911	gas	EM	5
	2		1465	gas	EM	5
	3		1039.1	gas	EM,EF	5,12
			1043	Ne	LF	15
	4		592.1	gas	EM,LF	7
			596	Ne	LF	5,7
<i>e</i> '	9		1665	gas	EM	12,15
			1664	Ne	LF	7
	10		1533	gas	EM	7
	12		945	Ne	LF	5
	13		550.0	gas	EM,LF	7
			557	Ne	LF	12,15
	14		334	Ne	LF	7,14

$B_0 = 1.769(3)$; $C_0 = 0.885(2)$ LF¹⁶

1,3,5-C₆D₃F₃⁺**B²A₂'** D_{3h}

$T_0 = 21923.8$ gas EM⁶LF^{4,15} $\tilde{B}-\tilde{X}$ 437–544 nm
 21831 Ne LF⁷ $\tilde{B}-\tilde{X}$ 400–458 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₁ '	3		923	gas	EM	6
			932	Ne	LF	7
	4		560	gas	LF,EM	4,6
			569	Ne	LF	7
<i>e</i> '	9		1470	gas	LF	4
			1475	Ne	LF	7
	12		777	Ne	LF	7
	13		458	gas	LF,EM	4,6
			469	Ne	LF	7,14
	14		320	Ne	LF	7
	17		198 ^a	Ne	LF	7

X²E'' D_{3h}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₁ '	1		2247	gas	EM	6
	3		976.1	gas	EM,EF	6,15
	4		586.5	gas	EM,EF	6,15
			592	Ne	LF	7
<i>e</i> '	9		1625	gas	EM	6
			1612	Ne	LF	7
	10		1484	gas	EM	6
	11		1053.0	gas	EF	15
	12		780	Ne	EM	7
	13		532.3	gas	EM,EF	6,15
			541	Ne	LF	7,14
	14		334	Ne	LF	7,14

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

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CF₃(C≡C)₂F⁺**A²E** C_{3v}

$T_0 = 20400(10)$ gas EF² $\tilde{A}-\tilde{X}$ 480–635 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a</i> ₁	4	CF stretch	1160(40)	gas	PE	1,2
	6	C–C stretch	760(40)	gas	PE	1,2
	7	CF ₃ deform.	340(10)	gas	EF	2

$\tau_0 = 30(3)$ ns gas EF²

$\tilde{X}^2E$		C_{3v}	Structure: PE^1			
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CC stretch	2280(10)	gas	EF	2
	3	C—C a-stretch	1440(10)	gas	EF	2
	4	CF stretch	1140(10)	gas	EF	2
	5	CF stretch	880(10)	gas	EF	2
	6	C—C stretch	710(10)	gas	EF	2
	7	CF ₃ deform.	340(10)	gas	EF	2

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CF₃(C≡C)₂CF₃⁺ **$\tilde{B}$** $T_0 = 33160(240)$ gas PE^1

$\tilde{A}^2E_u$		D_{3d}				
$T_0 = 19534(3)$ gas $EF^{2,3}LF^3$			$\tilde{A}-\tilde{X}$ 448–595 nm			
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1	C≡C stretch	2085(5)	gas	LF	3
	3	C—C stretch	1033(5)	gas	LF	3
	4	C—C stretch	743(5)	gas	LF	3
	5	CF ₃ deform.	232(2)	gas	EF	2,3

 $\tau_0 = 46(2)$ ns gas EF^2PEPCO^3

$\tilde{X}^2E_g$		D_{3d}				
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1	CC stretch	2239(2)	gas	EF	2,3
	2	C—F stretch	1262(2)	gas	EF	2,3
	3	C—C stretch	1095(2)	gas	EF	2,3
	4	C—C stretch	752(2)	gas	EF	3
	5	CF ₃ deform.	235(2)	gas	EF	3

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C₆F₆⁺ $\tilde{C}^2B_{2u}$ D_{6h} $T_0 \sim 32300$ gas PE^{10} $\tau_0 < 15$ ns gas $PEPCO^{10}$

$\tilde{B}^2A_u$		D_{6h}				
$T_0 = 21616.16$ gas $EF^{1,11}EM^4LF^{5,9,14,16}$					$\tilde{B}-\tilde{X}$ 426–510 nm	
21553.7		Ne	$LF^{7,8,15}$		$\tilde{B}-\tilde{X}$ 405–523 nm	
21372		Ar	$LF^{3,6}$		$\tilde{B}-\tilde{X}$ 418–468 nm	
21027		Kr	LF^8			

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1		1520.0	Ne	LF	8,15
			1561	Ar	LF	3,6
	2		535.5	gas	EM,LF	4,9,14
a_{2g}			538.3	Ne	LF	8,15
			547	Ar	LF	3,6
	3		603.6	gas	LF	14
			629.1	Ne	LF	15
	4		203.7	gas	LF	14
b_{1u}	6		611.0	gas	LF	14
	7		706.2	gas	LF	14
b_{2g}	8		166.8	gas	LF	14
	10		274.0	gas	LF	14
e_{1g}	11		299.0	gas	LF	14
	14		308.4	gas	LF	14
e_{2g}	15		1554.0	gas	LF	9
			1552	Ne	LF	8
			1603	Ar	LF	6
	16		1187.0	gas	LF	9,15
			1185.7	Ne	LF	8,15
			1196	Ar	LF	6
	17		421.86	gas	EM,LF	4,5,9,14
			424.4	Ne	LF	8,15
			428	Ar	LF	3,6
	18		262.02	gas	EM,LF	4,5,9,14
			264.4	Ne	LF	8,15
			270	Ar	LF	3,6
e_{2u}	19		573.8	gas	LF	14
	20		114.1	gas	LF	14

$\tau_0 = 48(2)$ ns gas $EF^2PEFCO^{10,13}$
 42(2) ns Ne LF^{12}

 $B_0 = 1.01; C_0 = 0.50$ LF^{16}

$\tilde{X}^2E_{1g}$		D_{6h}				
Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	2		556	gas	UV,LF	4,9
					EF	11
			554	Ne	LF	8
e_{2g}			557	Ar	LF	3,6
	15		1698	Ne	LF	8
	16		1226	Ne	LF	8
	17		406	gas	UV,EF	9,11
			417	Ne	LF	8
			444	Ar	LF	3,6
	18		284	gas	UV,LF	4,9
					EF	11
			289	Ne	LF	8
			300	Ar	LF	3,6

 $B_0 = 1.02; C_0 = 0.51$ LF^{16}

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C₆H₅CF $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			1595s	Ar	IR	1
			1450m	Ar	IR	1
			1311m	Ar	IR	1
			1222s	Ar	IR	1
			1164s	Ar	IR	1
			1107s	Ar	IR	1
			1082s	Ar	IR	1
			1061s	Ar	IR	1
			1020m	Ar	IR	1
			834m	Ar	IR	1
			758s	Ar	IR	1
			690m	Ar	IR	1
			678m	Ar	IR	1
			623m	Ar	IR	1

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cyc-1-C₇H₅F $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			3060w	Ar	IR	1
			3025w	Ar	IR	1
			1810m	Ar	IR	1
			1528w	Ar	IR	1
			1502m	Ar	IR	1
			1460w	Ar	IR	1
			1443m	Ar	IR	1
			1403s	Ar	IR	1

 $\bar{\chi}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			1388m	Ar	IR	1
			1248m	Ar	IR	1
			1228m	Ar	IR	1
			1188s	Ar	IR	1
			1182s	Ar	IR	1
			937m	Ar	IR	1
			839w	Ar	IR	1
			823m	Ar	IR	1
			789m	Ar	IR	1
			759m	Ar	IR	1
			732s	Ar	IR	1
			661w	Ar	IR	1
			598w	Ar	IR	1
			532w	Ar	IR	1
			474w	Ar	IR	1

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C₆H₅CCl

In an argon matrix, C₆H₅CCl has a prominent absorption maximum at 300 nm^{2,3} and a weaker absorption maximum at 276 nm.³

 $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			1600m	Ar	IR	2-4
			1582s	Ar	IR	2-4
			1477w	Ar	IR	1-4
			1440m	Ar	IR	1-4
			1318w	Ar	IR	1-4
			1301m	Ar	IR	1-4
			1244m	Ar	IR	1-4
			1222vs	Ar	IR	1-4
			1205w	Ar	IR	2
			1168s	Ar	IR	1-4
			995w	Ar	IR	2,4
			840vs	Ar	IR	1-4
			761m	Ar	IR	1-4
			744vs	Ar	IR	1-4
			671s	Ar	IR	1-4
			563w	Ar	IR	1-4

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(2-ClC₆H₄)CH

In an argon matrix, this species contributes prominent absorptions with maxima at 239.5 and 245.5 nm, a less intense absorption at 308 nm, and a relatively weak absorption at 456 nm.

 $\tilde{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			1058s	Ar	IR	1
			739s	Ar	IR	1
			680m	Ar	IR	1

The positions of weaker absorptions are not given in Ref. 1.

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¹W. Sander, *Spectrochim. Acta* **43A**, 637 (1987).

cyc-1-C₇H₅Cl $\tilde{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			1809m	Ar	IR	1,2
			1425w	Ar	IR	1
			1387m	Ar	IR	2
			1360w	Ar	IR	1
			1222w	Ar	IR	1
			1061s	Ar	IR	1,2
			920m	Ar	IR	1
			881w	Ar	IR	1
			798s	Ar	IR	1,2
			726s	Ar	IR	1,2
			714s	Ar	IR	1,2
			590w	Ar	IR	1
			553w	Ar	IR	1
			497w	Ar	IR	1

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¹R. J. McMahon, C. J. Abelt, O. L. Chapman, J. W. Johnson, C. L. Kreil, J.-P. LeRoux, A. M. Mooring, and P. R. West, *J. Am. Chem. Soc.* **109**, 2456 (1987).

²W. Sander, *Spectrochim. Acta* **43A**, 637 (1987).

H₂C=CH—CH=NH^a $\tilde{\chi}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	4	CH ₂ s-stretch	2955	gas	IR	2
	5	CH stretch	~2885	gas	IR	2
	6	C=N stretch	1651	gas	IR	2
	7	C=C stretch	1600	gas	IR	2
	8	CH ₂ scissors	~1416	gas	IR	2
	9	CH bend	1368	gas	IR	2
	10	CH bend	1260	gas	IR	2
	11	CNH bend	1251	gas	IR	2
	12	CH ₂ rock	1089	gas	IR	2
	13	C—C stretch	~855	gas	IR	2

 $\tilde{\chi}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a''	16	C=N torsion	1096	gas	IR	2
	17	CH OPLA	991	gas	IR	2
	18	CH ₂ OPLA	979	gas	IR	2
	19	CH OPLA	839	gas	IR	2
	20	C=C torsion	568	gas	IR	2

$A_0 = 1.527$; $B_0 = 0.152$; $C_0 = 0.138$ MW¹

^aTwo or more rotational isomers contribute to the observed microwave and infrared spectra.

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H₂C=C=NCH₃ $\tilde{\chi}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	1	CH ₂ s-stretch	2984	gas	IR	1
	2	CH ₃ stretch	~2941	gas	IR	1
	3	CH ₃ s-stretch	2889	gas	IR	1
	4	CCN a-stretch	2060vs	gas	IR	1
	5	CH ₃ deform.	1470	gas	IR	1
	6	CH ₂ scissors	1410	gas	IR	1
	7	CH ₃ s-deform.	1363	gas	IR	1
	8	CCN s-stretch	1233	gas	IR	1
	10	N—C stretch	875	gas	IR	1
	11	CH ₂ wag	693s	gas	IR	1
	12	C=C=N bend	595	gas	IR	1
	13	C=N-C bend	207	gas	IR	1
a''	14	CH ₂ a-stretch	3050	gas	IR	1
	16	CH ₃ deform.	1464	gas	IR	1
	18	CH ₂ rock	1015	gas	IR	1

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¹Y. Amatatsu, Y. Hamada, and M. Tsuboi, *J. Mol. Spectrosc.* **123**, 476 (1987).

H₂C=CHN=CH₂ $\tilde{\chi}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	2	CH ₂ a-stretch	3035	gas	IR	1
	4	CH stretch	2871	gas	IR	1
	5	CH ₂ s-stretch	2832	gas	IR	1
	6	C=N stretch	1635	gas	IR	1
	7	C=C stretch	1618	gas	IR	1
	8	CH ₂ scissors	~1452w	gas	IR	1
	9	CH ₂ scissors	1382	gas	IR	1
	10	CH bend	1298	gas	IR	1
	11	CH ₂ rock	1233	gas	IR	1
	14	CNC bend	~523w	gas	IR	1

$\bar{X}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a''</i>	16	CH ₂ OPLA	1015	gas	IR	1
	17	CH OPLA	965	gas	IR	1
	18	CH ₂ OPLA	913	gas	IR	1
	20	C=C torsion	585	gas	IR	1

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cyc-C₃H₅N

(1-Azetine)

 $\bar{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	1	CH stretch	~3015	gas	IR	2
	3	CH ₂ s-stretch	2870	gas	IR	2
	4	C=N stretch	1575s	gas	IR	1,2
	5	CH ₂ scissors	1460	gas	IR	2
	6	CH ₂ scissors	~1430	gas	IR	1,2
	7	CH ₂ wag	1279s	gas	IR	1,2
	8	CH bend	1220	gas	IR	2
	9	CH ₂ wag	1208	gas	IR	1,2
	10	C-N stretch	1020	gas	IR	1,2
	11	Ring deform.	895	gas	IR	2
	12	C-C stretch	888s	gas	IR	1,2
	13	C-C stretch	866	gas	IR	1,2
<i>a''</i>	16	CH ₂ twist	1142	gas	IR	2
	17	CH ₂ twist	1102s	gas	IR	1,2
	18	CH ₂ rock	~1038	gas	IR	2
	19	CH OPLA	873	gas	IR	2
	20	CH ₂ rock	711s	gas	IR	1,2

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²Y. Amatatsu, Y. Hamada, and M. Tsuboi, *J. Mol. Spectrosc.* **123**, 267 (1987).

CH₃CH=CHNH₂ $\bar{X}$ C_s (approximate)

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	1	NH ₂ a-stretch	3500	gas	IR	1
	2	NH ₂ s-stretch	3415	gas	IR	1
	3	1-CH stretch	3070	gas	IR	1
	5	CH ₃ stretch	2970	gas	IR	1
	6	CH ₃ s-stretch	2877	gas	IR	1
	7	C=C stretch	1666s	gas	IR	1
	8	NH ₂ scissors	~1615m	gas	IR	1
	10	CH ₃ s-deform.	1375	gas	IR	1
	11	2-CH bend	1280	gas	IR	1
	12	1-CH bend	1270	gas	IR	1
	13	CH ₃ rock	1078	gas	IR	1

 $\bar{X}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a''</i>	14	CN stretch	1067	gas	IR	1
	15	C-C stretch	920	gas	IR	1
	16	C ₃ bend	480	gas	IR	1
	18	CH ₃ stretch	2935	gas	IR	1
	19	CH ₃ deform.	1457	gas	IR	1
	20	NH ₂ twist	1210	gas	IR	1
	21	CH ₃ rock	~1108	gas	IR	1
	22	1-CH OPLA	~993	gas	IR	1
	24	NH ₂ wag	675m	gas	IR	1

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¹Y. Hamada, Y. Amatatsu, and M. Tsuboi, *J. Mol. Spectrosc.* **110**, 369 (1985).

C₂H₃NHCH₃ $\bar{X}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
<i>a'</i>	1	NH stretch	3485	gas	IR	1
	2	CH ₂ a-stretch	3120	gas	IR	1
	3	CH ₂ s-stretch	3037	gas	IR	1
	4	CH stretch	2990	gas	IR	1
	5	CH ₃ stretch	~2928	gas	IR	1
	6	CH ₃ s-stretch	~2868	gas	IR	1
	7	C=C stretch	1655s	gas	IR	1
	8	CH ₃ deform.	1495	gas	IR	1
	9	NH bend	1465	gas	IR	1
	10	CH ₂ scissors	~1430	gas	IR	1
	11	CH ₃ s-deform.	1405	gas	IR	1
	12	CCH bend	1315	gas	IR	1
	13	CNC a-stretch	1230	gas	IR	1
<i>a''</i>	14	CH ₃ rock	1150	gas	IR	1
	15	CH ₂ rock	1029	gas	IR	1
	16	CNC s-stretch	920	gas	IR	1
	17	CNC bend	527	gas	IR	1
	19	CH ₃ stretch	~2822	gas	IR	1
	20	CH ₃ deform.	~1445	gas	IR	1
	21	CH ₃ rock	~1063	gas	IR	1
	22	CH OPLA	966	gas	IR	1
	23	CH ₂ OPLA	795s	gas	IR	1
	24	C=C torsion	788s	gas	IR	1
	25	NH wag	408	gas	IR	1

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¹Y. Amatatsu, Y. Hamada, M. Tsuboi, and M. Sugie, *J. Mol. Spectrosc.* **111**, 29 (1985).

(CH₃)₂C=C=NH**(3,3-Dimethylketenimine)** **$\tilde{X}$**

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CCN a-stretch	2032vs	Ar	IR	1
			2026s	Xe	IR	1
			2018s			
			2008wm	Ar	IR	1
			1424wm	Ar	IR	1
			1350m	Ar	IR	1
			1352m	Xe	IR	1
			1315s	Xe	IR	1
			1309s			
		NH deform.	1075m	Ar	IR	1
			1050m	Ar	IR	1
			1050vs	Xe	IR	1
			1016ms	Xe	IR	1
			744w	Ar	IR	1
		Torsion	735m	Ar	IR	1
			734s	Xe	IR	1

References¹S. T. Collins and G. C. Pimentel, J. Phys. Chem. **88**, 4258 (1984).**CH₃C≡C—NH(CH₃)****(N-Methyl-1-amino-1-propyne)** **$\tilde{X}$**

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		C≡C stretch	2037wm	Xe	IR	1
			1429w	Xe	IR	1
		NH deform.	1329m	Xe	IR	1
			1114wm	Xe	IR	1
			1062wm	Xe	IR	1
			966vw	Xe	IR	1
		C—N stretch	860vs	Xe	IR	1
			851m	Xe	IR	1
		NH deform. + CH ₃ rock	750w	Xe	IR	1
		NH deform. + CH ₃ rock	707m	Xe	IR	1

References¹S. T. Collins and G. C. Pimentel, J. Phys. Chem. **88**, 4258 (1984).**cyc-C₅H₃N****3,4-Pyridyne** **$\tilde{X}$**

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			2085	N ₂	IR	1
			1558	N ₂	IR	1
			1387	N ₂	IR	1

 $\tilde{X}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			1355	N ₂	IR	1
			1216	N ₂	IR	1
			1055	N ₂	IR	1
			996	N ₂	IR	1
			853	N ₂	IR	1
			848	N ₂	IR	1
			802	N ₂	IR	1
			489	N ₂	IR	1

References¹H.-H. Nam and G. E. Leroi, J. Am. Chem. Soc. **110**, 4096 (1988).**CH₃(C≡C)₂CN⁺** **$\tilde{C}^2E$** C_{3v}T₀ = 28720(160) gas PE¹ **$\tilde{B}^2A_1$** C_{3v}T₀ = 23960(160) gas PE¹ **$\tilde{A}^2E$** C_{3v}T₀ = 17694(2) gas EF^{1,2}LF² $\tilde{A}-\tilde{X}$ 449–646 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a ₁	2	C≡C stretch	2253(4)	gas	LF	2
	3	C≡C,C≡N str.	2080(4)	gas	LF	2
	4	C≡C,C≡N str.	1895(4)	gas	LF	2
	5	CH ₃ deform.	1205(40) ^a	gas	LF	2
	8	C—C stretch	486(2)	gas	EF	2

τ₀ = 8(2) ns gas EF¹ **$\tilde{X}^2E$** C_{3v}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a ₁	2	C≡C stretch	2207(2)	gas	EF	1,2
	3	C≡C,C≡N str.	2093(2)	gas	EF	1,2
	4	C≡C,C≡N str.	1980(2)	gas	EF	1,2
	5	CH ₃ deform.	1340(2) ^a	gas	EF	1,2
	8	C—C stretch	513(2)	gas	EF	1,2

^aAlternatively, may be assigned to ν₆, a C—C stretching mode.**References**¹G. Bieri, E. Kloster-Jensen, S. Kvisle, J. P. Maier, and O. Marthaler, J. Chem. Soc., Faraday Trans. 2 **76**, 676 (1980).²D. Klapstein, J. P. Maier, L. Misev, F. Thommen, and W. Zambach, J. Electron Spectrosc. Relat. Phenom. **31**, 283 (1983).

(C₆F₅)N $\tilde{X}$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			1575m	N ₂	IR	1
			1565m	N ₂	IR	1
			1502vs	N ₂	IR	1
			1462vs	N ₂	IR	1
			1454vs	N ₂	IR	1
			1359s	N ₂	IR	1
			1284m	N ₂	IR	1
			1204w	N ₂	IR	1
			1149w	N ₂	IR	1
			1029vs	N ₂	IR	1
			1007s	N ₂	IR	1
			990m	N ₂	IR	1
			981vs	N ₂	IR	1

References

¹I. R. Dunkin and P. C. P. Thomson, J. Chem. Soc., Chem. Commun. 1192 (1982).

NC(C≡C)₂CN⁺ $\tilde{E}^{\prime} \Pi_u$ D_{∞h}T₀ = 30420(160) gas PE¹ $\tilde{D}^{\prime} \Pi_g$ D_{∞h}T₀ = 25580(160) gas PE¹ $\tilde{B}, \tilde{C}^{\prime} \Sigma_g^+, \tilde{A}^{\prime} \Sigma_g^+$ D_{∞h}T₀ = 22190(160) gas PE¹ $\tilde{A}^{\prime} \Pi_u$ D_{∞h}T₀ = 15260(10) gas EF¹ $\tilde{A}-\tilde{X}$ 630–770 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ_g^+			1940(80)	gas	PE	1

 $\tilde{X}^{\prime} \Pi_g$ D_{∞h}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
Σ_g^+	1	C≡N stretch	2180(10)	gas	EF	1
	2	C≡C stretch	2100(10)	gas	EF	1
	3	C–C stretch	1360(10)	gas	EF	1
	4	C–C stretch	460(10)	gas	EF	1

References

¹E. Kloster-Jensen, J. P. Maier, O. Marthaler, and M. Mohraz, J. Chem. Phys. 71, 3125 (1979).

C₂H₅(C≡C)₂CN⁺ $\tilde{C}, \tilde{D}^{\prime} A^{\prime}, \tilde{A}^{\prime} C_s$ T₀ ~ 29530 gas PE¹ $\tilde{B}^{\prime} A^{\prime} C_s$ T₀ = 24450(160) gas PE¹ $\tilde{A}^{\prime} A^{\prime} C_s$ T₀ = 17530(10) gas EF¹ $\tilde{A}-\tilde{X}$ 570–720 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'		C≡C stretch	2000(160)	gas	PE	1
			1050(160)	gas	PE	1

τ₀ < 6 ns gas EF¹ $\tilde{X}^{\prime} A^{\prime\prime} C_s$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
a'	2	C≡N, C≡C str.	2180(10)	gas	EF	1
	3	C≡N, C≡C str.	2080(10)	gas	EF	1
	5	C–C stretch	1320(10)	gas	EF	1
	6	C–C stretch	550(10)	gas	EF	1
			460(10)	gas	EF	1

^aFrom vertical ionization potential.**References**

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

H₇O⁺ $\tilde{X}$ C_{2v} ?

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		H ₂ O a-stretch	3721.6	gas	PF	1
		H ₃ O ⁺ O–H str.	3667.0	gas	PF	1
		H ₂ O s-stretch	3637.4	gas	PF	1

References

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

H₉O⁺ $\tilde{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		H ₂ O in-phase a-stretch	3730.4	gas	PF	1
		H ₂ O out-of-phase s-stretch	3644.9	gas	PF	1

References

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

***t*-CH₃C—OCH₃**

In a nitrogen matrix, a broad absorption with maximum near 390 nm behaves appropriately for assignment to CH₃C—OCH₃.¹

 $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			1330	N ₂	IR	1
			1288	N ₂	IR	1
			1160	N ₂	IR	1
			1100	N ₂	IR	1
			550	N ₂	IR	1

References

- ¹R. S. Sheridan, R. A. Moss, B. K. Wilk, S. Shen, M. Wlostowski, M. A. Kesselmayr, R. Subramanian, G. Kmiecik-Lawrynowicz, and K. Krogh-Jespersen, *J. Am. Chem. Soc.* **110**, 7563 (1988).

***c*-CH₃C—OCH₃**

In a nitrogen matrix, a broad absorption with maximum near 390 nm behaves appropriately for assignment to CH₃C—OCH₃.¹

 $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			1320	N ₂	IR	1
			1275	N ₂	IR	1

References

- ¹R. S. Sheridan, R. A. Moss, B. K. Wilk, S. Shen, M. Wlostowski, M. A. Kesselmayr, R. Subramanian, G. Kmiecik-Lawrynowicz, and K. Krogh-Jespersen, *J. Am. Chem. Soc.* **110**, 7563 (1988).

***n*-C₃H₇O** $\bar{A}$

$T_0 = 29000$ gas LF¹ $\bar{A}$ - $\bar{\chi}$ 340–450 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CO stretch	450(50)	gas	LF	1

$\tau = 0.70(8)$ μ s gas LF¹

 $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CO stretch	1065	gas	LF	1

References

- ¹J. Bai, H. Okabe, and M. K. Emadi-Babaki, *J. Photochem. Photobiol., A: Chem.* **50**, 163 (1989).

(CH₃)₂CHO

$\bar{A}$ $T_0 \sim 27167$ gas EM^{1,4}LF^{2,3} $\bar{A}$ - $\bar{\chi}$ 330–520 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		C—O stretch	560(10)	gas	LF	2,3

$\tau = 0.64(9)$ μ s gas EM⁴

 $\bar{\chi}$ C_s

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		C—O stretch	960(20)	gas	EM	4

References

- ¹K. Ohbayashi, H. Akimoto, and I. Tanaka, *J. Phys. Chem.* **81**, 798 (1977).
²R. J. Balla, H. H. Nelson, and J. R. McDonald, *Chem. Phys.* **99**, 323 (1985).
³S. C. Foster, Y.-C. Hsu, C. P. Damo, X. Liu, C.-Y. Kung, and T. A. Miller, *J. Phys. Chem.* **90**, 6766 (1986).
⁴J. Bai, H. Okabe, and J. B. Halpern, *Chem. Phys. Lett.* **149**, 37 (1988).

(CH₃)₂SiO $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		Si=O stretch	1209.6	Ar	IR	1–3

References

- ¹C. A. Arrington, R. West, and J. Michl, *J. Am. Chem. Soc.* **105**, 6176 (1983).
²R. Withnall and L. Andrews, *J. Am. Chem. Soc.* **108**, 8118 (1986).
³R. Withnall and L. Andrews, *J. Phys. Chem.* **92**, 594 (1988).

CH₃SiH₂OH $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OH stretch	3716.0m	Ar	IR	1
		SiH stretch	2138.0s	Ar	IR	1
		SiH stretch	2127.4s	Ar	IR	1
		SiH ₂ bend	976.7ms	Ar	IR	1
		CH ₃ rock	797.4m	Ar	IR	1
		SiOH bend	718.5s	Ar	IR	1
		SiH ₂ rock	509.7w	Ar	IR	1

References

¹R. Withnall and L. Andrews, *J. Phys. Chem.* **92**, 594 (1988).

SiH₃SiH₂OH $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OH stretch	3708.5	Ar	IR	1
		SiH ₃ deform.	961.6	Ar	IR	1
		SiH ₂ bend	950.6	Ar	IR	1
		SiH ₂ twist	855.0	Ar	IR	1
		SiOH bend	748br	Ar	IR	1
		SiH ₂ rock	521.7	Ar	IR	1

SiD₃SiD₂OD $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OD stretch	2733.5	Ar	IR	1
		SiO stretch	862.0	Ar	IR	1
		SiD ₃ deform.	704.4	Ar	IR	1
		SiD ₂ twist	637.4	Ar	IR	1
		SiOD bend	556.9	Ar	IR	1

References

¹R. Withnall and L. Andrews, *J. Phys. Chem.* **92**, 594 (1988).

CH₃OSiCH₃

In an argon matrix, an absorption maximum has been observed¹ at 357 nm. Irradiation in that spectral region results in photoisomerization to CH₃OSiH=CH₂.

 $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			2842.2wm	Ar	IR	1
			1470.0wm	Ar	IR	1
			1218.8m	Ar	IR	1
			1106.5m	Ar	IR	1
			1086.7s	Ar	IR	1
			1084.3vs	Ar	IR	1
			844.2wm	Ar	IR	1
			791.7m	Ar	IR	1
			709.2wm	Ar	IR	1

References

¹G. Maier, H. P. Reisenauer, K. Schöttler, and U. Wessolek-Kraus, *J. Organomet. Chem.* **366**, 25 (1989).

CH₃OSiH=CH₂

In an argon matrix, an absorption maximum has been observed¹ at 245 nm. Irradiation in that spectral region results in photoisomerization to CH₃OSiCH₃.

 $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		SiH stretch	2241.9m	Ar	IR	1
			1464.2w	Ar	IR	1
			1462.3wm	Ar	IR	1
			1318.1wm	Ar	IR	1
			1199.0w	Ar	IR	1
			1119.0m	Ar	IR	1
			1100.2vs	Ar	IR	1
			1002.5wm	Ar	IR	1
			862.5s	Ar	IR	1
			752.1w	Ar	IR	1
			671.1m	Ar	IR	1
			561.8wm	Ar	IR	1

References

¹G. Maier, H. P. Reisenauer, K. Schöttler, and U. Wessolek-Kraus, *J. Organomet. Chem.* **366**, 25 (1989).

CH₂=Si(OH)CH₃^a $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OH stretch	3737br	Ar	IR	1
			3715.4			
		Si=C stretch + CH ₃ rock	899vs	Ar	IR	1
		SiO stretch	781.0	Ar	IR	1
			777.5			
		SiOH bend	729.7vs	Ar	IR	1
		Torsion	360.2	Ar	IR	1
		CSiC bend	285.1	Ar	IR	1

^aTentative identification.

References

¹R. Withnall and L. Andrews, *J. Phys. Chem.* **92**, 594 (1988).

(CH₃)₂SiHOH $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OH stretch	3717.1	Ar	IR	1
		SiH stretch	2111.0	Ar	IR	1
			925vs	Ar	IR	1
			819.4	Ar	IR	1
			808.8			
		HSiO bend	764.5	Ar	IR	1
			757.2			

$\bar{X}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		SiOH bend	711.0 707.3	Ar	IR	1
		CSiC bend	616.2 283	Ar Ar	IR IR	1 1

References

¹R. Withnall and L. Andrews, *J. Phys. Chem.* **92**, 594 (1988).**cyc-C₄H₄O⁺**

(Furan Cation)

 $\bar{X}^2A_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			1776	gas	LF	2
			1585	gas	LF	2
			1409	gas	PE,LF	1,2
			1225	gas	LF	2
			1068	gas	PE,LF	1,2
			846	gas	PE,LF	1,2
			644	gas	LF	2
			459	gas	LF	2
			287	gas	LF	2
			133	gas	LF	2

References

¹P. J. Derrick, L. Åsbrink, O. Edqvist, B. O. Jonsson, and E. Lindholm, *Int. J. Mass Spectrom. Ion Phys.* **6**, 161 (1971).²R. S. Smith, M. Anselment, L. F. DiMauro, J. M. Frye, and T. J. Sears, *J. Chem. Phys.* **87**, 4435 (1987).**(cyc-C₅H₄)O**

(Cyclopentadienone)

In an argon matrix, a very prominent absorption maximum at 195 nm and a weaker absorption maximum at 360 nm have been attributed¹ to cyclopentadienone.

 $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			1870wm	Ar	IR	1,2
			1789w	Ar	IR	1,2
			1727vs	Ar	IR	1,2
			1724vs			
			1678wm	Ar	IR	1,2
			1332s	Ar	IR	1,2
			1136s	Ar	IR	1,2
			1068wm	Ar	IR	1,2
			822vs	Ar	IR	1,2
			632s	Ar	IR	1,2
			458wm	Ar	IR	1,2

References

¹G. Maier, L. H. Franz, H.-G. Hartan, K. Lanz, and H. P. Reisenauer, *Chem. Ber.* **118**, 3196 (1985).²G. Maier, *Pure Appl. Chem.* **58**, 95 (1986).**(CH₂)₃C=C=Se**

(Trimethyleneselenoketene)

 $\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CH stretch	2967s	Ar	IR	1
		CH stretch	2863s	Ar	IR	1
			1757m			
		CCSe a-stretch	1746vs	Ar	IR	1
			1432w	Ar	IR	1
			1232m	Ar	IR	1

References

¹W. W. Sander and O. L. Chapman, *J. Org. Chem.* **50**, 543 (1985).**C₆H₅O** $\bar{B}$ C_{2v}

gas AB^{1,2} $\bar{B}-\bar{X}$ 380–395 nm
 T₀ = 25175(10) Ar AB⁴ $\bar{B}-\bar{X}$ 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

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

T₀ ~ 16360 gas AB^{2,3} $\bar{A}-\bar{X}$ 559–612 nm
 Ar AB⁴ $\bar{A}-\bar{X}$ 573–629 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			~500	gas	AB	3
			504(10)	Ar	AB	4

C₆D₅O $\bar{B}$ C_{2v}

T₀ = 25240(10) Ar AB⁴ $\bar{B}-\bar{X}$ 349–397 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			1349(20)	Ar	AB	4
			809(20)	Ar	AB	4

References

- ¹G. Porter and F. J. Wright, *Trans. Faraday Soc.* **51**, 1469 (1955).
²G. Porter and B. Ward, *J. Chim. Phys.* **61**, 1517 (1964).
³B. Ward, *Spectrochim. Acta* **24a**, 813 (1968).
⁴D. Pullin and L. Andrews, *J. Mol. Struct.* **95**, 181 (1982).

C₆H₅S**C** $T_0 \sim 32260$ gas AB¹**B**C_{2v} $T_0 = 19328(4)$ gas LF² $\tilde{B}-\tilde{X}$ 490–600 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		Ring deform.	483(5)	gas	LF	2
		CS stretch	410(5)	gas	LF	2
		CH deform.	275(5)	gas	LF	2

 $\tau_0 < 20$ ns gas LF²**X̃**C_{2v}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CH deform.	1165(20)	gas	LF	2
		Ring deform.	610(20)	gas	LF	2
		CS stretch	430(20)	gas	LF	2

References

- ¹G. Porter and F. J. Wright, *Trans. Faraday Soc.* **51**, 1469 (1955).
²K. Shibuya, M. Nemoto, A. Yanagibori, M. Fukushima, and K. Obi, *Chem. Phys.* **121**, 237 (1988).

C₆H₅OH⁺**X̃**C_{2v}

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			1669(33)	gas	PE	1
			1500(30)	gas	PE	1
			1395(28)	gas	PE	1
			1210(24)	gas	PE	1
			1040(21)	gas	PE	1
			1027(21)	gas	PE	1
			976(20)	gas	PE	1
			815(16)	gas	PE	1
			556(12)	gas	PE	1
			516(12)	gas	PE	1
		Ring torsion ?	169(12)	gas	PE	1

References

- ¹S. L. Anderson, L. Goodman, K. Krogh-Jespersen, A. G. Ozkabak, R. N. Zare, and C.-F. Zheng, *J. Chem. Phys.* **82**, 5329 (1985).

C₆H₅OCCL

In a nitrogen matrix, an absorption maximum at 320 nm has been assigned¹ to C₆H₅OCCL.

X̃

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			1285B	N ₂	IR	1
			1275B	N ₂	IR	1
			1251A	N ₂	IR	1
			850A	N ₂	IR	1
			800B	N ₂	IR	1

The infrared spectrum between 400 and 2000 cm⁻¹ is shown in Ref. 1, but the positions of only a few very prominent absorptions are given. There is evidence for the stabilization of two rotational isomers, labelled A and B.

References

- ¹M. A. Kesselmayr and R. S. Sheridan, *J. Am. Chem. Soc.* **108**, 844 (1986).

C₂H₅O₂

An unstructured gas-phase absorption between 215 and 280 nm, with maximum at 235 nm, has been assigned^{1,3-5} to C₂H₅O₂.

Ā $T_0 = 7593(6)$ gas AB² $\tilde{A}-\tilde{X}$ 1175–1317 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OO stretch	918(9)	gas	AB	2

X̃

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CH ₂ a-stretch	3016wm	Ar	IR	6
		CH ₂ scissors	1474m	Ar	IR	6
		CH ₃ deform.	1451sh	Ar	IR	6
		CH ₃ deform.	1389vs	Ar	IR	6
		CH ₃ deform.	1380sh	Ar	IR	6
		CH ₂ wag	1351m	Ar	IR	6
		CH ₂ twist	1242w	Ar	IR	6
		CH ₃ rock	1136m,br	Ar	IR	6
		OO stretch	1112ms	Ar	IR	6
		CC stretch	1009s	Ar	IR	6
		CO stretch	838m	Ar	IR	6
		CH ₂ rock	800m	Ar	IR	6
		Skel. bend	499vs	Ar	IR	6

References

- ¹D. A. Parkes, D. M. Paul, C. P. Quinn, and R. C. Robson, *Chem. Phys. Lett.* **23**, 425 (1973).
²H. E. Hunziker and H. R. Wendt, *J. Chem. Phys.* **64**, 3488 (1976).
³H. Adachi, N. Basco, and D. G. L. James, *Int. J. Chem. Kinet.* **11**, 1211 (1979).

⁴C. Anastasi, D. J. Waddington, and A. Woolley, *J. Chem. Soc., Faraday Trans. 1* **79**, 505 (1983).

⁵J. Munk, P. Pagsberg, E. Ratajczak, and A. Sillesen, *J. Phys. Chem.* **90**, 2752 (1986).

⁶G. Chettur and A. Snelson, *J. Phys. Chem.* **91**, 3483 (1987).

$(\text{CH}_3)_2\text{CHO}_2$

A gas-phase absorption between 220 and 290 nm, with maximum near 240 nm, has been attributed^{2,3} to $(\text{CH}_3)_2\text{CHO}_2$.

$\bar{A}$

$T_0 = 7564(11)$ gas AB¹

$\bar{A}-\bar{X}$ 1178–1322 nm

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OO stretch	924(9)	gas	AR	1

$\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CH bend	1372	Ar	IR	4
		CH bend	1310	Ar	IR	4
			1178	Ar	IR	4
			1153	Ar	IR	4
			1130	Ar	IR	4
		OO stretch	1101vs	Ar	IR	4
		CC stretch	884ms	Ar	IR	4
		CO stretch	789m	Ar	IR	4
		Skel. bend	515s	Ar	IR	4
		Skel. bend	450wm	Ar	IR	4
		Skel. bend	348m	Ar	IR	4
		Skel. bend	305m	Ar	IR	4

References

¹H. E. Hunziker and H. R. Wendt, *J. Chem. Phys.* **64**, 3488 (1976).

²L. J. Kirsch, D. A. Parkes, D. J. Waddington, and A. Woolley, *J. Chem. Soc., Faraday Trans. 1* **74**, 2293 (1978).

³H. Adachi and N. Basco, *Int. J. Chem. Kinet.* **14**, 1125 (1982).

⁴G. Chettur and A. Snelson, *J. Phys. Chem.* **91**, 913 (1987).

$(\text{CH}_3\text{O})_2\text{Si}$

In an argon matrix, an absorption maximum has been observed¹ at 243 nm. Irradiation in that spectral region results in photoisomerization to $\text{CH}_3\text{SiOOCH}_3$.

$\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			2948.2w	Ar	IR	1
			2828.0w	Ar	IR	1
			1460.9w	Ar	IR	1
			1191.6wm	Ar	IR	1
			1178.1w	Ar	IR	1
			1074.7vs	Ar	IR	1
			752.4wm	Ar	IR	1
			737.9wm	Ar	IR	1

References

¹G. Maier, H. P. Reisenauer, K. Schöttler, and U. Wessolek-Kraus, *J. Organomet. Chem.* **366**, 25 (1989).

$\text{CH}_3\text{SiOOCH}_3$ ^a

In an argon matrix, an absorption maximum has been observed¹ at 232 nm.

$\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
			2981.0wm	Ar	IR	1
			2851.1wm	Ar	IR	1
			1453.9wm	Ar	IR	1
			1237.6wm	Ar	IR	1
			1182.5m	Ar	IR	1
			1174.0m	Ar	IR	1
			1121.2s	Ar	IR	1
			1104.8m	Ar	IR	1
			1094.4vs	Ar	IR	1

^aTentative assignment.

References

¹G. Maier, H. P. Reisenauer, K. Schöttler, and U. Wessolek-Kraus, *J. Organomet. Chem.* **366**, 25 (1989).

t-C₄H₉O₂

A gas-phase absorption between 210 and 300 nm, with maximum near 240 nm, has been attributed² to *t*-C₄H₉O₂.

$\bar{X}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CH ₃ rock	1187vs	Ar	IR	3
		CH ₃ rock	1139m	Ar	IR	3
		OO stretch	1124s	Ar	IR	3
		CC stretch	808ms	Ar	IR	3
			760(2)	gas	IR	1
		CO stretch	730m	Ar	IR	3
			693.7(5)	gas	IR	1
		Skel. bend	539ms	Ar	IR	3
		Skel. bend	403wm	Ar	IR	3
		Skel. bend	361m	Ar	IR	3
		Skel. bend	337m	Ar	IR	3

References

¹D. A. Parkes and R. J. Donovan, *Chem. Phys. Lett.* **36**, 211 (1975).

²C. Anastasi, I. W. M. Smith, and D. A. Parkes, *J. Chem. Soc., Faraday Trans. 1* **74**, 1693 (1978).

³G. Chettur and A. Snelson, *J. Phys. Chem.* **91**, 5873 (1987).

CH₃O₄CH₃ $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CO stretch	978(2)	Ar	IR	1
		CO stretch	960(2)	Ar	IR	1
		OO stretch	775(2)	Ar	IR	1
		OOO bend	580(2)	Ar	IR	1
		COO bend	457(2)	Ar	IR	1
		OOO bend	296(2)	Ar	IR	1

CD₃O₄CD₃ $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CO stretch	902(2)	Ar	IR	1
		CO stretch	893(2)	Ar	IR	1
		OOO bend	570(2)	Ar	IR	1
		COO bend	416(2)	Ar	IR	1

References¹P. Ase, W. Bock, and A. Snelson, *J. Phys. Chem.* **90**, 2099 (1986).**c-CH₃CH(NO)OH** $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OH stretch	3458.5m	Ar	IR	1
		NO stretch	1552s	Ar	IR	1
		CO stretch	1176vs	Ar	IR	1
		CH ₃ rock	1080ms	Ar	IR	1
		CH ₃ rock	999m	Ar	IR	1
		CNO bend + CN stretch	793.5m	Ar	IR	1
		OH torsion	326m	Ar	IR	1
		OCN scissors	303.5w	Ar	IR	1

References¹R. P. Muller, S. Murata, M. Nonella, and J. R. Huber, *Helv. Chim. Acta* **67**, 953 (1984).**CH₃NHCH₂NO (A)**

(Methyl(nitrosomethyl)amine—Conformer A)

 $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		NH stretch	3399w ^a	Ar	IR	1
		NO stretch	1552vs	Ar	IR	1
		CH ₃ deform.	1483wm	Ar	IR	1
		CH ₃ deform.	1455wm	Ar	IR	1

 $\bar{\chi}$ — Continued

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		CH ₃ deform.	1428vw	Ar	IR	1
		CH ₃ rock	1105wm	Ar	IR	1
		CNO bend + CN stretch	821w	Ar	IR	1
		NH deform.	662vs ^b	Ar	IR	1
		NCN scissors	318wm	Ar	IR	1

^aND stretch of CD₃NDCD₂NO at 2537 cm⁻¹.^bND deform. of CD₃NDCD₂NO at 540 cm⁻¹.**References**¹R. P. Muller, S. Murata, M. Nonella, and J. R. Huber, *Helv. Chim. Acta* **67**, 953 (1984).**CH₃NHCH₂NO (B)**

(Methyl(nitrosomethyl)amine—Conformer B)

 $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		NH stretch	3393w	Ar	IR	1
		NO stretch	1568vs	Ar	IR	1
		CH ₃ deform.	1486wm	Ar	IR	1
		CH ₃ deform.	1465wm	Ar	IR	1
		CH ₃ deform.	1428vw	Ar	IR	1
		CH ₃ rock	1102wm	Ar	IR	1
		CNO bend + CN stretch	761w	Ar	IR	1
		NH deform.	657vs	Ar	IR	1
		NCN scissors	308wm	Ar	IR	1

References¹R. P. Muller, S. Murata, M. Nonella, and J. R. Huber, *Helv. Chim. Acta* **67**, 953 (1984).**HOCH₂OONO₂** $\bar{\chi}$

Vib. sym.	No.	Approximate type of mode	cm ⁻¹	Med.	Type meas.	Refs.
		OH stretch	3645wm	gas	IR	2
			3006w	gas	IR	2
			2951w	gas	IR	2
			2899w	gas	IR	2
		NO ₂ a-stretch	1725vs	gas	IR	1,2
			1404wm	gas	IR	1,2
		NO ₂ s-stretch	1299s	gas	IR	1,2
			1106m	gas	IR	1,2
			1054m	gas	IR	1,2
			943m	gas	IR	1,2
			796ms	gas	IR	1,2
			721w	gas	IR	2
			610wm	gas	IR	2

References

- ¹H. Niki, P. D. Maker, C. M. Savage, and L. P. Breitenbach, *Chem. Phys. Lett.* **72**, 71 (1980).
²I. Barnes, K. H. Becker, E. H. Fink, A. Reimer, F. Zabel, and H. Niki, *Chem. Phys. Lett.* **115**, 1 (1985).

7. Master Index

Formula	Structure	Page Nos.
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AlCl ₂	AlCl ₂	S-1417
AlCl ₂ H	HAICl ₂	V-993
AlCl ₃ ⁺	AlCl ₃ ⁺	E-400
AlFO	FAIO	V-970
AlF ₃ ⁺	AlF ₃ ⁺	E-400
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AsH ₃ O	H ₂ AsOH	S-1463
As ₄ O	As ₄ O	S-1476
As ₄ O	<i>br</i> - As ₄ O	S-1476
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BBr ₂	BBr ₂	V-971
BBr ₂ H ⁺	HBBBr ₂ ⁺	E-378
BBr ₂ H ₂ N ⁺	NH ₂ BBr ₂ ⁺	E-470
BBr ₃ ⁺	BBr ₃ ⁺	V-1001,E-399
BClF ₃ ⁻	BF ₃ Cl ⁻	V-1020
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BCl ₂ H ⁺	HBCl ₂ ⁺	E-378
BCl ₂ H ₂ N ⁺	NH ₂ BCl ₂ ⁺	E-470
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BFH ⁺	HBF ⁺	S-1400

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BF ₂ O	F ₂ BO	V-1001,E-398
BF ₃ ⁺	BF ₃ ⁺	E-398
BF ₄ ⁻	BF ₄ ⁻	V-1020
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BHO	HBO	V-954,S-1399
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BaH ₂ O ₂	Ba(OH) ₂	S-1468
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BrF ₂ ⁻	FFBr ⁻	V-981
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BrNO ⁺	BrNO ⁺	E-331
BrNO ₂	BrNO ₂	V-1004,S-1453

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BrOP	BrPO	S-1421	CBr ₂	CBr ₂	V-974,E-337,S-1420
BrO ₂	BrOO	V-977	CBr ₂ Cl ⁺	CClBr ₂ ⁺	V-1003
BrO ₂	OBBrO	V-979	CBr ₂ Cl	CClBr ₂	V-1007
BrPS	BrPS	S-1422	CBr ₂ F ⁺	CFBr ₂ ⁺	V-1003
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Br ₂ Cl ⁻	ClBrBr ⁻	V-983	CBr ₃ ⁺	CBr ₃ ⁺	V-1003
Br ₂ F	BrBrF	V-980	CBr ₃	CBr ₃	V-1007
Br ₂ F ₂	Br ₂ F ₂	V-1009	CBr ₃ F ⁺	CFBr ₃ ⁺	V-1019,E-458
Br ₂ Ge ⁺	GeBr ₂ ⁺	E-330	CBr ₃ F ⁻	CFBr ₃ ⁻	V-1021
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Br ₂ O	BrBrO	V-980	CClFS ⁺	FCICS ⁺	E-403
Br ₂ OP	OPBr ₂	S-1455	CClF ₂ ⁺	CF ₂ Cl ⁺	V-1002
Br ₂ P	PBr ₂	V-976	CClF ₂	CF ₂ Cl	V-1006,S-1453
Br ₂ S ⁺	SBr ₂ ⁺	V-978	CClF ₂ NO ⁺	CF ₂ CINO ⁺	E-503
Br ₂ S	SBr ₂	V-979	CClF ₃ ⁺	CF ₃ Cl ⁺	V-1018,E-454,S-1479
Br ₂ S ₂ ⁺	S ₂ Br ₂ ⁺	E-413	CClF ₃ ⁻	CF ₃ Cl ⁻	V-1020
Br ₂ S ₂	SSBr ₂	V-1009	CClF ₄	CF ₃ ClF	V-1029,E-504
Br ₂ Se ⁺	SeBr ₂ ⁺	E-347	CCIN ⁺	ClCN ⁺	E-322,S-1414
Br ₂ Si	SiBr ₂	V-975,E-339	CCIN	ClNC	V-970
Br ₃ ⁻	Br ₃ ⁻	V-983	CCINO ⁺	ClNCO ⁺	E-392
Br ₃ P ⁺	PBr ₃ ⁺	E-409	CCINO	ClCNO	S-1451
Br ₃ PO ⁺	Br ₃ PO ⁺	E-463	CCINO	ClNCO	S-1450
Br ₃ PS ⁺	Br ₃ PS ⁺	E-465	CCINS ⁺	ClSCN ⁺	V-999,E-394
Br ₃ Sb ⁺	SbBr ₃ ⁺	E-411	CCINS	ClSCN	S-1451
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CBrCl ₂ ⁺	CCl ₂ Br ⁺	V-1003	CCl ₂ FNO ⁺	CFCl ₂ NO ⁺	E-504
CBrCl ₂	CCl ₂ Br	V-1007	CCl ₂ F ₂ ⁺	CF ₂ Cl ₂ ⁺	V-1019,E-456,S-1479
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CBrF ₂ ⁺	CF ₂ Br ⁺	V-1002	CCl ₂ O ⁺	Cl ₂ CO ⁺	E-401
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CBrF ₃ ⁻	CF ₃ Br ⁻	V-1021	CCl ₃	CCl ₃	V-1006,S-1454
CBrF ₄	CF ₃ BrF	V-1029,E-505	CCl ₃ F ⁺	CFCl ₃ ⁺	V-1019,E-457
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CBrN	BrNC	V-971	CCl ₃ NO ⁺	CCl ₃ NO ⁺	E-504
CBrNO ⁺	BrNCO ⁺	E-393	CCl ₃ O ₂	CCl ₃ O ₂	S-1492

<i>Formula</i>	<i>Structure</i>	<i>Page Nos.</i>	<i>Formula</i>	<i>Structure</i>	<i>Page Nos.</i>
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CFI ₂ ⁺	CFI ₂ ⁺	V-1003	CHCl ₂ ⁺	HCCl ₂ ⁺	V-994,E-380
CFI ₂	CFI ₂	V-1006	CHCl ₂	HCCl ₂	V-998,E-383
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CFN	FNC	V-970	CHCl ₃ ⁺	HCCl ₃ ⁺	E-444
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CFNS ⁺	FSCN ⁺	V-999,E-393	CHF	HCF	V-957,E-297,S-1402
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CF ₂ ⁺	CF ₂ ⁺	V-971,E-328	CHF ₂ ⁺	HCF ₂ ⁺	V-994
CF ₂	CF ₂	V-973,E-334,S-1419	CHF ₂	HCF ₂	V-997
CF ₂ ⁻	CF ₂ ⁻	S-1423	CHF ₂ N	<i>c</i> -HFC=NF	S-1472
CF ₂ I ⁺	CF ₂ I ⁺	V-1002	CHF ₂ P	CF ₂ =PH	S-1472
CF ₂ I	CF ₂ I	V-1006	CHF ₃ ⁺	HCF ₃ ⁺	E-443,S-1473
CF ₂ N	F ₂ CN	V-1001,E-400	CHI	HCI	S-1403
CF ₂ NOP ⁺	PF ₂ NCO ⁺	E-503	CHI ⁻	HCI ⁻	S-1404
CF ₂ NP ⁺	PF ₂ CN ⁺	E-452	CHI ₂	HCl ₂	V-998
CF ₂ NPS ⁺	PF ₂ NCS ⁺	E-503	CHN ⁺	HCN ⁺	E-292
CF ₂ N ₂ ⁺	CF ₂ N ₂ ⁺	E-452	CHN	HNC	V-955,E-295
CF ₂ O ⁺	F ₂ CO ⁺	E-401	CHNO ⁺	HNCO ⁺	E-375
CF ₂ OS	F ₂ CSO	S-1477	CHNO ⁺	HCNO ⁺	E-376
CF ₂ S ⁺	F ₂ CS ⁺	E-402	CHNO	HNCO	S-1441
CF ₂ Se ⁺	F ₂ CSe ⁺	E-404	CHNO	HOCN	V-992,S-1441
CF ₃ ⁺	CF ₃ ⁺	V-1002	CHNO	HCNO	S-1442
CF ₃	CF ₃	V-1005,E-407	CHNO	HONC	S-1442
CF ₃ I ⁺	CF ₃ I ⁺	V-1018,E-455	CHNP	HPCN	E-375
CF ₃ I ⁻	CF ₃ I ⁻	V-1021	CHNS ⁺	HNCS ⁺	E-375
CF ₃ IO	CF ₃ IO	S-1494	CHN ₂	HCNN	V-992,S-1440
CF ₃ IO	CF ₃ OI	S-1495	CHN ₂	HNCN	E-374,S-1440
CF ₃ NO ⁺	CF ₃ NO ⁺	E-503	CHO ⁺	HCO ⁺	V-955,S-1400
CF ₃ NO ₃	CF ₃ ONO ₂	S-1508	CHO ⁺	HOC ⁺	S-1401
CF ₃ O	CF ₃ O	S-1478	CHO	HCO	V-956,E-296,S-1402
CF ₃ O ⁻	CF ₃ O ⁻	V-1020	CHOS ⁺	HOCS ⁺	S-1443
CF ₃ O ₂	CF ₃ O ₂	V-1028,S-1492	CHO ₂ ⁺	HOCO ⁺	S-1443
CF ₄ ⁺	CF ₄ ⁺	E-453,S-1478	CHO ₂	<i>c</i> -HOCO	V-993
CF ₄ I	CF ₃ IF	V-1029,E-505	CHO ₂	<i>t</i> -HOCO	V-993,S-1444
CF ₄ O ⁺	CF ₃ OF ⁺	E-504	CHO ₂ Sr	HCOOSr	S-1471
CHBr	HBr	S-1403	CHO ₃	HC(O)OO	V-1016,S-1472
CHBr ⁻	HBr ⁻	S-1404	CHP ⁺	HCP ⁺	V-954,E-293
CHBrCl ⁺	HCClBr ⁺	V-995	CHS ⁺	HCS ⁺	S-1400
CHBrCl	HCClBr	V-998	CH ₂	CH ₂	V-951,E-279,S-1395
CHBrF ⁺	HCBrF ⁺	V-994	CH ₂ ⁻	CH ₂ ⁻	E-282
CHBrF	HCBrF	V-997	CH ₂ Br ⁺	H ₂ CB ⁺	V-989
CHBrO	HCOBr	S-1446	CH ₂ Br	H ₂ CBr	V-990
CHBr ₂ ⁺	HCB ₂ ⁺	V-995	CH ₂ BrF ⁺	CH ₂ FBr ⁺	V-1015
CHBr ₂	HCB ₂	V-998	CH ₂ BrI	H ₂ CBr-I	E-440
CHBr ₃ ⁺	HCB ₃ ⁺	E-444	CH ₂ Br ₂ ⁺	CH ₂ Br ₂ ⁺	V-1015,E-437
CHCaO ₂	HCOOCa	S-1471	CH ₂ CaNO	HCONHCa	S-1488
CHCl	HCCl	V-957,E-298,S-1403	CH ₂ Cl ⁺	H ₂ CCl ⁺	V-988
CHCl ⁻	HCCl ⁻	S-1404	CH ₂ Cl	H ₂ CCl	V-990,S-1437
CHClF ⁺	HCFCI ⁺	V-994	CH ₂ ClF ⁺	CH ₂ FCI ⁺	V-1015,E-436
CHClF	HCFCI	V-997	CH ₂ ClI	H ₂ CCl-I	E-439
CHClF ₂ ⁺	HCF ₂ Cl ⁺	E-443	CH ₂ CIN	CH ₂ =NCl	S-1470

Formula	Structure	Page Nos.	Formula	Structure	Page Nos.
CH ₂ ClP	CH ₂ =PCl	S-1470	CH ₃ N	CH ₂ NH	V-1010,E-418
CH ₂ Cl $\frac{1}{2}$	CH ₂ Cl $\frac{1}{2}$	V-1015,E-436	CH ₃ NO ⁺	CH ₃ NO ⁺	E-478
CH ₂ Cl ₂ Si	CH ₂ =SiCl ₂	V-1026,E-491	CH ₃ NO ⁺	H ₂ CNOH ⁺	E-479
CH ₂ Cu	CuCH ₂	S-1430	CH ₃ NO ⁺	HCONH $\frac{1}{2}$	E-479
CH ₂ F ⁺	H ₂ CF ⁺	V-988	CH ₃ NO	CH ₃ NO	V-1025
CH ₂ F	H ₂ CF	V-989,E-367	CH ₃ NO	CH ₂ NOH	S-1485
CH ₂ FI ⁺	CH ₂ FI ⁺	V-1015	CH ₃ NO ₂	<i>c</i> -CH ₂ (NO)OH	V-1033
CH ₂ F $\frac{1}{2}$	CH ₂ F $\frac{1}{2}$	V-1015,E-435	CH ₃ NO ₂	<i>t</i> -CH ₂ (NO)OH	V-1033
CH ₂ Fe	FeCH ₂	S-1429	CH ₃ NO ₅	HOCH ₂ OONO ₂	S-1535
CH ₂ Fe	HFeCH	S-1430	CH ₃ NS ⁺	HCSNH $\frac{1}{2}$	E-480
CH ₂ I	H ₂ CI	V-990,S-1437	CH ₃ O ⁺	CH ₂ OH ⁺	S-1459
CH ₂ I $\frac{1}{2}$	CH ₂ I $\frac{1}{2}$	E-437	CH ₃ O	CH ₃ O	V-1010,E-419,S-1459
CH ₂ I ₂	H ₂ CI-I	E-400	CH ₃ O	CH ₂ OH	V-1011,E-420,S-1460
CH ₂ N ⁺	HCNH ⁺	V-987,S-1433	CH ₃ O ⁻	CH ₃ O ⁻	V-1012
CH ₂ N	H ₂ CN	E-360	CH ₃ OSr	SrOCH ₃	E-476,S-1484
CH ₂ NOSr	HCONHSr	S-1489	CH ₃ O ₂	CH ₃ O ₂	E-482,S-1485
CH ₂ NO ₂	CH ₂ NO ₂	V-1026,E-485	CH ₃ S	CH ₃ S	V-1011,E-421,S-1460
CH ₂ N $\frac{1}{2}$	CH ₂ N $\frac{1}{2}$	E-431	CH ₃ S	CH ₂ SH	V-1011
CH ₂ N $\frac{1}{2}$	<i>cyc</i> -CH ₂ N $\frac{1}{2}$	E-432	CH ₃ S ⁻	CH ₃ S ⁻	V-1012,S-1462
CH ₂ N $\frac{1}{2}$	NH ₂ CN ⁺	E-431	CH ₃ S ₂	CH ₃ S ₂	S-1485
CH ₂ N ₂	HN=C=NH	V-1013,S-1468	CH ₃ S $\frac{1}{2}$	CH ₃ S $\frac{1}{2}$	S-1486
CH ₂ N ₂ O	H ₂ NNCO	S-1490	CH ₃ Sr	SrCH ₃	E-417
CH ₂ O ⁺	H ₂ CO ⁺	E-361	CH ₃ Te	CH ₃ Te	S-1461
CH ₂ OS ⁺	H ₂ CSO ⁺	E-435	CH ₃ Zn	ZnCH ₃	S-1457
CH ₂ OS	H ₂ CSO	V-1014	CH $\frac{1}{4}$	CH $\frac{1}{4}$	E-415
CH ₂ O $\frac{1}{2}$	HCOOH ⁺	E-434	CH ₄ Fe	HFeCH ₃	S-1482
CH ₂ S ⁺	H ₂ CS ⁺	V-987,E-362	CH ₄ N ⁺	CH ₂ NH $\frac{1}{2}$	S-1483
CH ₂ S	H ₂ CS	V-988,E-363	CH ₄ Ni	HNiCH ₃	S-1482
CH ₂ S ⁻	H ₂ CS ⁻	S-1437	CH ₄ NiO	HNiOCH ₃	S-1497
CH ₂ Se ⁺	H ₂ CSe ⁺	E-362	CH ₄ NiO	CH ₃ NiOH	S-1497
CH ₂ Se	H ₂ CSe	E-365,S-1434	CH ₄ O ⁺	CH ₃ OH ⁺	E-471
CH ₂ Si	H ₂ CSi	E-359	CH ₄ OSi	HCH ₃ SiO	S-1497
CH ₂ Zn	ZnCH ₂	S-1429	CH ₄ O ₃	HO ₂ CH ₂ OH	S-1506
CH ₂ Zn	HZnCH	S-1429	CH ₄ S ⁺	CH ₃ SH ⁺	E-472
CH $\frac{1}{3}$	CH $\frac{1}{3}$	V-985,E-352	CH ₄ Si ⁺	CH ₂ =SiH $\frac{1}{2}$	V-1022
CH ₃	CH ₃	V-985,E-352,S-1426	CH ₄ Si	CH ₂ =SiH ₂	V-1022,E-470
CH $\frac{1}{3}$	CH $\frac{1}{3}$	E-355	CH ₄ Si	CH ₃ SiH	V-1023,E-471
CH ₃ BO ⁺	BH ₃ CO ⁺	E-473	CH ₆ OSi	CH ₃ SiH ₂ OH	S-1530
CH ₃ BaO	BaOCH ₃	E-477	CIN ⁺	ICN ⁺	E-324
CH ₃ Br ⁺	CH ₃ Br ⁺	E-423	CINO ⁺	INCO ⁺	E-393
CH ₃ BrF	CH ₃ BrF	S-1487	CINO	INCO	S-1451
CH ₃ Ca	CaCH ₃	E-416,S-1457	CINS ⁺	ISCN ⁺	E-395
CH ₃ CaO	CaOCH ₃	E-475	CINS	ISCN	S-1451
CH ₃ Cd	CdCH ₃	S-1457	Cl ₃	Cl ₃	V-1007
CH ₃ Cl ⁺	CH ₃ Cl ⁺	E-422	CNO ⁺	NCO ⁺	V-966,E-314
CH ₃ ClF	CH ₃ ClF	S-1487	CNO	CNO	E-325
CH ₃ ClO ⁺	CH ₃ OCi ⁺	E-483	CNO	NCO	V-968,E-318,S-1412
CH ₃ ClSi	CH ₂ =SiHCl	V-1024,E-482	CNO ⁻	NCO ⁻	S-1416
CH ₃ ClSi	CH ₃ SiCl	V-1025,E-482	CNOSr	SrNCO	E-386
CH ₃ F ⁺	CH ₃ F ⁺	E-422	CNP	PCN	E-313
CH ₃ FI	CH ₃ IF	S-1487	CNS	NCS	V-968,E-319,S-1412
CH ₃ I ⁺	CH ₃ I ⁺	E-423,S-1461	CNS ⁻	NCS ⁻	S-1416
CH ₃ IO	CH ₃ IO	S-1486	CNSr	SrCN	E-308
CH ₃ IO	CH ₃ OI	S-1486	CN ₂	NCN	V-966,E-313,S-1410
CH ₃ IO	ICH ₂ OH	S-1486	CN ₂	CNN	V-966,E-314,S-1410
CH ₃ N ⁺	CH ₂ NH ⁺	E-417	CN ₂ O ⁺	ONCN ⁺	E-388
CH ₃ N	CH ₃ N	E-418,S-1459	CN ₂ O	NCNO	E-388

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CN ⁺	N ₃ CN ⁺	E-446	C ₂ H ₂ F ₂ ⁺	<i>t</i> -CHF=CHF ⁺	E-487
COS ⁺	OCS ⁺	V-968,E-320,S-1413	C ₂ H ₂ Fe	HFeCCH	S-1464
COSi	SiCO	V-966,E-312	C ₂ H ₂ Li	LiC ₂ H ₂	S-1464
CO ₂ ⁺	CO ₂ ⁺	V-968,E-320,S-1412	C ₂ H ₂ N	H ₂ CCN	S-1467
CO ₂ ⁻	CO ₂ ⁻	V-971,S-1418	C ₂ H ₂ N	H ₂ CNC	S-1467
CO ₃	CO ₃	V-1000,E-397	C ₂ H ₂ N ⁻	H ₂ CCN ⁻	E-430,S-1468
CO ₃ ⁻	CO ₃ ⁻	V-1001	C ₂ H ₂ N ⁻	H ₂ CNC ⁻	E-430
CS ₂ ⁺	CS ₂ ⁺	V-969,E-321,S-1413	C ₂ H ₂ N ₂	<i>t</i> -HN=CHCN	S-1490
CSi ₂	Si ₂ C	V-965,S-1410	C ₂ H ₂ N ₂ O ₂	HON=CHCNO	S-1507
C ₂ BrCl ⁺	ClCCBr ⁺	E-390	C ₂ H ₂ N ₂ O ₂	HON=CHNCO	S-1507
C ₂ BrN	BrCCN	V-999	C ₂ H ₂ Ni	C ₂ H ₂ Ni	E-427
C ₂ Br ₂ ⁺	C ₂ Br ₂ ⁺	V-1044,E-390	C ₂ H ₂ Ni	NiC=CH ₂	E-427
C ₂ ClF ₃ ⁺	CF ₂ =CFCI ⁺	E-501	C ₂ H ₂ O ⁺	H ₂ CCO ⁺	E-429
C ₂ ClN	ClCCN	V-999	C ₂ H ₂ O	HCCOH	S-1469
C ₂ Cl ₂ ⁺	C ₂ Cl ₂ ⁺	V-1044,E-389	C ₂ H ₂ OS	CHOCHS	V-1026
C ₂ Cl ₂ F ₂ ⁺	CF ₂ =CCl ₂ ⁺	E-501	C ₂ H ₂ O ₂ ⁺	(HCO) ₂ ⁺	E-484
C ₂ Cl ₂ O ⁺	Cl ₂ CCO ⁺	V-1017,E-452	C ₂ H ₂ O ₃	(HCO) ₂ O	V-1034
C ₂ Cl ₂ O	Cl ₂ CCO	V-1017	C ₂ H ₂ S ⁺	H ₂ CCS ⁺	V-1012,E-430
C ₂ Cl ₂ O ₂ ⁺	<i>t</i> -(ClCO) ₂ ⁺	E-499	C ₂ H ₂ S	H ₂ CCS	V-1013,E-433
C ₂ Cl ₄ ⁺	C ₂ Cl ₄ ⁺	E-502	C ₂ H ₂ S	HCCSH	V-1013,S-1469
C ₂ F ₂ ⁺	C ₂ F ₂ ⁺	E-389	C ₂ H ₂ S	<i>cyc</i> -C ₂ H ₂ S	V-1014,S-1469
C ₂ F ₂	C ₂ F ₂	V-1000,S-1450	C ₂ H ₂ S ₂	HS-CH=C=S	V-1026
C ₂ F ₂ N ₂	F ₂ C=C=N=N	S-1494	C ₂ H ₃ ⁺	C ₂ H ₃ ⁺	S-1458
C ₂ F ₂ O ₂ ⁺	<i>t</i> -(FCO) ₂ ⁺	E-499	C ₂ H ₃	C ₂ H ₃	E-417,S-1458
C ₂ F ₄ ⁺	C ₂ F ₄ ⁺	E-500	C ₂ H ₃ Cl ⁺	CH ₂ =CHCl ⁺	E-481
C ₂ F ₅	C ₂ F ₅	V-1035	C ₂ H ₃ ClO	CH ₃ OCCL	V-1032,S-1499
C ₂ F ₅ P	CF ₂ =PCF ₃	S-1508	C ₂ H ₃ F ⁺	CH ₂ =CHF ⁺	E-480
C ₂ H	HCC	V-954,E-291,S-1398	C ₂ H ₃ N ⁺	CH ₃ CN ⁺	E-474
C ₂ H ⁻	HCC ⁻	S-1400	C ₂ H ₃ N ⁺	CH ₃ NC ⁺	E-474
C ₂ HBr ⁺	HCCBr ⁺	V-1044,E-373	C ₂ H ₃ N ⁺	CH ₂ =C=NH ⁺	S-1484
C ₂ HCa	CaCCH	E-370,S-1439	C ₂ H ₃ N	CH ₂ =C=NH	V-1023,S-1484
C ₂ HCl ⁺	HCCCl ⁺	V-1044,E-372	C ₂ H ₃ N	HCCNH ₂	S-1484
C ₂ HClF ₂ ⁺	CHCl=CF ₂ ⁺	E-494	C ₂ H ₃ NO	CH ₃ CNO	S-1498
C ₂ HCl ₃ ⁺	CHCl=CCl ₂ ⁺	E-494	C ₂ H ₃ NO	HOCH ₂ CN	S-1499
C ₂ HF ₃ ⁺	CHF=CF ₂ ⁺	E-493	C ₂ H ₃ NO ₂	CH ₃ ONCO	S-1506
C ₂ HF ⁺	HCCF ⁺	E-372	C ₂ H ₃ O	CH ₃ CO	V-1024,E-477
C ₂ HI ⁺	HCCI ⁺	E-374	C ₂ H ₃ O	CH ₂ CHO	V-1024,E-477
C ₂ HN	HCCN	V-992,E-370	C ₂ H ₃ O ⁻	CH ₂ CHO ⁻	V-1024,E-481
C ₂ HNO	HCOCN	E-442,S-1472	C ₂ H ₃ O ₃	CH ₃ COO ₂	S-1507
C ₂ HO	HCCO	E-370,S-1440	C ₂ H ₃ P ⁺	CH ₃ CP ⁺	V-1023,E-475
C ₂ HS	HCCS	E-371	C ₂ H ₃ P	CH ₃ CP	S-1485
C ₂ HS	HSCC	E-371	C ₂ H ₄ ⁺	C ₂ H ₄ ⁺	E-468
C ₂ HSr	SrCCH	E-370	C ₂ H ₄ Al	AlC ₂ H ₄	S-1496
C ₂ H ₂ ⁺	C ₂ H ₂ ⁺	E-357	C ₂ H ₄ F	FCH ₂ CH ₂	V-1032
C ₂ H ₂	H ₂ C=C	V-987,E-359,S-1433	C ₂ H ₄ Fe	HFeC ₂ H ₃	S-1496
C ₂ H ₂ ⁻	H ₂ C=C ⁻	S-1434	C ₂ H ₄ FeO	CH ₂ =CHFeOH	S-1506
C ₂ H ₂ Br	CHBr=CH	S-1470	C ₂ H ₄ FeO	<i>cyc</i> -C ₂ H ₄ OFe	S-1505
C ₂ H ₂ ClF ⁺	CH ₂ =CFCI ⁺	E-488	C ₂ H ₄ Li	C ₂ H ₄ Li	S-1496
C ₂ H ₂ ClN ⁺	CH ₂ ClCN ⁺	E-485	C ₂ H ₄ Li ₂	1,2-C ₂ H ₄ Li ₂	S-1505
C ₂ H ₂ Cl ₂ ⁺	CH ₂ =CCl ₂ ⁺	E-488	C ₂ H ₄ N ⁺	CH ₃ CNH ⁺	S-1497
C ₂ H ₂ Cl ₂ ⁺	<i>c</i> -CHCl=CHCl ⁺	E-489	C ₂ H ₄ O	CH ₂ =CHOH	V-1032
C ₂ H ₂ Cl ₂ ⁺	<i>t</i> -CHCl=CHCl ⁺	E-489	C ₂ H ₄ O ₃	1,2,3- <i>cyc</i> -C ₂ H ₄ O ₃	V-1059
C ₂ H ₂ F	<i>t</i> -CHF=CH	V-1014	C ₂ H ₄ O ₃	1,2,4- <i>cyc</i> -C ₂ H ₄ O ₃	V-1059
C ₂ H ₂ FN ⁺	CH ₂ FCN ⁺	E-485	C ₂ H ₄ O ₃	<i>c</i> -HCOOCH ₂ OH	V-1060
C ₂ H ₂ FO ⁻	CH ₂ COF ⁻	S-1490	C ₂ H ₄ O ₃	<i>t</i> -HCOOCH ₂ OH	V-1061
C ₂ H ₂ F ₂ ⁺	CH ₂ =CF ₂ ⁺	E-486	C ₂ H ₄ S ⁺	CH ₃ CHS ⁺	V-1032
C ₂ H ₂ F ₂ ⁺	<i>c</i> -CHF=CHF ⁺	V-1026,E-486	C ₂ H ₅ ⁺	C ₂ H ₅ ⁺	V-1031,S-1495

<i>Formula</i>	<i>Structure</i>	<i>Page Nos.</i>	<i>Formula</i>	<i>Structure</i>	<i>Page Nos.</i>
C ₂ H ₅	C ₂ H ₅	V-1031,S-1495	C ₃ HF ₃ S	CF ₃ H(<i>cyc</i> -CCS)	V-1037
C ₂ H ₅ N	<i>c</i> -CH ₃ CH=NH	S-1503	C ₃ H ₂	HCCCH	V-1012,E-428,S-1466
C ₂ H ₅ N	<i>t</i> -CH ₃ CH=NH	S-1502	C ₃ H ₂	<i>cyc</i> -C ₃ H ₂	E-427,S-1466
C ₂ H ₅ N	C ₂ H ₃ NH ₂	S-1503	C ₃ H ₂	H ₂ C=C=C:	E-428,S-1466
C ₂ H ₅ N	H ₂ C=NCH ₃	S-1504	C ₃ H ₂	HCCH=C:	S-1467
C ₂ H ₅ NO ₂	<i>c</i> -CH ₃ CH(NO)OH	S-1535	C ₃ H ₂ N ⁺	HCCCNH ⁺	S-1488
C ₂ H ₅ O	C ₂ H ₅ O	V-1036,S-1504	C ₃ H ₂ O ⁺	H ₂ C=C=C=O ⁺	S-1489
C ₂ H ₅ O ₂	C ₂ H ₅ O ₂	S-1533	C ₃ H ₂ O	H ₂ C=C=C=O	S-1489
C ₂ H ₅ S	C ₂ H ₅ S	S-1504	C ₃ H ₂ S	H ₂ C=C=C=S	S-1490
C ₂ H ₆ Ge	(CH ₃) ₂ Ge	S-1520	C ₃ H ₂ Se	H ₂ C=C=C=Se	S-1490
C ₂ H ₆ N ₂ O	CH ₃ NHCH ₂ NO(A)	S-1535	C ₃ H ₂ Se	HCC-CHSe	S-1490
C ₂ H ₆ N ₂ O	CH ₃ NHCH ₂ NO(B)	S-1535	C ₃ H ₃	CH ₂ CCH	V-1023,E-473,S-1484
C ₂ H ₆ OSi	(CH ₃) ₂ SiO	V-1062,S-1530	C ₃ H ₃ Br ⁺	CH ₃ CCBr ⁺	S-1498
C ₂ H ₆ OSi	CH ₂ =Si(OH)CH ₃	S-1531	C ₃ H ₃ Cl ⁺	CH ₃ CCCl ⁺	S-1497
C ₂ H ₆ OSi	CH ₃ OSiCH ₃	S-1531	C ₃ H ₄ Li	CH ₃ CCHLi	S-1505
C ₂ H ₆ OSi	CH ₃ OSiH=CH ₂	S-1531	C ₃ H ₄ O	<i>cyc</i> -(H ₂ COC)=CH ₂	S-1506
C ₂ H ₆ O ₂ Si	(CH ₃ O) ₂ Si	S-1534	C ₃ H ₄ S	HCH ₃ (<i>cyc</i> -CCS)	V-1037
C ₂ H ₆ O ₂ Si	CH ₃ SiOOCH ₃	S-1534	C ₃ H ₅ ⁺	CH ₂ CHCH ₂ ⁺	V-1036
C ₂ H ₆ O ₄	CH ₃ O ₄ CH ₃	S-1535	C ₃ H ₅ ⁺	<i>cyc</i> -C ₃ H ₅ ⁺	S-1501
C ₂ H ₆ Si	(CH ₃) ₂ Si	V-1056,S-1519	C ₃ H ₅	CH ₂ CHCH ₂	V-1036,S-1501
C ₂ H ₆ Si	CH ₃ SiH=CH ₂	V-1056,S-1520	C ₃ H ₅ N	H ₂ C=CH-CH=NH	S-1526
C ₂ H ₆ Sn	(CH ₃) ₂ Sn	V-1058,S-1520	C ₃ H ₅ N	H ₂ C=C=NCH ₃	S-1526
C ₂ H ₇ ⁺	C ₂ H ₇ ⁺	S-1508	C ₃ H ₅ N	H ₂ C=CHN=CH ₂	S-1526
C ₂ H ₇ ⁺	<i>br</i> -C ₂ H ₇ ⁺	S-1508	C ₃ H ₅ N	<i>cyc</i> -C ₃ H ₅ N	S-1527
C ₂ H ₈ OSi	(CH ₃) ₂ SiHOH	S-1531	C ₃ H ₆ O	<i>t</i> -CH ₃ C-OCH ₃	S-1530
C ₂ I ₂ ⁺	C ₂ I ₂ ⁺	V-1044,E-391	C ₃ H ₆ O	<i>c</i> -CH ₃ C-OCH ₃	S-1530
C ₂ N	CCN	V-965,E-310,S-1410	C ₃ H ₇ ⁺	1-C ₃ H ₇ ⁺	S-1508
C ₂ N	CNC	V-965,E-311	C ₃ H ₇ ⁺	2-C ₃ H ₇ ⁺	V-1038,S-1508
C ₂ N ₂ ⁺	NCCN ⁺	E-387	C ₃ H ₇	CH ₃ CH ₂ CH ₂	V-1038
C ₂ N ₂ ⁺	CNCN ⁺	S-1446	C ₃ H ₇	(CH ₃) ₂ CH	V-1038,S-1508
C ₂ N ₂	CNCN	S-1447	C ₃ H ₇ N	CH ₃ CH=CHNH ₂	S-1527
C ₂ N ₂	CNNC	S-1447	C ₃ H ₇ N	C ₂ H ₃ NHCH ₃	S-1527
C ₂ N ₂ O ⁺	NCNCO ⁺	E-447	C ₃ H ₇ O	<i>n</i> -C ₃ H ₇ O	S-1530
C ₂ N ₂ O	NC-CNO	S-1475	C ₃ H ₇ O	(CH ₃) ₂ CHO	S-1530
C ₂ N ₂ O	NC-NCO	S-1475	C ₃ H ₇ O ₂	(CH ₃) ₂ CHO ₂	S-1534
C ₂ N ₂ S ⁺	S(CN ₂) ⁺	E-447	C ₃ H ₈ Si ⁺	(CH ₃) ₂ Si-CH ₂ ⁺	V-1056
C ₂ N ₂ S ⁺	NCNCS ⁺	E-448	C ₃ H ₈ Si	(CH ₃) ₂ Si=CH ₂	V-1056,S-1520
C ₂ N ₂ S	NC-NCS	S-1475	C ₃ IN ⁺	ICCCN ⁺	E-450
C ₂ N ₂ S ₂ ⁺	(SCN) ₂ ⁺	V-1027,E-497	C ₃ N ₂	C(CN) ₂	V-1017
C ₂ N ₂ Se ⁺	Se(CN) ₂ ⁺	E-451	C ₃ N ₂ O ⁺	CO(CN) ₂ ⁺	E-495
C ₂ O	CCO	V-965,E-312	C ₃ O	CCCO	V-999,S-1447
C ₂ O ⁻	CCO ⁻	V-967,E-316	C ₃ O ₂ ⁺	C ₃ O ₂ ⁺	E-446
C ₂ O ₂ ⁺	<i>t</i> -OCCO ⁺	S-1447	C ₄	C ₄	S-1446
C ₂ O ₂ ⁻	<i>t</i> -OCCO ⁻	S-1449	C ₄ Br ₂ ⁺	Br(CC) ₂ Br ⁺	V-1046,E-496
C ₂ O ₂ Si	Si(CO) ₂	V-1017	C ₄ Cl ₂ ⁺	Cl(CC) ₂ Cl ⁺	V-1046,E-496
C ₂ Si	SiCC	V-964,E-309,S-1409	C ₄ F ₂ ⁺	F(CC) ₂ F ⁺	V-1045,E-495
C ₃	C ₃	V-964,E-308,S-1408	C ₄ F ₆ O	CF ₃ CCOCF ₃	V-1062
C ₃ BrN ⁺	BrCCCN ⁺	E-450	C ₄ F ₆ O	(CF ₃) ₂ (<i>cyc</i> -CCO)	V-1062
C ₃ ClN ⁺	ClCCCN ⁺	E-449	C ₄ H	C ₄ H	V-1016,E-441,S-1471
C ₃ FN ⁺	FCCCN ⁺	E-448	C ₄ HBr ⁺	H(CC) ₂ Br ⁺	V-1045,E-492
C ₃ F ₂ O	F ₂ C=C=C=O	S-1493	C ₄ HCl ⁺	H(CC) ₂ Cl ⁺	V-1045,E-492
C ₃ F ₂ O	<i>cyc</i> -(CF=CFC)=O	S-1494	C ₄ HF ⁺	H(CC) ₂ F ⁺	E-491
C ₃ F ₆ ⁺	C ₃ F ₆ ⁺	V-1054	C ₄ HI ⁺	H(CC) ₂ I ⁺	E-493
C ₃ F ₇	<i>n</i> -C ₃ F ₇	V-1054	C ₄ H ₂ ⁺	C ₄ H ₂ ⁺	V-1025,E-483,S-1487
C ₃ F ₇	<i>i</i> -C ₃ F ₇	V-1055	C ₄ H ₄	<i>cyc</i> -C ₄ H ₄	V-1036,S-1505
C ₃ H	HC ₃	V-992,S-1440	C ₄ H ₄	H ₂ C=(<i>cyc</i> -C ₃ H ₂)	S-1505
C ₃ HN ⁺	HCCCN ⁺	E-441	C ₄ H ₄ O ⁺	<i>cyc</i> -C ₄ H ₄ O ⁺	S-1532

Formula	Structure	Page Nos.	Formula	Structure	Page Nos.
C ₄ H ₆ S	(CH ₃) ₂ (cyc-CCS)	V-1062	C ₆ H ₅	C ₆ H ₅	V-1040,S-1511
C ₄ H ₇ N	(CH ₃) ₂ C=C=NH	S-1528	C ₆ H ₅ N	3-CH(cyc-C ₅ H ₄ N)	V-1059
C ₄ H ₇ N	CH ₃ CC-NHCH ₃	S-1528	C ₆ H ₅ N	cyc-C ₆ H ₅ N	V-1058
C ₄ H ₉ ⁺	<i>t</i> -C ₄ H ₉ ⁺	V-1038	C ₆ H ₅ O	C ₆ H ₅ O	S-1532
C ₄ H ₉	<i>n</i> -C ₄ H ₉	V-1038	C ₆ H ₅ S	C ₆ H ₅ S	S-1533
C ₄ H ₉	<i>i</i> -C ₄ H ₉	V-1039	C ₆ H ₆ ⁺	C ₆ H ₆ ⁺	S-1512
C ₄ H ₉	<i>t</i> -C ₄ H ₉	V-1039,S-1509	C ₆ H ₆ ⁺	CH ₃ (CC) ₂ CH ₃ ⁺	V-1041,S-1514
C ₄ H ₉ O ₂	<i>t</i> -C ₄ H ₉ O ₂	V-1061,S-1534	C ₆ H ₆ F	C ₆ H ₆ F	V-1055
C ₄ H ₁₀ Si	(CH ₃) ₂ Si=CHCH ₃	V-1057	C ₆ H ₆ Li	LiC ₆ H ₆	S-1521
C ₄ I ₂ ⁺	I(CC) ₂ I ⁺	V-1046,E-497	C ₆ H ₆ O ⁺	C ₆ H ₅ OH ⁺	S-1533
C ₄ N ₂ ⁺	NCCCCN ⁺	V-1045,E-494	C ₆ H ₇ N ⁺	C ₆ H ₅ NH ₂ ⁺	V-1048
C ₄ O	C ₄ O	S-1475	C ₆ H ₈ ⁺	<i>t</i> -CH ₂ (CH) ₄ CH ₂ ⁺	V-1041
C ₅	C ₅	S-1475	C ₆ H ₈ Si	1-CH ₃ C ₅ SiH ₅	V-1058
C ₅ F ₄ ⁺	CF ₃ (CC) ₂ F ⁺	V-1047,S-1523	C ₆ N ₂ ⁺	NC(CC) ₂ CN ⁺	V-1046,S-1529
C ₅ F ₆ O	(CF ₃) ₂ (cyc-CCO)	V-1062	C ₇ F ₈ ⁺	C ₆ F ₅ CF ₃ ⁺	V-1053
C ₅ F ₈ O	CF ₃ (cyc-CCO)C ₂ F ₅	V-1062	C ₇ H ₃ F ₃ ⁺	C ₆ F ₅ CH ₃ ⁺	V-1053
C ₅ HN ⁺	H(CC) ₂ CN ⁺	V-1045,S-1500	C ₇ H ₃ Cl	C ₆ H ₅ CCl	S-1525
C ₅ H ₃ Br ⁺	CH ₃ (CC) ₂ Br ⁺	V-1046,S-1522	C ₇ H ₃ Cl	(2-ClC ₆ H ₄)CH	S-1526
C ₅ H ₃ Cl ⁺	CH ₃ (CC) ₂ Cl ⁺	V-1046,S-1522	C ₇ H ₃ Cl	cyc-1-C ₇ H ₃ Cl	S-1526
C ₅ H ₃ F ₂ N ⁺	cyc-C ₅ H ₃ F ₂ N ⁺	V-1058	C ₇ H ₃ ClO	C ₆ H ₅ OCCL	S-1533
C ₅ H ₃ N	cyc-C ₅ H ₃ N	S-1528	C ₇ H ₃ F	C ₆ H ₅ CF	S-1525
C ₅ H ₄ ⁺	CH ₃ (CC) ₂ H ⁺	V-1039,S-1509	C ₇ H ₃ F	cyc-1-C ₇ H ₃ F	S-1525
C ₅ H ₄	cyc-C ₅ H ₄	V-1039	C ₇ H ₃ F ₃ ⁺	sym-C ₆ H ₂ F ₃ CH ₃ ⁺	V-1051
C ₅ H ₄ O	(cyc-C ₅ H ₄)O	S-1532	C ₇ H ₃ N ⁺	C ₂ H ₅ (CC) ₂ CN ⁺	V-1047,S-1529
C ₅ H ₄ O ₂	cyc-C ₅ H ₄ O-1-O	V-1061	C ₇ H ₆	C ₆ H ₅ CH	V-1041,S-1514
C ₅ H ₅	cyc-C ₅ H ₅	V-1040,S-1510	C ₇ H ₆	cyc-C ₇ H ₆	V-1042,S-1514
C ₅ H ₆ Se	(CH ₂) ₃ C=C=Se	S-1532	C ₇ H ₆	cyc-C ₇ H ₆ :	S-1515
C ₅ H ₆ Si ⁺	C ₅ SiH ₆ ⁺	S-1521	C ₇ H ₇ ⁺	cyc-C ₇ H ₇ ⁺	V-1042
C ₅ H ₆ Si	C ₅ SiH ₆	V-1057,S-1521	C ₇ H ₇ ⁺	C ₆ H ₅ CH ₂ ⁺	V-1042
C ₅ H ₆ Si	C ₅ SiH ₆ (Dewar)	V-1057,S-1521	C ₇ H ₇	C ₆ H ₅ CH ₂	V-1042,S-1515
C ₅ H ₁₁	<i>n</i> -C ₅ H ₁₁	V-1040	C ₇ H ₇ ⁻	C ₆ H ₅ CH ₂ ⁻	S-1516
C ₅ H ₁₁	(CH ₃) ₃ CCH ₂	V-1040	C ₈ H ₈	<i>o</i> -(CH ₂) ₂ C ₆ H ₄	V-1043,S-1517
C ₅ O ₂	C ₅ O ₂	S-1500	C ₈ H ₈	C ₆ H ₅ CCH ₃	S-1518
C ₆ Br ₃ F ₃ ⁺	sym-C ₆ F ₃ Br ₃ ⁺	V-1051	C ₈ H ₈	<i>m</i> -CH ₃ C ₆ H ₄ CH:	S-1517
C ₆ ClF ₅ ⁺	C ₆ F ₅ Cl ⁺	V-1053	C ₈ H ₈	<i>o</i> -CH ₃ C ₆ H ₄ CH:	S-1517
C ₆ Cl ₃ F ₃ ⁺	sym-C ₆ F ₃ Cl ₃ ⁺	V-1050	C ₈ H ₈	<i>p</i> -CH ₃ C ₆ H ₄ CH:	S-1516
C ₆ F ₅ N	(C ₆ F ₅)N	S-1529	C ₈ H ₈	1-CH ₃ (cyc-C ₇ H ₅)	S-1518
C ₆ F ₆ ⁺	CF ₃ (CC) ₂ CF ₃ ⁺	V-1047,S-1524	C ₈ H ₈	4-CH ₃ (cyc-C ₇ H ₅)	S-1519
C ₆ F ₆ ⁺	C ₆ F ₆ ⁺	V-1053,S-1524	C ₈ H ₈	5-CH ₃ (cyc-C ₇ H ₅)	S-1518
C ₆ HF ₅ ⁺	C ₆ HF ₅ ⁺	V-1052	CaHO	CaOH	E-288
C ₆ HF ₅ O ⁺	C ₆ F ₅ OH ⁺	V-1053	CaH ₂ N	CaNH ₂	E-356,S-1430
C ₆ H ₂ ⁺	C ₆ H ₂ ⁺	V-1037,S-1507	CaH ₂ O	HCaOH	S-1431
C ₆ H ₂ F ₄ ⁺	1,2,3,4-C ₆ H ₂ F ₄ ⁺	V-1051	CaH ₂ O ₂	Ca(OH) ₂	S-1467
C ₆ H ₂ F ₄ ⁺	1,2,3,5-C ₆ H ₂ F ₄ ⁺	V-1051	CaN ₃	CaN ₃	E-386
C ₆ H ₂ F ₄ ⁺	1,2,4,5-C ₆ H ₂ F ₄ ⁺	V-1052	Ca ₂ H ₂ O	HCaOCaH	S-1465
C ₆ H ₃ Cl ₂ F ⁺	1,3,5-C ₆ H ₃ Cl ₂ F ⁺	V-1050	Ca ₂ H ₂ O	HCa ₂ OH	S-1465
C ₆ H ₃ Cl ₃ ⁺	1,3,5-C ₆ H ₃ Cl ₃ ⁺	V-1050	ClFH ⁻	FHCl ⁻	V-961
C ₆ H ₃ F ₃ ⁺	1,2,3-C ₆ H ₃ F ₃ ⁺	V-1048	ClFO	FCIO	V-979
C ₆ H ₃ F ₃ ⁺	1,2,4-C ₆ H ₃ F ₃ ⁺	V-1048	ClFO ₂ S ⁺	FCISO ₂ ⁺	E-467
C ₆ H ₃ F ₃ ⁺	1,3,5-C ₆ H ₃ F ₃ ⁺	V-1049,S-1522	ClFO ₃ ⁺	FCIO ₃ ⁺	E-466
C ₆ H ₃ N ⁺	CH ₃ (CC) ₂ CN ⁺	V-1047,S-1528	ClFS	FSCI	S-1424
C ₆ H ₄	C ₆ H ₄	V-1040,S-1510	ClFXe	XeClF	V-984
C ₆ H ₄ ⁻	C ₆ H ₄ ⁻	S-1511	ClF ₂	ClF ₂	V-980
C ₆ H ₄ F ₂ ⁺	1,3-C ₆ H ₄ F ₂ ⁺	V-1048	ClF ₂ ⁻	FCIF ⁻	V-981
C ₆ H ₄ F ₂ O ⁺	3,5-F ₂ C ₆ H ₃ OH ⁺	V-1049	ClF ₂ ⁻	FFCl ⁻	V-981
C ₆ H ₄ S ₂	<i>p</i> -C ₆ H ₄ S ₂	V-1063	ClF ₂ P ⁺	PF ₂ Cl ⁺	E-409
C ₆ H ₅ ⁺	C ₆ H ₅ ⁺	S-1511	ClF ₃ ⁺	ClF ₃ ⁺	E-414

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ClF ₃ P ⁻	PClF ₃ ⁻	V-1022	Cl ₂ P	PCl ₂	V-976
ClF ₃ S	SClF ₃	S-1481	Cl ₂ S ⁺	SCl ₂ ⁺	E-346
ClF ₃ Si ⁺	SiF ₃ Cl ⁺	E-460	Cl ₂ S ₂ ⁺	S ₂ Cl ₂ ⁺	E-413
ClF ₄ Si ⁻	SiF ₄ Cl ⁻	V-1029	Cl ₂ S ₂	SSCl ₂	V-1009
ClFeH	HFeCl	S-1399	Cl ₂ Se ⁺	SeCl ₂ ⁺	V-978,E-346
ClGeH	HGeCl	V-958,E-300	Cl ₂ Se ₂ ⁺	Se ₂ Cl ₂ ⁺	E-413
ClGeH ₂	H ₂ GeCl	V-990	Cl ₂ Si ⁺	SiCl ₂ ⁺	E-329
ClGeH ₃ ⁺	GeH ₃ Cl ⁺	E-426	Cl ₂ Si	SiCl ₂	V-974,E-338,S-1420
ClHI ⁻	ClHI ⁻	V-962	Cl ₂ Xe	XeCl ₂	V-984
ClHO ⁺	HOCl ⁺	E-306	Cl ₃	Cl ₃	V-982,S-1424
ClHSi	HSiCl	V-958,E-299	Cl ₃ FS	SCl ₃ F	S-1482
ClH ₂ ⁺	H ₂ Cl ⁺	S-1398	Cl ₃ F ₂ Si ⁻	SiF ₂ Cl ₃ ⁻	V-1030
ClH ₂ N ⁺	H ₂ NCl ⁺	E-368	Cl ₃ Ge	GeCl ₃	S-1455
ClH ₃ Si ⁺	SiH ₃ Cl ⁺	E-425	Cl ₃ HSi ⁺	HSiCl ₃ ⁺	E-445
ClIO	OICl	S-1424	Cl ₃ N ⁺	NCl ₃ ⁺	E-408
ClIO ₂	O ₂ ICl	S-1456	Cl ₃ OP ⁺	Cl ₃ PO ⁺	E-463
ClKrNe	NeKrCl	E-350	Cl ₃ O ₂ P	OPCl ₂ OCl	S-1494
ClKrXe	KrXeCl	E-350	Cl ₃ P ⁺	PCl ₃ ⁺	E-409
ClKr ₂	Kr ₂ Cl	E-350	Cl ₃ PS ⁺	Cl ₃ PS ⁺	E-464
ClNO ⁺	CINO ⁺	E-331	Cl ₃ Sb ⁺	SbCl ₃ ⁺	E-411
ClNO ₂ ⁺	CINO ₂ ⁺	E-405	Cl ₃ Si ⁺	SiCl ₃ ⁺	V-1004
ClNO ₂	CIONO	V-1004,S-1453	Cl ₃ Si	SiCl ₃	V-1008
ClNO ₂	OCINO	V-1004	Cl ₄ FSi ⁻	SiFCl ₄ ⁻	V-1030
ClNS ⁺	NSCl ⁺	E-332	Cl ₄ Ge ⁺	GeCl ₄ ⁺	E-462,S-1481
ClN ₃ ⁺	CIN ₃ ⁺	E-396	Cl ₄ Si ⁺	SiCl ₄ ⁺	E-461,S-1480
ClOP	ClPO	V-975,S-1421	Cl ₅ P ⁺	PCl ₅ ⁺	E-505
ClO ₂ ⁺	ClO ₂ ⁺	E-340	CoH ₂	CoH ₂	E-278
ClO ₂	ClOO	V-977,E-344	CoH ₂ O	HCoOH	S-1432
ClO ₂ ⁻	OCIO ⁻	V-979	CrH ₂	CrH ₂	S-1395
ClO ₂ P	PO ₂ Cl	S-1453	CrH ₂ O	HCrOH	S-1432
ClPS	CIPS	V-975	CrH ₃ O ₂	HCr(OH) ₂	S-1485
ClS ₂	SSCl	V-978,E-345	CuHO	CuOH	E-290
ClXe ₂	Xe ₂ Cl	E-350	CuH ₂ N	CuNH ₂	S-1430
Cl ₂ F	ClClF	V-980	CuH ₂ O	HCuOH	S-1433
Cl ₂ F ⁻	ClFCl ⁻	V-982	CuH ₃ N	HCuNH ₂	S-1458
Cl ₂ F ⁻	FClCl ⁻	V-982	Cu ₂ H ₂	Cu ₂ H ₂	S-1428
Cl ₂ F ₂	Cl ₂ F ₂	V-1009	Cu ₃ H ₂	Cu ₃ H ₂	S-1463
Cl ₂ F ₂ S	SCl ₂ F ₂	S-1482	DOSc	ScOD	S-1398
Cl ₂ F ₃ Si ⁻	SiF ₃ Cl ₂ ⁻	V-1029	FFeH	HFeF	S-1399
Cl ₂ Ga	GaCl ₂	S-1417	FFe ₂ H	HFe ₂ F	S-1440
Cl ₂ Ge ⁺	GeCl ₂ ⁺	E-329	FGaO	OGaF	V-970
Cl ₂ Ge	GeCl ₂	E-339,S-1421	FGeH ₃ ⁺	GeH ₃ F ⁺	E-426
Cl ₂ GeH ₂ ⁺	GeH ₂ Cl ₂ ⁺	E-439	FHI ⁻	FHI ⁻	V-961
Cl ₂ H ⁻	ClHCl ⁻	V-962,S-1406	FHN	HNF	V-960,E-303
Cl ₂ HN ⁺	HNCl ₂ ⁺	E-384	FHO ⁺	HO ⁺	E-306
Cl ₂ H ₂ Si ⁺	SiH ₂ Cl ₂ ⁺	E-438	FHSi	HSiF	V-958,E-299
Cl ₂ N	NCl ₂	V-976,E-343	FH ₂ ⁺	H ₂ F ⁺	V-953,S-1397
Cl ₂ O ⁺	Cl ₂ O ⁺	E-345	FH ₂ N ⁺	NH ₂ F ⁺	S-1438
Cl ₂ O	ClClO	V-980	FH ₂ N	NH ₂ F	S-1438
Cl ₂ OP	OPCl ₂	S-1455	FH ₂ P	PH ₂ F	S-1438
Cl ₂ OS ⁺	Cl ₂ SO ⁺	E-412	FH ₃ N ₂	NH ₂ NHF	S-1487
Cl ₂ OSi	Cl ₂ SiO	V-1004	FH ₃ Si ⁺	SiH ₃ F ⁺	E-424
Cl ₂ O ₂	ClOOCl	S-1456	FI ₂	IIF	V-981
Cl ₂ O ₂ S ⁺	Cl ₂ SO ₂ ⁺	E-467	FKrXe	KrXeF	E-350
Cl ₂ O ₂ Si	cyc-Cl ₂ SiO ₂	S-1477	FKr ₂	Kr ₂ F	E-349,S-1425
Cl ₂ O ₃	Cl ₂ O ₃	S-1478	FNO ⁺	FNO ⁺	E-331
Cl ₂ O ₄	ClOCIO ₃	S-1494	FNO	FON	V-975

<i>Formula</i>	<i>Structure</i>	<i>Page Nos.</i>	<i>Formula</i>	<i>Structure</i>	<i>Page Nos.</i>
FNO_2^+	FNO_2^+	E-405	F_3S	SF_3	V-1009
FNO_2	FONO	V-1004	F_3Sb^+	SbF_3^+	E-410
FNS^+	NSF^+	E-331	F_3Si	SiF_3	V-1007,S-1455
FN_3^+	FN_3^+	S-1449	F_4Ge^+	GeF_4^+	E-461,S-1481
FNeXe	NeXeF	E-350	F_4OXe^+	XeOF_4^+	E-506
FNe_2	Ne_2F	E-349	F_4P^-	PF_4^-	V-1022
FOP	FPO	S-1421	F_4P_2^+	P_2F_4^+	E-504
FOS	FSO	V-978	F_4P_2	$\text{PF}_3=\text{PF}$	S-1494
FO_2	FOO	V-977,E-343,S-1423	F_4Si^+	SiF_4^+	E-459,S-1479
FO_2S^-	FSO_2^-	V-1008	F_4Xe^+	XeF_4^+	E-467
FO_3S^+	FSO_3^+	E-453	F_5I^+	IF_5^+	E-506
FO_3S	FSO_3	V-1020,E-465	F_5P^+	PF_5^+	E-505
FPS	FPS	S-1422	F_5S	SF_5	V-1030
F_2Ge^+	GeF_2^+	E-329	F_5S^-	SF_5^-	V-1030
F_2GeH_2^+	GeH_2F_2^+	E-439	F_5Si^-	SiF_5^-	V-1029
F_2GeO	F_2GeO	S-1453	FeHI	HFeI	S-1399
F_2H^-	FHF^-	V-961,S-1405	FeH_2	FeH_2	E-277
F_2HN^+	HNF_2^+	E-383	FeH_2O	HFeOH	S-1432
F_2HP^+	HPF_2^+	E-384	FeH_2O_2	Fe(OH)_2	S-1468
$\text{F}_2\text{H}_2\text{Si}^+$	SiH_2F_2^+	E-438	FeH_3N	HFeNH_2	S-1457
$\text{F}_2\text{H}_3\text{P}$	PH_3F_2	S-1487	$\text{Fe}_2\text{H}_2\text{O}$	HFeOFeH	S-1465
F_2I^-	FIF^-	V-982	$\text{Fe}_2\text{H}_2\text{O}$	HFe_2OH	S-1465
F_2I^-	FFI^-	V-982	$\text{Fe}_2\text{H}_3\text{N}$	HFe_2NH_2	S-1483
F_2I_2	I_2F_2	V-1009	GaHO	GaOH	E-294
F_2Kr^+	KrF_2^+	E-347	GaH_2O	HGaOH	S-1434
F_2Kr	KrF_2	V-984,E-348	Ga_2H_6	Ga_2H_6	S-1501
F_2N^+	NF_2^+	V-975,E-340	GeH_2	GeH_2	V-952
F_2N	NF_2	V-976,E-342	GeH_2I_2^+	GeH_2I_2^+	E-439
F_2N_2^+	$t\text{-N}_2\text{F}_2^+$	E-404	GeH_2O	H_2GeO	S-1436
F_2O^+	OF_2^+	E-345	GeH_2O	HGeOH	S-1436
F_2OS^+	F_2SO^+	E-411	GeH_2O_3	H_2GeO_3	S-1491
F_2OSi	F_2SiO	V-1004	GeH_3^+	GeH_3^+	S-1425
$\text{F}_2\text{O}_2\text{S}^+$	F_2SO_2^+	E-466	GeH_3	GeH_3	V-986,S-1427
$\text{F}_2\text{O}_2\text{Si}$	$\text{cyc-F}_2\text{SiO}_2$	S-1477	GeH_3I^+	GeH_3I^+	E-426
$\text{F}_2\text{O}_2\text{Xe}$	XeO_2F_2	S-1482	GeH_4^+	GeH_4^+	E-416
$\text{F}_2\text{O}_3\text{Xe}$	XeO_3F_2	V-1030	GeH_4O	GeH_3OH	S-1483
F_2P^+	PF_2^+	V-975	GeH_4S^+	GeH_3SH^+	E-472
F_2P	PF_2	S-1423	GeI_2^+	GeI_2^+	E-330
F_2S^+	SF_2^+	V-978,E-346	$\text{Ge}_2\text{H}_2\text{O}$	HGe_2OH	S-1470
F_2S	SF_2	V-979,S-1424	Ge_2O_2	Ge_2O_2	S-1448
F_2S_2^+	F_2SS^+	E-412	Ge_3O_3	$(\text{GeO})_3$	S-1493
F_2S_2^+	FSSF^+	E-412	HIO	HOI	S-1405
F_2Se^+	SeF_2^+	V-978	HISi	HSiI	V-958,E-300
F_2Si^+	SiF_2^+	E-329	HI_2^-	IHI^-	V-963
F_2Si	SiF_2	V-974,E-337	HInO	InOH	E-294
F_2Xe^+	XeF_2^+	E-347	HKO^+	KOH^+	E-288
F_2Xe	XeF_2	V-984,E-348	HKr_2^+	HKr_2^+	V-964
F_3^-	F_3^-	V-981	HNO	HNO	V-959,E-301,S-1403
F_3HSi^+	HSiF_3^+	E-445	HNO^-	HNO^-	V-959,S-1404
F_3N^+	NF_3^+	E-407	HNOS^+	HNSO^+	E-379
F_3NO^+	F_3NO^+	E-462	HNOS	$t\text{-HONS}$	E-380
F_3NS^+	F_3NS^+	E-462	HNOS	$t\text{-HSNO}$	V-996,E-381
F_3OP^+	F_3PO^+	E-463	HNOS	$c\text{-HSNO}$	V-995,E-380
F_3OS^-	SOF_3^-	V-1022	HNOS	$c\text{-HNSO}$	V-996,E-381
$\text{F}_3\text{O}_2\text{S}^-$	SO_2F_3^-	V-1030	HNOS	$t\text{-HNSO}$	V-996,E-382
F_3P^+	PF_3^+	E-408	HNOS	$c\text{-HOSN}$	V-997,E-382
F_3PS^+	F_3PS^+	E-464	HNO_2	$t\text{-HONO}$	S-1444

<i>Formula</i>	<i>Structure</i>	<i>Page Nos.</i>	<i>Formula</i>	<i>Structure</i>	<i>Page Nos.</i>
HNO ₂	<i>c</i> -HONO	S-1445	H ₂ OV	HVOH	E-358
HNO ₃ ⁺	HNO ₃ ⁺	E-442	H ₂ O ₂ ⁺	H ₂ O ₂ ⁺	E-369
HNO ₄	HOONO ₂	S-1491	H ₂ O ₂	H ₂ O ₂	S-1439
HNSi	HNSi	V-956	H ₂ O ₂ Si	HSiOOH	S-1471
HN ₂ ⁺	HN ₂ ⁺	V-956,S-1401	H ₂ O ₃ Si	H ₂ SiO ₃	S-1491
HN ₂ O ⁺	HONN ⁺	S-1443	H ₂ OP	H ₂ PO	S-1437
HN ₃ ⁺	HN ₃ ⁺	E-376	H ₂ OP	HPOH	S-1438
HNaO ⁺	NaOH ⁺	E-288	H ₂ P ⁺	PH ₂ ⁺	E-282,S-1396
HNiO	NiOH	S-1398	H ₂ P	PH ₂	V-953,E-283,S-1397
HOP	HPO	V-959,E-302	H ₂ S ⁺	H ₂ S ⁺	E-286
HOS	HSO	V-961,E-305,S-1405	H ₂ S ₂ ⁺	H ₂ S ₂ ⁺	E-369
HOSi ⁺	HOSi ⁺	S-1401	H ₂ Sb	SbH ₂	E-285,S-1397
HOSr	SrOH	E-289	H ₂ Se ⁺	H ₂ Se ⁺	E-286
HOXe	XeOH	E-307	H ₂ Si ⁺	SiH ₂ ⁺	E-279
HOZn	ZnOH	S-1398	H ₂ Si	SiH ₂	V-951,E-280,S-1396
HO ₂ ⁺	HO ₂ ⁺	V-959	H ₂ Si ⁻	SiH ₂ ⁻	V-952,E-282
HO ₂	HO ₂	V-960,E-303,S-1404	H ₂ Te ⁺	H ₂ Te ⁺	E-287
HO ₂ ⁻	HO ₂ ⁻	E-306	H ₃ ⁺	H ₃ ⁺	V-951,S-1393
HO ₂ P	<i>c</i> -HOPO	S-1446	H ₃	H ₃	E-276,S-1393
HO ₃ P	HOPO ₂	S-1473	H ₃ ISi ⁺	SiH ₃ I ⁺	E-425
HO ₃ P	HOPO	S-1473	H ₃ N ⁺	NH ₃ ⁺	E-354,S-1428
HO ₃ P	HP(O ₂)O	S-1473	H ₃ NNi	HNiNH ₂	S-1458
HO ₃ S	HOSO ₂	V-1016,S-1474	H ₃ NO ⁺	NH ₂ OH ⁺	E-426
HO ₃ Sb	HSbO ₃	S-1474	H ₃ NSi	HSiNH ₂	S-1459
HO ₃ Sb	HOSbO ₂	S-1474	H ₃ O ⁺	H ₃ O ⁺	V-986,S-1428
HS ₂	HS ₂	E-305	H ₃ OP	PH ₃ O	S-1462
HS ₂ ⁻	HS ₂ ⁻	S-1405	H ₃ OP	<i>c</i> -H ₂ POH	S-1462
H ₂ I ₂ Si ⁺	SiH ₂ I ₂ ⁺	E-438	H ₃ OSb	H ₃ SbO	S-1463
H ₂ InO	HIInOH	S-1434	H ₃ OSb	H ₂ SbOH	S-1463
H ₂ Mg	MgH ₂	S-1395	H ₃ O ₃ P	(HO) ₂ HPO	S-1500
H ₂ MgO	HMgOH	S-1431	H ₃ P ⁺	PH ₃ ⁺	E-354
H ₂ Mg ₂ O	HMgOMgH	S-1464	H ₃ S ⁺	H ₃ S ⁺	S-1428
H ₂ Mg ₂ O	HMg ₂ OH	S-1464	H ₃ Sb ⁺	SbH ₃ ⁺	E-355
H ₂ Mn	MnH ₂	E-277	H ₃ Si ⁺	SiH ₃ ⁺	V-985,S-1425
H ₂ MnO	HMnOH	S-1432	H ₃ Si	SiH ₃	V-986,E-354,S-1426
H ₂ Mn ₂ O	HMn ₂ OH	S-1465	H ₃ Si ⁻	SiH ₃ ⁻	E-355
H ₂ Mn ₂ O	HMnOMnH	S-1465	H ₄ N ⁺	NH ₄ ⁺	V-1010,S-1456
H ₂ N ⁺	NH ₂ ⁺	V-952,E-281,S-1396	H ₄ N	NH ₄	E-416
H ₂ N	NH ₂	V-952,E-282,S-1396	H ₄ N ₂ ⁺	N ₂ H ₄ ⁺	E-472
H ₂ N ⁻	NH ₂ ⁻	E-287,S-1397	H ₄ N ₂ O	NH ₂ NHOH	S-1497
H ₂ NSr	SrNH ₂	E-356	H ₄ OSi	SiH ₃ OH	S-1483
H ₂ N ₂ ⁺	<i>t</i> -N ₂ H ₂ ⁺	V-987,E-362	H ₄ P ₂ ⁺	P ₂ H ₄ ⁺	E-473
H ₂ N ₂	<i>t</i> -N ₂ H ₂	V-989,E-365	H ₄ SSi ⁺	SiH ₃ SH ⁺	E-472
H ₂ N ₂	H ₂ NN	E-366,S-1436	H ₄ Si ⁺	SiH ₄ ⁺	E-415,S-1456
H ₂ N ₂ O ₂	NH ₂ NO ₂	E-490	H ₅ ⁺	H ₅ ⁺	S-1456
H ₂ NiO	HNiOH	S-1433	H ₅ O ₂ ⁺	H ₅ O ₂ ⁺	S-1496
H ₂ NiO ₂	Ni(OH) ₂	S-1468	H ₆ OSi	SiH ₃ SiH ₂ OH	S-1531
H ₂ Ni ₂ O	HNi ₂ OH	S-1466	H ₇ O ₃ ⁺	H ₇ O ₃ ⁺	S-1529
H ₂ O ⁺	H ₂ O ⁺	V-953,E-285,S-1397	H ₉ O ₄ ⁺	H ₉ O ₄ ⁺	S-1529
H ₂ OS	HSOH	V-991	IKrXe	KrXeI	E-351
H ₂ OSc	HScOH	E-358	INO ₂	INO ₂	V-1005
H ₂ OSi	HSiOH	V-989,S-1435	INS ⁺	NSI ⁺	S-1418
H ₂ OSi	H ₂ SiO	S-1435	INS	NSI	S-1422
H ₂ OSn	HSnOH	S-1436	I ₂ S	SI ₂	V-979
H ₂ OSn ₂	HSn ₂ OH	S-1470	I ₃ ⁻	I ₃ ⁻	V-983
H ₂ OSr	HSrOH	S-1431	Li ₃	Li ₃	S-1406
H ₂ OTi	HTiOH	E-358	Mn ₃	Mn ₃	S-1407

<i>Formula</i>	<i>Structure</i>	<i>Page Nos.</i>	<i>Formula</i>	<i>Structure</i>	<i>Page Nos.</i>
NOP	PNO	S-1417	O ₃ ⁺	O ₃ ⁺	E-332
NOS	SNO	V-972	O ₃ ⁻	O ₃ ⁻	V-977,E-343,S-1423
NOS	NSO	V-972	O ₃ P	PO ₃	S-1452
NO ₂ ⁺	NO ₂ ⁺	E-326	O ₃ S ⁺	SO ₃ ⁺	E-406
NO ₂ ⁻	NO ₂ ⁻	V-975,S-1421	O ₃ S ⁻	SO ₃ ⁻	S-1456
NO ₃	NO ₃	V-1002,E-404,S-1452	O ₃ Se	SeO ₃	S-1453
N ₂ O ⁺	N ₂ O ⁺	V-969,E-326,S-1415	O ₃ Si ₃	(SiO) ₃	S-1493
N ₂ O ₂ ⁺	(NO) ₂ ⁺	E-396	O ₄ ⁺	<i>t</i> -O ₄ ⁺	S-1452
N ₂ O ₂	<i>c</i> -(NO) ₂	V-1000,S-1450	O ₄ ⁻	<i>t</i> -O ₄ ⁻	V-1008,S-1455
N ₂ O ₂	<i>t</i> -(NO) ₂	V-1000	O ₄ S	SO ₄	V-1018
N ₂ O ₂ S	ON-NSO	S-1477	O ₅ P ₂	P ₂ O ₅	S-1501
N ₂ O ₂ S	ONSNO	S-1477	P ₃	P ₃	S-1415
N ₂ O ₃	O ₂ N-NO	V-1017,S-1476	P ₄ ⁺	P ₄ ⁺	E-388,S-1448
N ₂ O ₃	O=N-O-N=O	V-1018,S-1476	Pd ₃	Pd ₃	S-1408
N ₂ O ₄ ⁺	N ₂ O ₄ ⁺	E-502	Pt ₃	Pt ₃	S-1408
N ₂ O ₄	N ₂ O ₄	V-1027,S-1492	S ₂ Si	SiS ₂	S-1416
N ₂ O ₄	N ₂ O ₄ (V _d)	V-1027	S ₃	S ₃	E-342
N ₂ O ₄	ONO-NO ₂ (D)	V-1028,S-1492	S ₄	S ₄	V-1005,E-406
N ₂ O ₄	ONO-NO ₂ (D')	V-1028	Sb ₃	Sb ₃	S-1415
N ₂ O ₅	O ₂ N-O-NO ₂	V-1035,S-1500	Sb ₄	Sb ₄	S-1448
N ₂ S ⁺	NNS ⁺	S-1416	Sc ₃	Sc ₃	S-1407
N ₂ S	NNS	S-1417	Se ₃	Se ₃	S-1422
N ₂ S ₂ ⁺	N ₂ S ₂ ⁺	E-396	Te ₃	Te ₃	S-1423
N ₂ S ₄ ⁺	N ₂ S ₄ ⁺	E-502			
N ₂ Si	SiNN	V-967,E-315			
N ₃ ⁺	N ₃ ⁺	V-967,E-315			
N ₃	N ₃	E-325,S-1415			
N ₃ ⁻	N ₃ ⁻	E-326,S-1416			
N ₃ P ₃	(PN) ₃	S-1493			
N ₃ S ₃ ⁺	S ₃ N ₃ ⁺	E-498			
N ₃ Sr	SrN ₃	E-387			
N ₄ ⁺	N ₄ ⁺	S-1447			
Na ₃	Na ₃	E-307,S-1406			
Ni ₃	Ni ₃	S-1407			
OP ₂	P ₂ O	S-1417			
OP ₄	P ₄ O	S-1475			
OP ₄	<i>br</i> -P ₄ O	S-1476			
OSSi	OSiS	S-1416			
OS ₂ ⁺	SSO ⁺	E-334,S-1418			
OS ₂	SSO	E-341,S-1422			
OS ₂ ⁻	SSO ⁻	E-344			
O ₂ P	PO ₂	V-972,E-330,S-1418			
O ₂ P ⁻	PO ₂ ⁻	S-1421			
O ₂ P ₂	(PO) ₂	S-1450			
O ₂ S ⁺	SO ₂ ⁺	V-972,E-333			
O ₂ S ⁻	SO ₂ ⁻	V-977,E-344			
O ₂ Si	SiO ₂	V-970			
O ₂ Si ₂	Si ₂ O ₂	S-1448			

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