Ground-State Vibrational Energy Levels of Polyatomic Transient Molecules

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The experimentally determined ground-state vibrational energy levels of approximately 480 covalently bonded transient molecules possessing from 3 to 16 atoms are tabulated, together with references to the pertinent literature. The types of measurement surveyed include laser-based high resolution gas phase infrared absorption and visible-ultraviolet emission techniques, ultraviolet photoelectron spectroscopy, and matrix isolation spectroscopy. An assessment of the magnitude of the uncertainty of observations in neon, argon, and nitrogen matrices is given.

Key words: emission spectra; experimental data; free radicals; gas phase; infrared absorption; matrix isolation; molecular ions; polyatomic molecules; transient molecules; ultraviolet photoelectron spectroscopy; vibrational energy levels.

Contents

1. Introduction

Knowledge of the vibrational energy levels of small polyatomic molecules in their ground states, of intrinsic interest to the spectroscopist, is of widespread importance. In the rapidly developing field of quantum chemistry, correspondence of the calculated vibrational energy levels for a moderately complicated molecule with the observed values remains one of the more stringent tests for a computational procedure. The thermochemist uses vibrational data, together with the rotational constants of the molecule, to obtain the temperature variation in the thermodynamic properties, of especial importance to the modeling of high-temperature processes. Chemical kineticists and photochemists frequently have used infrared absorption for following the course of a reaction or for end-product analysis. Spectroscopy also provides a vital tool for measuring the changes which result from the formation of hydrogen bonds or of van der Waals clusters and from the adsorption of molecules on surfaces.

The use of specific, highly sensitive laser-based techniques has opened a new era in chemical kinetics. The ability to probe directly for reaction intermediates permits verification of reaction mechanisms and provides previously inaccessible information on the role of inhibitors and promoters in complex chemical processes. The availability of ground-state spectroscopic data for short-lived molecules greatly facilitates the identification

of band systems observed by laser-excited fluorescence and the application of such high resolution techniques as laser difference frequency spectroscopy, infrared diode laser spectroscopy, and infrared-based laser magnetic resonance and laser Stark spectroscopy for studying specific reaction intermediates.

Although vibrational data are readily available for most small, stable molecules, there are very few collections of vibrational energy level data for chemically reactive species such as free radicals and molecular ions. Noteworthy is the compilation by Herzberg[1], published in 1966. Although the primary focus of these tables is on electronic energy levels, they include authoritative data, with key references to the experimental literature, on the ground-state vibrational energy levels of molecules possessing from three to twelve atoms, arranged in a sequence which facilitates the correlation of spectroscopic properties with electronic structure. While the values cited for most stable molecules have much more often been refined than revised, such experimental tools as matrix isolation sampling, Fourier transform spectroscopy, and laser-based absorption and emission techniques have provided new data on the vibrational and electronic energy levels of many transient molecules.

Often, generalizations regarding characteristic group frequencies have been used to help to fill gaps in our knowledge of the vibrational spectra of transient molecules. However, these generalizations are not universally valid for molecules with atypical chemical bonding properties, including species with either a deficiency or an excess of electrons. In Fig. 1, stretching vibration

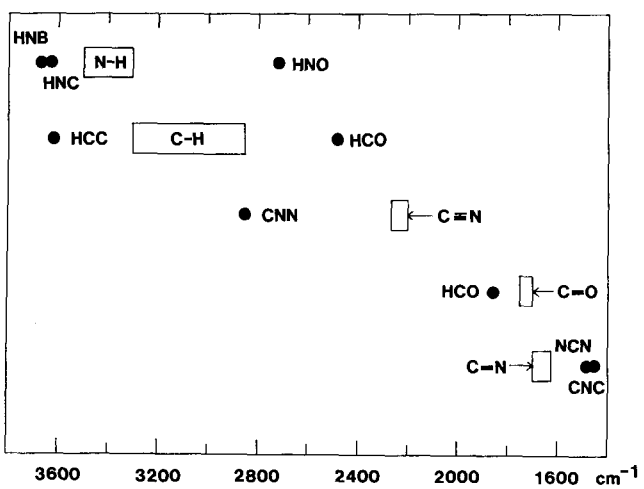

FIG. 1. Characteristic group frequencies[2] (ranges shown in rectangles) compared with values observed for small free radicals.

frequencies for several electron-deficient species, for which experimental evidence will be summarized in the following tables, are plotted together with the frequency range cited by Bellamy[2] as typical for the types of chemical bond associated with these stretching vibrations. It may be concluded that, despite their great usefulness, characteristic group frequencies can neither be assumed to be valid for all transient molecules nor used to provide a definitive identification of such species.

In the past few years, great strides have been made in the use of ab initio molecular orbital calculations to predict molecular properties. While even semi-empirical calculations frequently are very useful for predicting approximate ground-state molecular structures, the depth of the potential minimum often varies substantially as a function of the basis set chosen for the calculation. At this time, ab initio calculations for small polyatomic species are generally cited as yielding ground-state vibrational frequencies which correspond within 10 to 15% with the experimentally determined values[3–5]. While uncertainties of this magnitude may still permit valid predictions of anomalously large or small vibrational frequencies, a much smaller range of uncertainty is generally necessary in order to provide a positive spectroscopic identification of a transient molecule by the correspondence between its calculated and observed vibrational spectra or to provide a guide for tuning a laser system to probe a specific vibrational transition of a reaction intermediate.

2. Scope of Review

In this review, the definition of a transient molecule as one whose lifetime is less than a few minutes in the pressure range encountered in its production (typically 0.1–1.0 Torr), suggested by Dyke and co-workers[6], will be adopted. Many free radicals and molecular ions can be categorized as transient molecules. However, such important small free radicals as NO and NO_2 do not fit the definition. On the other hand, there are many examples of species that obey the familiar rules of chemical bonding, such as H_2CS and $CH_2{=}NH$, which must be regarded as transient molecules.

Experimental data are summarized in this review for the ground-state vibrational fundamentals of covalently bonded transient molecules composed of from 3 to 16 atoms. With only a few exceptions, data are limited to molecules formed from hydrogen, elements in the first two full rows of the Periodic Table, bromine, iodine, krypton, and xenon. A few covalently bonded species which possess heavier atoms (e.g., Ga, Ge, Se) and which are closely related to other species meeting the criteria for inclusion are also listed. Compounds such as LiO_2 and LiON, in which the metal bond is largely ionic, are considered to be diatomic anions which are somewhat perturbed by the metal cation and are not included. On the other hand, spectral data for covalently bonded polyatomic anions are within the scope of this review. In general, the vibrational data for these anions are included.

Because of the enhanced reactivity of most molecules at high temperatures, the definition of transient molecule would include the vapors of many compounds that are solid at room temperature. This review includes electron-deficient high-temperature molecules which are expected to possess substantially covalent bonding, such as C_3 and SiF_2, and species which are formed in chemical reactions with high-temperature reactants but are not

known to exist in equilibrium with the solid of that composition, such as SiO_2 and $HAlCl_2$. On the other hand, species which are expected to possess predominantly ionic bonds, such as MgF_2, are omitted.

A number of interesting compounds which may be regarded as bimolecular complexes (e.g., $CH_3 \cdots LiX$ and $CH_3 \cdots MgX$, as well as a large number of hydrogen-bonded species) do not fall within the scope of this review. Several species which were initially identified as molecular anions have since been found to have the structure $(R \cdots HX)^-$. It is frequently uncertain whether the complex is more adequately described $R^- \cdots HX$ or as $R \cdots HX^-$. Such species have been excluded. Many of the bihalide anions exist in both a relatively weakly hydrogen-bonded Type I (i.e., $(X \cdots HY)^-$) and a more strongly bonded Type II (i.e, XHY^-) form, in which extensive electron delocalization occurs. Spectral data are included only for the Type II structures of these species. Many electron acceptors have a high affinity for F^-, with which they form covalently bonded anions. Spectral data for a number of such anions, exemplified by BF_4^- and SiF_5^-, are included.

3. Types of Measurement

High resolution gas-phase observations potentially provide the highest precision data, with minimal perturbation by intermolecular interactions. Until recently, sensitive, fast time response detection systems were not available for infrared absorption studies. Therefore, vibrational data for transient molecules in their ground states were obtained from analysis of electronic emission spectra or from contributions of "hot bands" to visible or ultraviolet absorption spectra. Analysis of the emission spectrum, frequently complicated even for a diatomic molecule, has heretofore been possible only for a few small polyatomic species. The contribution of "hot bands" to absorption spectra generally is limited to low-frequency vibrations which may experience significant thermal excitation under the conditions necessary for the production of a detectable concentration of transient molecules. The recent introduction of free-jet expansion techniques has great potential for simplifying emission spectra. Excitation by electron bombardment and by broad-band radiation sources, as well as by lasers, has yielded ground-state vibrational data for even complicated molecules in free-jet experiments.

While direct infrared absorption measurements have generally not been amenable to the study of ground-state spectra of transient molecules, recent improvements in the design of Fourier transform infrared instrumentation have permitted the detection of a number of transient molecules. Spectral subtraction is a useful technique for eliminating overlapping absorptions of other products. However, it is often difficult to be certain that the absorptions which remain after those of known species have been removed are contributed by a single species.

As has already been noted, a variety of infrared and ultraviolet laser-based techniques possess high sensitivity and rapid time response. Such techniques as infrared diode laser spectroscopy, laser magnetic resonance, laser difference frequency spectroscopy, and laser-excited fluorescence have proved to be powerful tools for the study of the ground-state vibrational energy levels of transient molecules. These techniques, which often afford very high resolution spectra, are characterized by a limited range of tunability.

The appearance of structure in the lowest energy transition of the ultraviolet photoelectron spectrum also provides information on the vibrational energy levels of the species which results on electron detachment. Although this species usually is a molecular cation, Lineberger and co-workers have obtained vibrational data for several free radicals produced by electron detachment from the mass-selected anion. While photoelectron spectroscopy often has provided otherwise inaccessible vibrational data for molecular ions in their ground states, it is not a universal tool, since the first transition often is unstructured. Moreover, the precision and resolution of the observations have usually been approximately 5 meV, or 40 cm^{-1}, although improved resolution is now being achieved in a few laboratories.

The matrix isolation technique provides a powerful tool for obtaining the broad spectral surveys of transient molecules needed for efficient use of laser-based systems in high resolution gas phase studies. Application of this technique has yielded spectroscopic data for the ground states of a large number of transient molecules. In such experiments, the species of interest is trapped in dilute solid solution in an inert, rigid material, permitting the storage of a sufficient concentration of the transient molecule for direct infrared detection. The most frequently used matrix materials, nitrogen and the rare gases, are transparent from the far infrared to the vacuum ultraviolet. With few exceptions, molecular rotation is not possible in these solids. The infrared absorptions are sharp, typically with band widths (FWHM) of approximately 5 cm^{-1}, permitting determination of the absorption maximum to within 1 cm^{-1} in most measurements. Structure usually consists of a simple splitting, amounting to only a few cm^{-1}, or of much weaker satellite absorptions near the major peak. Such structure may result from the occurrence of multiple trapping sites or from the contributions of residual molecular aggregates or of individual isotopic species.

As is shown by Fig. 2, which compares the band centers of the 69 transitions of diatomic and polyatomic transient molecules which have been reported with a precision of 1 cm^{-1} or better both in solid neon and in the gas phase, vibrational frequencies characteristic of the neon matrix usually correspond very closely to the gas-phase band centers. For many systems, argon matrix observations, which can conveniently be conducted using closed-cycle refrigeration systems, are almost as satisfactory. Fig. 3 shows a similar comparison for the 109

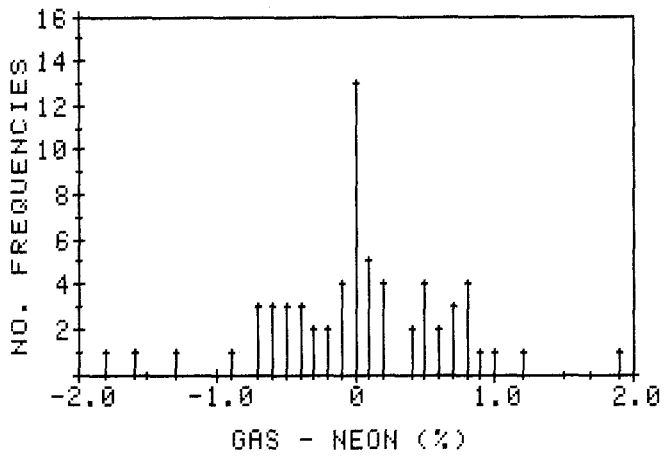

FIG. 2. Comparison of ground-state vibrational frequencies reported for transient molecules (2–16 atoms) in a neon matrix with corresponding values obtained from gas-phase measurements.

Beyond scale of plot:	XeF		−11.1%
	$C_6HF_5^+$	(ν_{10})	−3.6%
	$C_6F_6^+$	(ν_{17})	−2.7%
	SiC_2	(ν_2)	2.8%

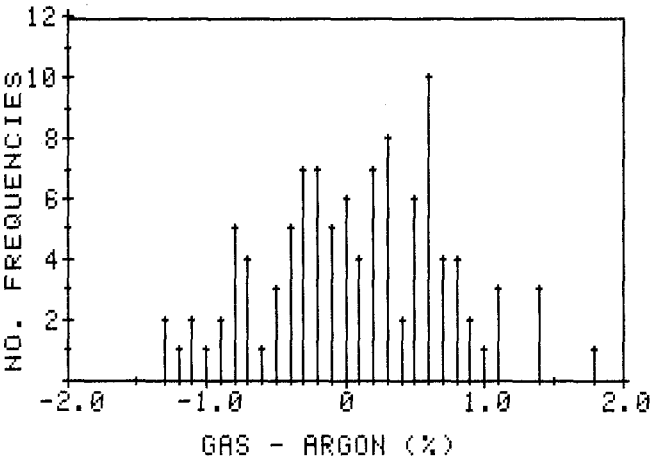

FIG. 3. Comparison of ground-state vibrational frequencies reported for transient molecules (2–16 atoms) in an argon matrix with corresponding values obtained from gas-phase measurements.

Beyond scale of plot:	$C_6F_6^+$	(ν_{17})	−9.4%
		(ν_{18})	−5.6%
	$C_6HF_5^+$	(ν_{11})	−2.5%

vibrational transitions of diatomic and polytomic transient molecules for which data are available from both gas-phase and argon-matrix observations. In approximately 90% of the argon-matrix observations correspondence is within ±1%, and for only 3 transitions is the agreement poorer than 2%. Krypton and xenon are relatively infrequently used as matrix materials, both because of their cost and because they tend to yield highly optically scattering samples. Comparison of krypton-matrix and gas-phase band centers for diatomic molecules[7] suggests that for covalently bonded species perturbations are similar in magnitude to those characteristic of the argon matrix. Because of the size of substitutional sites in the xenon lattice, small molecules may be less effectively isolated in this medium. As is shown in Fig. 4, the correspondence between gas-phase and nitrogen-matrix observations, for which data on 32 transitions are available, is somewhat less satisfactory. In part, the greater deviations may be attributed to the potential of nitrogen for hydrogen-bonding interaction.

Several types of spectral perturbation are important for molecular ions isolated in matrices. While vibrations associated with covalent bonds generally are relatively little perturbed by isolation of the species in neon or argon, ionic bonds may experience a much larger perturbation[7]. Because charge transfer interaction of the ion in its excited electronic state with argon and the heavier rare

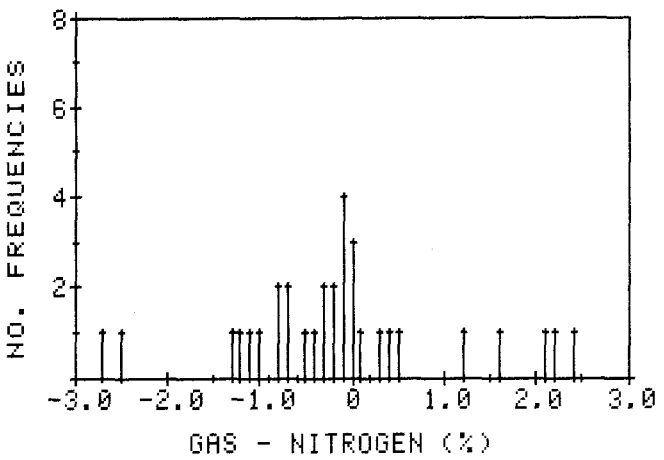

FIG. 4. Comparison of ground-state vibrational frequencies reported for transient molecules (2–16 atoms) in a nitrogen matrix with corresponding values obtained from gas-phase measurements.

gases may greatly distort its fluorescence spectrum,[8,9] neon is the preferred matrix material. Very recent studies[10] suggest that there may be a significant matrix perturbation of the Jahn-Teller splitting of degenerate energy levels even in solid neon. The unusually large deviations shown in Figs. 2 and 3 for $C_6F_6^+$ in neon and argon matrices can be attributed to this phenomenon. Infrared spectra have been reported for a number of molecular anions isolated in rare-gas matrices. Often, these anions are produced by spontaneous or photoinduced charge transfer interaction with an alkali metal atom. Usually, the absorption frequencies have a small dependence on the nature of the cation. Because of its relatively low ionization potential and relatively large size, cesium frequently has been found to perturb the anion somewhat less than do other metal atom electron donors. With few exceptions, degenerate vibrations are substantially split by the electric field of the cation, a phenomenon which has been studied for the infrared spectra of the matrix-isolated vapors of various metal salts by Devlin and co-workers[11–13]. This and other perturbations charactistic of the spectra of molecular anions formed by metal salt-molecule reactions in an argon matrix have been reviewed by Ault[14,15].

4. Guide to the Compilation

The following tables summarize experimentally determined ground-state vibrational energy levels for approximately 480 covalently bonded transient molecules observed in the gas phase or in various atomic or small molecule matrices. Studies using larger molecule matrices such as hydrocarbon glasses or alkali halide pellets are not included. The literature through June 1984 has been surveyed; only a few more recent additions have been possible. While much effort has been expended to provide a comprehensive compilation, certainly omissions will be discovered. The author invites communication of additions and revisions for inclusion in later editions of or supplements to this compilation.

It is the purpose of this review to bring together spectroscopic data for species which cannot readily be studied using conventional sampling techniques. In view of the availability of commercial instrumentation for the study of the photoelectron spectra of stable molecules, the criterion for the inclusion of photoelectron spectroscopic data in this compilation is that the species for which the photoelectron spectrum is studied itself be a transient molecule. Standard works such as those by Turner and co-workers[16] and by Rabalais[17] provide a wealth of information on the photoelectron spectra of small, stable molecules. More recent compilations including photoelectron spectroscopic data have been published by Kimura and co-workers[18] and by Levin and Lias[19].

Attempts have been made to provide a critically evaluated compilation. This is especially difficult for transient molecules, since often only a single set of observations has been reported. As newly developed techniques are applied and additional data become available, it is hoped that later versions of this compilation can be more definitive. Data have been omitted when later studies dictate reassignment and when the transient molecule identification is purely circumstantial. Included in thise catagory are identifications based solely on characteristic group frequencies or on vibrational spectra derived from either semiempirical or ab initio molecular orbital calculations. Because of the large difference in sensitivity between electron spin resonance and optical spectroscopic measurements, it is difficult to correlate observations in these two types of experimental system. Arguments supporting specific assignments generally are contained in the references cited. Isotopic substitution studies have been extremely valuable for obtaining definitive definitive identifications and assignments in both gas-phase and matrix isolation studies.

For molecules with from three to eight atoms, the order of appearance in the compilation is similar to that adopted by Herzberg[1]; the first criterion is the number of atoms in the molecule, the second is the number of hydrogen atoms, and the third is the number of valence electrons. Except for chain structures, it is generally possible to choose a central atom. When all three of these criteria match, the order of appearance in the compilation is that of the number of valence electrons on this central atom followed by its row in the Periodic Table. For molecules with more than eight atoms, families of related species (e.g., increasing methyl substitution in the silaethylenes) become increasingly important. Therefore, for these larger molecules the first determinant is the elemental composition, followed by molecular complexity. Because of the close relationships of carbon-halogen bonds to carbon-hydrogen bonds, halogen substitution is treated as a subset to other types of atomic substitution. Thus, boron compounds appear first, followed by halogen-substituted hydrocarbons and, successively, hydrogen- and halogen-substituted molecules in which silicon, nitrogen, phosphorus, oxygen, and sulfur are present. For convenience, an index is also provided. Vibrational data are given both for the normal and the fully deuterium-substituted molecule. Since the table for the deuterated species appears immediately after that for the unsubstituted molecule, only the hydrogen-containing species is listed in the index.

The heading for each molecule gives, as available, the symmetry of the ground electronic state, the symmetry of the molecule, and key references to the determination of its ground-state structure. Microwave and high resolution optical spectroscopy generally provide the most precise structural data, but estimates from molecular orbital calculations are often sufficiently precise for modelling molecular behavior.

Where feasible, vibrational assignments have been given. The convention in which the x axis is chosen perpendicular to the plane of the molecule, recommended by the Joint Commision for Spectroscopy of IAU and IUPAP[20], has been adopted. Frequently, this has required the interchange of assignments given in the literature for b_1 and b_2 vibrations of molecules with C_{2v} symmetry.

Since observations on transient molecules usually are not sufficiently extensive to permit derivation of anharmonic constants, the frequency values are uniformly given as $\Delta G(\frac{1}{2})$, except when the value of zero is within the range of uncertainty of $\omega_e x_e$.

For some systems, high resolution gas-phase data have been obtained with frequency accuracies of the order of 10^{-3} cm^{-1}. Such data have been rounded off at the second decimal place in the tables. Where no decimal places are given, accuracies are generally ± 1 cm^{-1} (± 2 cm^{-1} for matrix isolation observations between 2000 and 4000 cm^{-1}) unless other uncertainties are cited in footnotes. Where feasible, relative intensities have been estimated for infrared absorptions (vw—very weak; w—weak; m—medium; s—strong; vs—very strong). Antisymmetric vibrations are designated by the abbreviations "a-" or "asym."

5. Abbreviations

DL	Diode laser
ED	Electron diffraction
EF	Electron-excited fluorescence
ESR	Electron spin resonance
IR	Infrared absorption (conventional or Fourier transform)
LDF	Laser difference frequency
LF	Laser-excited fluorescence
LMR	Laser magnetic resonance
LSS	Laser Stark spectroscopy
MO	Molecular orbital calculations
MW	Microwave
PD	Electron photodetachment
PE	Photoelectron spectroscopy
PIR	Photoionization resonance
Ram	Raman
UV	Visible-ultraviolet absorption and emission
VMA	Velocity-modulated infrared absorption

6. Tables

6.1. H_3^+ and Triatomic Dihydrides

H_3^+ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Ring breathing	3185[a]	gas	MO	[3]
e'	2	Deformation	2521.6	gas	LDF	[1]

D_3^+

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Ring breathing	2307[a]	gas	MO	[3]
e'	2	Deformation	1826.4[b]	gas	MO	[2][3]

[a] Ab initio calculation [3] of gas-phase band center; calculated value of ν_2 of H_3^+ is 2516 cm^{-1}, in good agreement with observed value. Further support is provided by observation of ν_1 of H_2D^+ at 2992.486 cm^{-1} [4] and of ν_1 of D_2H^+ at 2736.997 cm^{-1} [5].

[b] Ab initio calculation [3] of gas-phase band center; calculated rotational structure for ν_2 of D_3^+ agrees within 9 cm^{-1} with that observed using Doppler-tuned fast-ion-beam laser spectroscopy [2].

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CH_2 $^3B_1$ C_{2v} Structure: ESR [1]-[3] UV [4] MW, IR [7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	963.10	gas	LMR, DL	[5][6] [8]

CD_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	752.37	gas	DL	[8]

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SiH_2 $^1A_1$ C_{2v} Structure: UV [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	2032vw	Ar	IR	[2]
	2	Bend	~1004	gas	UV	[1]
			990[a]	gas	LF	[3]
			1008w	Ar	IR	[2]
b_2	3	Asym. stretch	2022w	Ar	IR	[2]

SiD_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1472w	Ar	IR	[2]
	2	Bend	729m	Ar	IR	[2]
b_2	3	Asym. stretch	1468m	Ar	IR	[2]

[a] $\pm$ 20 cm^{-1}.

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GeH_2 C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		GeH stretch	1887wm	Ar	IR	[1]
		GeH stretch	1864wm	Ar	IR	[1]
		Bend	920wm	Ar	IR	[1]

GeD_2

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

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NH_2^+ $^3B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	840[a]	gas	PE	[1]

ND_2^+

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

[a] $\pm$ 50 cm^{-1}.

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SiH_2^-

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	Bend	1200[a]	gas	PE	[1]

[a] $\pm$ 160 cm^{-1}.

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NH_2 $^2B_1$ C_{2v} Structure: UV [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	3219.37	gas	LF,UV, LDF	[3][8] [9]
			3220w[a]	N_2	IR	[2]
	2	Bend	1497.32	gas	UV,LMR	[1][4] [5][7]
			1499m	N_2	IR	[2]
b_2	3	Asym. stretch	3301.11	gas	LDF	[9]

ND_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	1108.75	gas	LMR	[6]
			1110m	N_2	IR	[2]

[a] Assigned in [2] to ν_3. Gas-phase observation of ν_1 at 3219.36 cm^{-1} and demonstration [9] that ν_1 is more intense than ν_3 dictate reassignment to ν_1.

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PH_2 $^2B_1$ C_{2v} Structure: UV [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	2270[a]	gas	PE	[2]
	2	Bend	1101.91	gas	UV,LMR	[1][4]
			1103m	Ar	IR	[3]

PD_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	797w	Ar	IR	[3]

[a] $\pm$ 80 cm^{-1}.

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H_2O^+ $^2B_1$ C_{2v} Structure: UV [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	1408.4	gas	UV	[1]

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H_2F^+ C_{2v} Structure: VMA [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	3348.71	gas	VMA	[1][2]
b_2	3	Asym. stretch	3334.69	gas	VMA	[1][2]

References

[1] E. Schafer and R. J. Saykally, J. Chem. Phys. 80, 2973 (1984).

[2] E. Schafer and R. J. Saykally, J. Chem. Phys. (in press).

6.2. Triatomic Monohydrides

HBS^+ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	BS stretch	955[a]	gas	PE	[1][2]

[a] ± 40 cm^{-1}.

References

[1] T. P. Fehlner and D. W. Turner, J. Am. Chem. Soc. 95, 7175 (1973).

[2] H. W. Kroto, R. J. Suffolk, and N. P. C. Westwood, Chem. Phys. Lett. 22, 495 (1973).

HCC $C_{\infty v}$ Structure: ESR [2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3612m	Ar	IR	[3]
	3	CC stretch	1848m	Ar	IR	[1][3]

DCC

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2800m	Ar	IR	[3]
	3	CC stretch	1748m	Ar	IR	[1][3]

References

[1] D. E. Milligan, M. E. Jacox, and L. Abouaf-Marguin, J. Chem. Phys. 46, 4562 (1967).

[2] W. R. M. Graham, K. I. Dismuke, and W. Weltner, Jr., J. Chem. Phys. 60, 3817 (1974).

[3] M. E. Jacox, Chem. Phys. 7, 424 (1975).

HCP^+ $^2\Pi_i$ $C_{\infty v}$ Structure: UV [2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3120[a]	gas	EF	[3]
	3	C≡P stretch	1150[a]	gas	EF	[1][2]

DCP^+

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2355[a]	gas	EF	[3]
	3	C≡P stretch	1110[a]	gas	EF	[1][2]

[a] ± 10 cm^{-1}.

References

[1] M. A. King, H. W. Kroto, J. F. Nixon, D. Klapstein, J. P. Maier, and O. Marthaler, Chem. Phys. Lett. 82, 543 (1981).

[2] M. A. King, D. Klapstein, H. W. Kroto, J. P. Maier, and J. F. Nixon, J. Mol. Struct. 80, 23 (1982).

[3] M. A. King, D. Klapstein, H. W. Kroto, R. Kuhn, and J. P. Maier, XVI Internat. Symp. on Free Radicals, Lauzelle-Ottignies, Belgium (1983).

$HN^{11}B$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NH stretch	3675m	Ar	IR	[1]
	3	NB stretch	2035s	Ar	IR	[1]

$DN^{11}B$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	ND stretch	2770m	Ar	IR	[1]
	3	NB stretch	1963s	Ar	IR	[1]

References

[1] E. R. Lory and R. F. Porter, J. Am. Chem. Soc. 95, 1766 (1973).

$H^{11}BO$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	754m	Ar	IR	[1]
Σ^+	3	BO stretch	1817s	Ar	IR	[1]

$D^{11}BO$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BD stretch	2259w	Ar	IR	[1]
Π	2	Bend	606m	Ar	IR	[1]
Σ^+	3	BO stretch	1648m	Ar	IR	[1]

References

[1] E. R. Lory and R. F. Porter, J. Am. Chem. Soc. 93, 6301 (1971).

$H^{11}BS$ $C_{\infty v}$ Structure: MW [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BH stretch	2735.80	gas	IR	[2]
	3	BS stretch	1172.39	gas	IR	[3]

$D^{11}BS$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	BD stretch	2077.71	gas	IR	[3]
	3	BS stretch	1119.98[a]	gas	IR	[3]

[a] In Fermi resonance with $2\nu_2$, at 1098.60 cm^{-1}.

References

[1] E. F. Pearson and V. McCormick, J. Chem. Phys. 58, 1619 (1973).

[2] A. G. Maki and R. L. Sams, J. Mol. Struct. 26, 107 (1975).

[3] P. Turner and I. M. Mills, Mol. Phys. 46, 161 (1982).

HCO^+ $C_{\infty v}$ Structure: MW [2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3088.74	gas	VMA,LDF	[3][4]
Π	2	Bend	760[a]	gas	PE	[1]
Σ^+	3	CO stretch	2183.95	gas	DL	[5]

DCO^+

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	620[a]	gas	PE	[1]
Σ^+	3	CO stretch	1904.06	gas	DL	[6]

[a] $\pm$ 30 cm^{-1}.

References

[1] J. M. Dyke, N. B. H. Jonathan, A. Morris, and M. J. Winter, Mol. Phys. 39, 629 (1980).

[2] R. C. Woods, R. J. Saykally, T. G. Anderson, T. A. Dixon, and P. G. Szanto, J. Chem. Phys. 75, 4256 (1981).

[3] C. S. Gudeman, M. H. Begemann, J. Pfaff, and R. J. Saykally, Phys. Rev. Lett. 50, 727 (1983).

[4] T. Amano, J. Chem. Phys. 79, 3595 (1983).

[5] S. C. Foster, A. R. W. McKellar, and T. J. Sears, J. Chem. Phys. 81, 578 (1984).

[6] S. C. Foster and A. R. W. McKellar, J. Chem. Phys. (in press).

HNC $C_{\infty v}$ Structure: MW [4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NH stretch	3652.66	gas	IR	[3][5]
			3620s	Ar	IR	[2]
			3583s	Ar[a]	IR	[1][2]
			3567s	N_2	IR	[2]
Π	2	Bend	477s	Ar	IR	[2]
			535s	Ar[a]	IR	[1]
			559s	N_2	IR	[2]
Σ^+	3	NC stretch	2029w	Ar	IR	[2]
			2032w	Ar[a]	IR	[1]
			2035w	N_2	IR	[2]

DNC

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	ND stretch	2787.07	gas	IR	[3][5]
			2769s	Ar	IR	[2]
			2733s	Ar[a]	IR	[1]
			2728s	N_2	IR	[2]

DNC---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	374s	Ar	IR	[2]
			413s	Ar[a]	IR	[1]
			432s	N_2	IR	[2]
Σ^+	3	NC stretch	1940w	Ar	IR	[2]
			1940w	Ar[a]	IR	[1]
			1937w	N_2	IR	[2]

[a] N_2 trapped in adjacent site.

References

[1] D. E. Milligan and M. E. Jacox, J. Chem. Phys. 39, 712 (1963).

[2] D. E. Milligan and M. E. Jacox, J. Chem. Phys. 47, 278 (1967).

[3] C. A. Arrington and E. A. Ogryzlo, J. Chem. Phys. 63, 3670 (1975).

[4] E. F. Pearson, R. A. Creswell, M. Winnewisser, and G. Winnewisser, Z. Naturforsch. 31a, 1394 (1976).

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HNSi $C_{\infty v}$

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

DNSi

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

References

[1] J. F. Ogilvie and S. Cradock, Chem. Commun. 364 (1966).

HN_2^+ $C_{\infty v}$ Structure: MW [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NH stretch	3233.95	gas	VMA	[2]
	3	NN stretch	2257.87	gas	DL	[3]

DN_2^+

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	ND stretch	2636.98	gas	VMA	[4]
	3	NN stretch	2024.01	gas	DL	[3]

References

[1] P. G. Szanto, T. G. Anderson, R. J. Saykally, N. D. Piltch, T. A. Dixon, and R. C. Woods, J. Chem. Phys. 75, 4261 (1981).

[2] C. S. Gudeman, M. H. Begemann, J. Pfaff, and R. J. Saykally, J. Chem. Phys. 78, 5837 (1983).

[3] S. C. Foster and A. R. W. McKellar, J. Chem. Phys. (in press).

[4] D. J. Nesbitt, H. Petek, C. S. Gudeman, C. B. Moore, and R. J. Saykally, J. Chem. Phys. (in press).

HCO $^2A'$ C_s Structure: MW[5] UV[6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	CH stretch	2483m	Ar	IR	[4]
			2488m	CO	IR	[3]
	2	Bend	1080.76	gas	UV,LSS, LMR	[1][7] [8]
			1087s	Ar	IR	[4]
			1090s	CO	IR	[2][3]
	3	CO stretch	1868.17	gas	IR,LMR	[9][10]
			1863vs	Ar	IR	[4]
			1861vs	CO	IR	[2][3]

DCO

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	CD stretch	1909.77	gas	LMR	[11]
			1926s	Ar	IR	[4]
			1937s	CO	IR	[3]

DCO---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	Bend	847.4	gas	UV	[1]
			850s	Ar	IR	[4]
			852s	CO	IR	[2][3]
	3	CO stretch	1794.59	gas	LMR	[11]
			1803m	Ar	IR	[4]
			1800m	CO	IR	[2][3]

References

[1] J. W. C. Johns, S. H. Priddle, and D. A. Ramsay, Discuss. Faraday Soc. 35, 90 (1963).

[2] G. E. Ewing, W. E. Thompson, and G. C. Pimentel, J. Chem. Phys. 32, 927 (1960).

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[11] R. S. Lowe and A. R. W. McKellar, J. Chem. Phys. 74, 2686 (1981).

HCF^+ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′		CF stretch	1368m	Ar	IR	[1]

DCF^+

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′		CF stretch	1369m	Ar	IR	[1]

References

[1] L. Andrews and F. T. Prochaska, J. Chem. Phys. 70, 4714 (1979).

HCF $^1A'$ C_s Structure: UV [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	2	Bend	1406.87	gas	UV,LF	[1][3]
			1406vw	Ar	IR	[2]
	3	CF stretch	1181.5m	Ar	IR	[2]

DCF

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

References

[1] A. J. Merer and D. N. Travis, Can. J. Phys. 44, 1541 (1966).

[2] M. E. Jacox and D. E. Milligan, J. Chem. Phys. 50, 3252 (1969).

[3] K. Hakuta, J. Mol. Spectrosc. 106, 56 (1984).

HCCl $^1A'$ C_s Structure: UV [1]; LF [3]

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

DCCl

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

References

[1] A. J. Merer and D. N. Travis, Can. J. Phys. 44, 525 (1966).

[2] M. E. Jacox and D. E. Milligan, J. Chem. Phys. 47, 1626 (1967).

[3] M. Kakimoto, S. Saito, and E. Hirota, J. Mol. Spectrosc. 97, 194 (1983).

HSiF C_s

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

DSiF

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

References

[1] Z. K. Ismail, L. Fredin, R. H. Hauge, and J. L. Margrave, J. Chem. Phys. 77, 1626 (1982).

[2] H. U. Lee and J. P. Deneufville, Chem. Phys. Lett. 99, 394 (1983).

HSiCl $^1A'$ C_s Structure: UV [1]

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

References

[1] G. Herzberg and R. D. Verma, Can. J. Phys. 42, 395 (1964).

HSiBr $^1A'$ C_s Structure: UV [1]

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

References

[1] G. Herzberg and R. D. Verma, Can. J. Phys. 42, 395 (1964).

HSiI $^1A'$ C_s Structure: UV [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	Bend	727	gas	UV	[1]

References

[1] J. Billingsley, Can. J. Phys. 50, 531 (1972).

HGeCl C_s

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

DGeCl

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

References

[1] R. J. Isabel and W. A. Guillory, J. Chem. Phys. 55, 1197 (1971).

[2] R. I. Patel and G. W. Stewart, Can. J. Phys. 55, 1518 (1977).

HGeBr C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	GeH stretch	1858vs	Ar	IR	[1]
	2	Bend	701m	Ar	IR	[1]
	3	GeBr stretch	283s	Ar	IR	[1]

DGeBr

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

References

[1] R. J. Isabel and W. A. Guillory, J. Chem. Phys. 57, 1116 (1972).

HNO $^1A'$ C_s Structure: UV [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	NH stretch	2683.95	gas	IR	[3][5]
			2716wm	Ar	IR	[2]
			2756m	N_2	IR	[2]
	2	Bend	1500.82	gas	LSS	[4]
			1505w	Ar	IR	[2]
			1511w	N_2	IR	[2]
	3	NO stretch	1565.34	gas	LSS	[4]
			1563vs	Ar	IR	[2]
			1568.5s	N_2	IR	[2]

DNO

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	ND stretch	2025.14	gas	LSS,IR	[4][5]
			2043w-m	Ar	IR	[2]
			2074m	N_2	IR	[2]
	2	Bend	1153s	Ar	IR	[2]
			1158.5m	N_2	IR	[2]
	3	NO stretch	1546.88	gas	LSS	[4]
			1547vs	Ar	IR	[2]
			1548vs	N_2	IR	[2]

References

[1] F. W. Dalby, Can. J. Phys. 36, 1336 (1958).

[2] M. E. Jacox and D. E. Milligan, J. Mol. Spectrosc. 48, 536 (1973).

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[4] J. W. C. Johns and A. R. W. McKellar, J. Chem. Phys. 66, 1217 (1977).

[5] J. W. C. Johns, A. R. W. McKellar, and E. Weinberger, Can. J. Phys. 61, 1106 (1983).

HPO $^1A'$ C_s Structure: UV [3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	PH stretch	2095m-s	Ar	IR	[2]
	2	Bend	983	gas	UV	[1]
	3	PO stretch	1179	gas	UV	[1]
			1188s	Ar	IR	[2]

DPO

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	PD stretch	1530m	Ar	IR	[2]
	2	Bend	745	gas	UV	[1]
			750w	Ar	IR	[2]
	3	PO stretch	1177	gas	UV	[1]
			1186s	Ar	IR	[2]

References

[1] M. Lam Thanh and M. Peyron, J. Chim. Phys. 60, 1289 (1963).

[2] M. Larzilliere and M. E. Jacox, J. Mol. Spectrosc. 79, 132 (1980).

[3] M. Larzilliere, N. Damany, and M. Lam Thanh, Chem. Phys. 46, 401 (1980).

HO_2^+ $^3A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	3	OO stretch	1560[ab]	gas	PE	[1]

DO_2^+

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	3	OO stretch	1595[ac]	gas	PE	[1]

[a] $\pm$ 50 cm^{-1}.

[b] ω_e; $\omega_e x_e$ = 15 $\pm$ 20 cm^{-1}.

[c] ω_e; $\omega_e x_e$ = 25 $\pm$ 10 cm^{-1}.

References

[1] J. M. Dyke, N. B. H. Jonathan, A. Morris, and M. J. Winter, Mol. Phys. 44, 1059 (1981).

HNO^- C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′		NO stretch	1153[a]	gas	PE	[1]

DNO^-

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′		NO stretch	1113[a]	gas	PE	[1]

[a] ± 170 cm^{-1}.

References

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

HNF $^2A''$ C_s Structure: UV [2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	2	Bend	1419.3	gas	UV	[3]
			1432m	Ar	IR	[1]
	3	NF stretch	1000s	Ar	IR	[1]

DNF

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

[a] Overlapped by NF_2 absorption.

References

[1] M. E. Jacox and D. E. Milligan, J. Chem. Phys. 46, 184 (1967).

[2] C. M. Woodman, J. Mol. Spectrosc. 33, 311 (1970).

[3] D. M. Lindsay, J. L. Gole, and J. R. Lombardi, Chem. Phys. 37, 333 (1979).

HO_2 $^2A''$ C_s Structure: MW [5][6]
LMR [4][12]
UV [7][9][10]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	OH stretch	3436.20	gas	LDF	[14]
			3414s	Ar	IR	[1]-[3]
	2	Bend	1391.75	gas	DL	[13]
			1389vs	Ar	IR	[1]-[3]
	3	OO stretch	1097.63	gas	LMR	[8]
			1101s	Ar	IR	[1]-[3]

DO_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	OD stretch	2549.22	gas	LDF	[15]
			2530m	Ar	IR	[1]-[3]
	2	Bend	1120.2	gas	LMR	[11]
			1123vw	Ar	IR	[3]
	3	OO stretch	1020.16	gas	LMR	[11]
			1020s	Ar	IR	[1]-[3]

References

[1] D. E. Milligan and M. E. Jacox, J. Chem. Phys. 38, 2627 (1963).

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[15] K. G. Lubic and T. Amano, 38th Symposium on Molecular Spectroscopy, Columbus, Ohio, June 1983.

HSO $^2A''$ C_s Structure: UV [1]–[3] MW [4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	2	Bend	1063[a]	gas	UV	[1]
	3	SO stretch	1009.36	gas	LMR	[5]

DSO

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	2	Bend	770[b]	gas	UV	[1]
	3	SO stretch	1030[c]	gas	UV	[1]

[a] ± 5 cm^{-1}.

[b] ± 10 cm^{-1}.

[c] ± 15 cm^{-1}.

References

[1] U. Schurath, M. Weber, and K. H. Becker, J. Chem. Phys. 67, 110 (1977).

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FHF^- $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π_u	2	Bend	1217m	Ar[a]	IR	[1][2]
Σ_u^+	3	Asym. stretch	1377.0s	Ar	IR	[3]
			1364vs	Ar[a]	IR	[1][2]

FDF^-

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	965.5s	Ar	IR	[3]
			969vs	Ar[a]	IR	[1][2]

[a] Cs^+ in adjacent site.

References

[1] B. S. Ault, J. Phys. Chem. 82, 844 (1978).

[2] B. S. Ault, J. Phys. Chem. 83, 837 (1979).

[3] S. A. McDonald and L. Andrews, J. Chem. Phys. 70, 3134 (1979).

$FHCl^-$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	"Asym." stretch	933[a]	Ar	IR	[1]

$FDCl^-$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	"Asym." stretch	668[a]	Ar	IR	[1]

[a] Cs^+ in adjacent site.

References

[1] B. S. Ault, J. Phys. Chem. 83, 837 (1979).

$FHBr^-$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	"Asym." stretch	849[a]	Ar	IR	[1]

$FDBr^-$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	"Asym." stretch	609[a]	Ar	IR	[1]

[a] Cs^+ in adjacent site.

References

[1] B. S. Ault, J. Phys. Chem. 83, 837 (1979).

FHI^- $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	"Asym." stretch	763[a]	Ar	IR	[1]

FDI^-

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	"Asym." stretch	548[a]	Ar	IR	[1]

[a] Cs^+ in adjacent site.

References

[1] B. S. Ault, J. Phys. Chem. 83, 837 (1979).

$ClHCl^-$ $D_{\infty h}$

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	696s[a]	Ar	IR	[1]-[3]

$ClDCl^-$

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

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

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

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

References

[1] P. N. Noble and G. C. Pimentel, J. Chem. Phys. 49, 3165 (1968).

[2] D. E. Milligan and M. E. Jacox, J. Chem. Phys. 53, 2034 (1970).

[3] C. A. Wight, B. S. Ault, and L. Andrews, J. Chem. Phys. 65, 1244 (1976).

[4] M. Kneba and J. Wolfrum, J. Phys. Chem. 83, 69 (1979).

$ClHBr^-$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	"Asym." stretch	742[a]	Ar	IR	[1]

$ClDBr^-$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	"Asym." stretch	524[a]	Ar	IR	[1]

[a] Cs^+ in adjacent site.

References

[1] B. S. Ault and L. Andrews, J. Chem. Phys. 64, 1986 (1976).

$ClHI^-$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	"Asym." stretch	644[a]	Ar	IR	[1]

$ClDI^-$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	"Asym." stretch	456[a]	Ar	IR	[1]

[a] Cs^+ in adjacent site.

References

[1] C. M. Ellison and B. S. Ault, J. Phys. Chem. 83, 832 (1979).

$BrHBr^-$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	164[ab]	Ar	IR	[1][2]
Σ_u^+	3	Asym. stretch	728s[a]	Ar	IR	[1][2]

$BrDBr^-$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	170[ac]	Ar	IR	[1][2]
Σ_u^+	3	Asym. stretch	498s[a]	Ar	IR	[1][2]

[a] Attributed in [1] to the uncharged species. Reassigned to the anion by [2]. See $ClHCl^-$.

[b] Assignment deduced from combinations of this fundamental and of its first overtone with the 728 cm^{-1} fundamental which appear at 892 and 1053 cm^{-1}, respectively.

[c] Assignment deduced from moderately intense combination with 498 cm^{-1} fundamental that appears at 668 cm^{-1}.

References

[1] V. Bondybey, G. C. Pimentel, and P. N. Noble, J. Chem. Phys. 55, 540 (1971).

[2] D. E. Milligan and M. E. Jacox, J. Chem. Phys. 55, 2550 (1971).

$BrHI^-$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	"Asym." stretch	666[a]	Ar	IR	[1]

$BrDI^-$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	"Asym." stretch	470[a]	Ar	IR	[1]

[a] Cs^+ in adjacent site.

References

[1] C. M. Ellison and B. S. Ault, J. Phys. Chem. 83, 832 (1979).

IHI^- $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	121[ab]	Ar	IR	[1][2]
Σ_u^+	3	Asym. stretch	682m[a]	Ar	IR	[1][2]

IDI^-

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

[a] Attributed in [1] to the uncharged species. Reassigned by [2] to the anion. See $ClHCl^-$.

[b] Assignment deduced from combinations of this fundamental and of its first overtone with the 682 cm^{-1} fundamental which appear at 803 and 923 cm^{-1}, respectively.

[c] Assignment deduced from combination with 470 cm^{-1} fundamental that appears at 594 cm^{-1}.

References

[1] P. N. Noble, J. Chem. Phys. 56, 2088 (1972).

[2] C. M. Ellison and B. S. Ault, J. Phys. Chem. 83, 832 (1979).

HAr_2^+ [a] $D_{\infty h}$

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

DAr_2^+

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	644s[b]	Ar	IR	[1]-[4]

[a] May be complexed with two or four additional Ar atoms [2].

[b] Assigned in [1] to vibration of uncharged H (or D) atoms trapped in the Ar lattice. Reassigned by [2] to the cation. Peak at 644 cm^{-1} was prominent in deuteron radiolysis experiments [3], and [4] demonstrated that the absorptions did not appear when H or D atoms were present but a supplementary high energy source suitable for inducing photoionization or electron transfer was not.

References

[1] V. E. Bondybey and G. C. Pimentel, J. Chem. Phys. 56, 3832 (1972).

[2] D. E. Milligan and M. E. Jacox, J. Mol. Spectrosc. 46, 460 (1973).

[3] L. Andrews, B. S. Ault, J. M. Grzybowski, and R. O. Allen, J. Chem. Phys. 62, 2461 (1975).

[4] C. A. Wight, B. S. Ault, and L. Andrews, J. Chem. Phys. 65, 1244 (1976).

HKr_2^+ [a] $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	852m [b]	Kr	IR	[1]–[3]

DKr_2^+ [a]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	607m [b]	Kr	IR	[1]

[a] May be complexed with two or four additional Kr atoms [2].

[b] Assigned in [1] to vibration of uncharged H (or D) atoms trapped in the Kr lattice. Reassigned by [2] to the cation, and [3] demonstrated that the 852 cm^{-1} absorption did not appear when H atoms were present but a supplementary high energy source suitable for inducing photoionization or electron transfer was not.

References

[1] V. E. Bondybey and G. C. Pimentel, J. Chem. Phys. 56, 3832 (1972).

[2] D. E. Milligan and M. E. Jacox, J. Mol. Spectrosc. 46, 460 (1973).

[3] C. A. Wight, B. S. Ault, and L. Andrews, J. Chem. Phys. 65, 1244 (1976).

6.3. Triatomic Nonhydrides

C_3 $^1\Sigma_g^+$ $D_{\infty h}$ Structure: UV [1][4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1224.5	gas	UV	[5]
			1226	Ne	UV	[3]
Π_u	2	Bend	63	gas	UV	[4]
			~70 [a]	Ne,Ar	UV	[3]
Σ_u^+	3	Asym. stretch	2042	Ne	IR	[2]
			2038s	Ar	IR	[2][6]

[a] Greatly broadened in a rare-gas matrix by interaction with lattice modes [7].

References

[1] L. Gausset, G. Herzberg, A. Lagerqvist, and B. Rosen, Disc. Faraday Soc. 35, 113 (1963).

[2] W. Weltner, Jr., P. N. Walsh, and C. L. Angell, J. Chem. Phys. 40, 1299 (1964).

[3] W. Weltner, Jr., and D. McLeod, Jr., J. Chem. Phys. 40, 1305 (1964).

[4] L. Gausset, G. Herzberg, A. Lagerqvist, and B. Rosen, Astrophys. J. 142, 45 (1965).

[5] A. J. Merer, Can. J. Phys. 45, 4103 (1967).

[6] M. E. Jacox and D. E. Milligan, Chem. Phys. 4, 45 (1974).

[7] V. E. Bondybey and J. H. English, J. Chem. Phys. 68, 4641 (1978).

SiCC $^1A_1$ C_{2v} Structure: PIR [5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CC stretch	1742	gas	UV	[1][3]
			1746s	Ne	IR,LF	[2][4]
	2	CSi s-stretch	852	gas	UV	[3]
			836m	Ne	IR,LF	[2][4]
b_2	3	CSi a-stretch	354 [a]	gas	LF	[4]
			344	Ne	LF	[4]

SiCC---Footnote

[a] In [4] and earlier studies, this vibrational spacing was attributed to the excitation of two quanta of the ground-state bending vibration in the electronic transition, presumed by analogy with C_3 to be A $^1\Pi$ - X $^1\Sigma^+$. The demonstration by [5] that SiCC has C_{2v} symmetry and that the transition is A $^1B_2$ - X $^1A_1$ is consistent with assignment of the 354-cm^{-1} band spacing to a single quantum excitation of the ground-state vibrational fundamental of b_2 symmetry.

References

[1] B. Kleman, Astrophys. J. 123, 162 (1956).

[2] W. Weltner, Jr., and D. McLeod, Jr., J. Chem. Phys. 41, 235 (1964).

[3] R. D. Verma and S. Nagaraj, Can. J. Phys. 52, 1938 (1974).

[4] V. E. Bondybey, J. Phys. Chem. 86, 3396 (1982).

[5] D. L. Michalopoulos, M. E. Geusic, P. R. R. Langridge-Smith, and R. E. Smalley, J. Chem. Phys. 80, 3556 (1984).

Si_2C C_{2v} Structure: IR [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	1189s	Ar	IR	[1]

References

[1] Z. H. Kafafi, R. H. Hauge, L. Fredin, and J. L. Margrave, J. Phys. Chem. 87, 797 (1983).

CCN $^2\Pi$ $C_{\infty v}$ Structure: UV [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Sym. stretch	1060[a]	gas	LF	[3]
			1066	Ar	LF	[2]
Π	2	Bend	230[b]	Ar	LF	[2]
Σ^+	3	Asym. stretch	1917[c]	gas	LF	[3]
			1717	Ar	LF	[2]

CCN---Footnotes

[a] $\pm$ 3 cm^{-1}.

[b] Only sequence bands are seen in gas-phase UV studies [1]; analysis of perturbations suggests that this fundamental lies near 325 cm^{-1}. Reassignment in matrix studies [2] results from detection of 020-000 and 040-000 bands in excitation spectrum of A $^2\Delta$ - X $^2\Pi$ transition.

[c] $\pm$ 10 cm^{-1}.

References

[1] A. J. Merer and D. N. Travis, Can. J. Phys. 43, 1 (1965).

[2] V. E. Bondybey and J. H. English, J. Mol. Spectrosc. 236 (1978).

[3] K. Hakuta and H. Uehara, J. Chem. Phys. 78, 6484 (1983)

CNC $^2\Pi_g$ $D_{\infty h}$ Structure: UV [1]

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

[a] Very large Renner-Teller interaction; A = +26.41, $\epsilon\omega_2$ = +176.20 cm^{-1}. Calculated position of lowest frequency component ($^2\Sigma_u^-$) is 144 cm^{-1}. Moderately intense absorption at 134 cm^{-1} in an argon matrix is tentatively assigned to this transition.

References

[1] A. J. Merer and D. N. Travis, Can. J. Phys. 44, 353 (1966).

[2] M. E. Jacox, J. Mol. Spectrosc. 71, 369 (1978).

CCO $^3\Sigma^-$ $C_{\infty v}$ Structure: UV [2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CO stretch	1967	gas	LF	[4]
			1969s	Ar	IR	[1][3]
			1978	Ar[a]	IR	[1]
			1987	N_2	IR	[1]
Π	2	Bend	379.4	gas	UV	[2]
			381m	Ar	IR	[1]

CCO---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	CC stretch	1063	gas	LF	[4]
			1064w	Ar	IR	[1]
			1074	Ar[a]	IR	[1]
			1077	N_2	IR	[1]

[a] N_2 trapped in adjacent site.

References

[1] M. E. Jacox, D. E. Milligan, N. G. Moll, and W. E. Thompson, J. Chem. Phys. 43, 3734 (1965).

[2] C. Devillers and D. A. Ramsay, Can. J. Phys. 49, 2839 (1971).

[3] R. L. DeKock and W. Weltner, Jr., J. Am. Chem. Soc. 93, 7106 (1971).

[4] W. M. Pitts, V. M. Donnelly, A. P. Baronavski, and J. R. McDonald, Chem. Phys. 61, 451 (1981).

SiCO

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

References

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

NCN $^3\Sigma_g^-$ $D_{\infty h}$ Structure: UV [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1197[a]	Ar	IR	[4]
Π_u	2	Bend	423m	Ar	IR	[2][4]
Σ_u^+	3	Asym. stretch	1475vs	Ar	IR	[2][4]
			1478vs	N_2	IR	[2]-[4]

[a] Frequency deduced from weak combination with 1475 cm^{-1} fundamental which appears at 2672 cm^{-1}.

References

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

[2] D. E. Milligan, M. E. Jacox, and A. M. Bass, J. Chem. Phys. 43, 3149 (1965).

[3] N. G. Moll and W. E. Thompson, J. Chem. Phys. 44, 2684 (1966).

[4] D. E. Milligan and M. E. Jacox, J. Chem. Phys. 45, 1387 (1966).

NCO^+ $^3\Sigma^-$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Sym. stretch	1000[a]	gas	PE	[1]

[a] $\pm$ 30 cm^{-1}.

References

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

CNN $C_{\infty v}$ Structure: ESR [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CN stretch	2824	Ar	LF	[5]
			2847m	Ar[a]	IR	[2]
			2856m	N_2	IR	[2]-[4]
Π	2	Bend	394	Ar	LF	[5]
			393	Ar[a]	IR	[2]
			394	N_2	IR	[3][4]
Σ^+	3	CC stretch	1235	Ar	LF	[5]
			1241	Ar[a]	IR	[2]
			1252	N_2	IR	[2]-[4]

[a] N_2 trapped in adjacent site.

References

[1] E. Wasserman, L. Barash, and W. A. Yager, J. Am. Chem. Soc. 87, 2075 (1965).

[2] D. E. Milligan and M. E. Jacox, J. Chem. Phys. 44, 2850 (1966).

[3] N. G. Moll and W. E. Thompson, J. Chem. Phys. 44, 2684 (1966).

[4] R. L. DeKock and W. Weltner, Jr., J. Am. Chem. Soc. 93, 7106 (1971).

[5] V. E. Bondybey and J. H. English, J. Chem. Phys. 67, 664 (1977).

SiNN

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

References

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

N_3^+ $^3\Sigma^-$ $C_{\infty v}$ Structure: [1]

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

[a] $\pm$ 30 cm^{-1}.

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

References

[1] J. M. Dyke, N. B. H. Jonathan, A. E. Lewis, and A. Morris, Mol. Phys. 47, 1231 (1982).

$^{11}BO_2$ $^2\Sigma_u^+$ $D_{\infty h}$ Structure: UV [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1056.4	gas	UV,LF	[1] [3]-[5]
Π_u	2	Bend	447.4[a]	gas	UV,LF	[1] [3]-[5]
Σ_u^+	3	Asym. stretch	1278.26	gas	DL	[6]
			1276	Ar	IR	[2]

[a] Large Renner-Teller interaction; A = -150.9, $\epsilon\omega_2$ = -86.4 cm^{-1}.

References

[1] J. W. C. Johns, Can. J. Phys. 39, 1738 (1961).

[2] A. Sommer, D. White, M. J. Linevsky, and D. E. Mann, J. Chem. Phys. 38, 87 (1963).

[3] D. K. Russell, M. Kroll, and R. A. Beaudet, J. Chem. Phys. 66, 1999 (1977).

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[5] A. Fried and C. W. Mathews, Chem. Phys. Lett. 52, 363 (1977).

[6] K. Kawaguchi, E. Hirota, and C. Yamada, Mol. Phys. 44, 509 (1981).

$^{11}BS_2$ $^2\Sigma_u$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	510	Ne	UV	[1]
Π_u	2	Bend	~120[a]	Ne	UV	[1]
Σ_u^+	3	Asym. stretch	1015s	Ne	IR	[1]

[a] Estimated from isotope shift in origin of A - X transition.

References

[1] J. M. Brom, Jr., and W. Weltner, Jr., J. Mol. Spectrosc. 45, 82 (1973).

$ClBS^+$ $^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		B=S stretch	1375[a]	gas	PE	[1]

[a] $\pm$ 30 cm^{-1}.

References

[1] C. Kirby, H. W. Kroto, and N. P. C. Westwood, J. Am. Chem. Soc. 100, 3766 (1978).

CCO^-

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1625[a]	gas	PE	[1]

[a] $\pm$ 350 cm^{-1}.

References

[1] J. M. Oakes, M. E. Jones, V. M. Bierbaum, and G. B. Ellison, J. Phys. Chem. 87, 4810-4815 (1983).

NCO $^2\Pi$ $C_{\infty v}$ Structure: UV [1][6] MW [3]-[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Sym. stretch	1270	gas	LF	[9][10]
			1275vw	Ar	IR,LF	[2][7]
Π	2	Bend	535.4[a]	gas	UV,LF	[1][6] [10]
			529.5[b]	Ar	LF	[7]
Σ^+	3	Asym. stretch	1920.61	gas	LMR,LF	[8]-[10]
			1923m	Ar	IR,LF	[2][7]
			1935	N_2	IR	[2]

[a] Very large Renner-Teller interaction; A_{010} = -94.19, $\epsilon\omega_2$ = -76.9 cm^{-1} [6].

[b] Lowest frequency component ($^2\Sigma^+$) contributes a strong infrared absorption at 487 cm^{-1} [2]. Four components ($^2\Sigma^+$, $^2\Delta_{5/2}$, $^2\Delta_{3/2}$, $^2\Sigma^-$) observed at 484, 531, 626, and 672 cm^{-1} in LF experiments [7].

References

[1] R. N. Dixon, Phil. Trans. Roy. Soc. (London) A252, 165 (1960).

[2] D. E. Milligan and M. E. Jacox, J. Chem. Phys. 47, 5157 (1967).

[3] A. Carrington, A. R. Fabris, and N. J. D. Lucas, J. Chem. Phys. 49, 5545 (1968).

[4] S. Saito and T. Amano, J. Mol. Spectrosc. 34, 383 (1970).

[5] T. Amano and E. Hirota, J. Chem. Phys. 57, 5608 (1972).

[6] P. S. H. Bolman, J. M. Brown, A. Carrington, I. Kopp, and D. A. Ramsay, Proc. Roy. Soc. (London) A343, 17 (1975).

[7] V. E. Bondybey and J. H. English, J. Chem. Phys. 67, 2868 (1977).

[8] C. E. Barnes, J. M. Brown, A. D. Fackerell, and T. J. Sears, J. Mol. Spectrosc. 92, 485 (1982).

[9] K. N. Wong, W. R. Anderson, A. J. Kotlar, and J. A. Vanderhoff, J. Chem. Phys. (in press).

[10] R. A. Copeland and D. R. Crosley, Can. J. Phys. (in press).

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	387[a]	gas	UV	[1]
Σ^+	3	CS stretch	~715	gas	UV	[1]

NCS---Footnote

[a] ±10 cm^{-1}. Large Renner-Teller interaction; constants not precisely determined.

References

[1] R. N. Dixon and D. A. Ramsay, Can. J. Phys. 46, 2619 (1968).

CO_2^+ $^2\Pi_g$ $D_{\infty h}$ Structure: UV [1]-[4][7][8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	1280	gas	UV	[3][4] [6]
Π_u	2	Bend	513[a]	gas	UV	[8]
Σ_u^+	3	Asym. stretch	1469[b]	gas	UV	[5]

[a] Large Renner-Teller interaction; A = -159.92, $\epsilon\omega_2$ = -96.8 cm^{-1}.

[b] $(2\nu_3)/2$.

References

[1] S. Mrozowski, Phys. Rev. 60, 730 (1941).

[2] S. Mrozowski, Phys. Rev. 62, 270 (1942).

[3] S. Mrozowski, Phys. Rev. 72, 682 (1947).

[4] S. Mrozowski, Phys. Rev. 72, 691 (1947).

[5] J. W. C. Johns, Can. J. Phys. 42, 1004 (1964).

[6] D. L. Judge, G. S. Bloom, and A. L. Morse, Can. J. Phys. 47, 489 (1969).

[7] D. Gauyacq, M. Horani, S. Leach, and J. Rostas, Can. J. Phys. 53, 2040 (1975).

[8] D. Gauyacq, C. Larcher, and J. Rostas, Can. J. Phys. 57, 1634 (1979).

OCS^+ $^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CS stretch	685	gas	PIR	[2]
Π	2	Bend	417	gas	PIR	[2]
Σ^+	3	CO stretch	2069	gas	UV	[1]

References

[1] M. Horani, S. Leach, J. Rostas, and G. Berthier, J. Chim. Phys. 63, 1015 (1966).

[2] R. Frey, B. Gotchev, W. B. Peatman, H. Pollak, and E. W. Schlag, Int. J. Mass Spectrom. Ion Phys. 26, 137 (1978).

CS_2^+ $^2\Pi_g$ $D_{\infty h}$ Structure: UV [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	617[a]	gas	UV	[2]
			618[a]	Ne	LF	[3][4]
Π_u	2	Bend	348[b]	gas	UV	[2]
			349[b]	Ne	LF	[3][4]
Σ_u^+	3	Asym. stretch	1203[c]	gas	UV	[2]
			1224[c]	Ne	LF	[3][4]

[a] In Fermi resonance with $2\nu_2$.

[b] $(2\nu_2)/2$.

[c] $(2\nu_3)/2$.

References

[1] J. H. Callomon, Proc. Roy. Soc. (London) A244, 220 (1958).

[2] W. J. Balfour, Can. J. Phys. 54, 1969 (1976).

[3] V. E. Bondybey, J. H. English, and T. A. Miller, J. Chem. Phys. 70, 1621 (1979).

[4] V. E. Bondybey and J. H. English, J. Chem. Phys. 73, 3098 (1980).

$BrCN^+$ $^2\Pi$ $C_{\infty v}$ Structure: UV,PE [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+		CBr stretch	509[a]	gas	LF	[2]

[a] ± 16 cm^{-1}.

References

[1] M. Allan and J. P. Maier, Chem. Phys. Lett. 41, 231 (1976).

[2] F. J. Grieman, B. H. Mahan, and A. O'Keefe, J. Chem. Phys. 74, 857 (1981).

FCP^+ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	C≡P stretch	1729[a]	gas	PE,EF	[1][2]
Σ^+	3	CF stretch	765[b]	gas	PE,EF	[1][2]

[a] ± 2 cm^{-1}.

[b] ± 1 cm^{-1}.

References

[1] H. W. Kroto, J. F. Nixon, N. P. C. Simmons, and N. P. C. Westwood, J. Am. Chem. Soc. 100, 446 (1978).

[2] M. A. King, D. Klapstein, H. W. Kroto, R. Kuhn, J. P. Maier, and J. F. Nixon, J. Chem. Phys. 80, 2332 (1984).

N_2O^+ $^2\Pi$ $C_{\infty v}$ Structure: UV [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Sym. stretch	1126.5	gas	UV	[1]
Π	2	Bend	456.8[a]	gas	UV	[1]
Σ^+	3	Asym. stretch	1737.6	gas	UV	[1]

[a] Very large Renner-Teller interaction; $A = -133.59$, $\epsilon\omega_2 = -87.9$ cm^{-1}.

References

[1] J. H. Callomon and F. Creutzberg, Phil. Trans. Roy. Soc. (London) A277, 157 (1974).

$F^{11}BO$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	B=O stretch	2081	Ne	IR	[1]
			2071	Ar	IR	[1]
Π	2	Bend	502	Ne	IR	[1]
			493	Ar	IR	[1]

References

[1] A. Snelson, High Temp. Sci. 4, 141 (1972).

$Cl^{11}BO$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	B=O stretch	1958s	Ar	IR	[1]
	2	Bend	404s	Ar	IR	[1]
	3	BCl stretch	676.04	gas	DL	[2]
			673wm	Ar	IR	[1]

References

[1] A. Snelson, High Temp. Sci. 4, 318 (1972).

[2] K. Kawaguchi, Y. Endo, and E. Hirota, J. Mol Spectrosc. 93, 381 (1982).

$Br^{11}BO$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	B=O stretch	1937vs	Ar	IR	[1]
	2	Bend	374s	Ar	IR	[1]
	3	BBr stretch	535w	Ar	IR	[1]

References

[1] A. Snelson, High Temp. Sci. 4, 318 (1972).

FAlO

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	AlO stretch	1148vs	Ar	IR	[1]
	3	AlF stretch	740s	Ar	IR	[1]

References

[1] H. Schnockel, J. Mol. Struct. 50, 267 (1978).

OAlCl

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	AlO stretch	1094vs	Ar	IR	[1]
	3	AlCl stretch	490m	Ar	IR	[1]

References

[1] H. Schnockel, J. Mol. Struct. 50, 267 (1978).

$O^{69}GaF$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	GaO stretch	943	Ar	IR	[1]
	3	GaF stretch	690	Ar	IR	[1]

References

[1] H. Schnockel and H. J. Gocke, J. Mol. Struct. 50, 281 (1978).

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

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	2	Bend	650[a]	gas	PE	[1]

[a] $\pm$ 30 cm^{-1}.

References

[1] J. M. Dyke, N. Jonathan, A. Morris, and M. J. Winter, J. Chem. Soc., Faraday Trans. 2 77, 667 (1981).

SiO_2 $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	1416	Ar	IR	[1][2]

References

[1] H. Schnockel, Angew. Chem. 90, 638 (1978); Angew. Chem. Int. Ed. Engl. 17, 617 (1978).

[2] H. Schnockel, Z. Anorg. Allg. Chem. 460, 37 (1980).

FNC $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NC stretch	2123w	Ar	IR	[1]
Σ^+	3	NF stretch	928s	Ar	IR	[1]

References

[1] D. E. Milligan and M. E. Jacox, J. Chem. Phys. 47, 278 (1967).

ClNC $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NC stretch	2074s	Ar	IR	[1]
Σ^+	3	NCl stretch	615?	Ar	IR	[1]

References

[1] D. E. Milligan and M. E. Jacox, J. Chem. Phys. 47, 278 (1967).

BrNC $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	NC stretch	2067s	Ar	IR	[1]

References

[1] D. E. Milligan and M. E. Jacox, J. Chem. Phys. 47, 278 (1967).

$^{11}BCl_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	731w	Ar	IR	[1]
b_2	3	Asym. stretch	966vs	Ar	IR	[1]

References

[1] J. H. Miller and L. Andrews, J. Am. Chem. Soc. 102, 4900 (1980).

$^{11}BBr_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	597m	Ar	IR	[1]
b_2	3	Asym. stretch	833vs	Ar	IR	[1]

References

[1] J. H. Miller and L. Andrews, J. Am. Chem. Soc. 102, 4900 (1980).

CO_2^- C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	3	Asym. stretch	1596[a]	Ar	IR	[1]
			1608[b]	Ar	IR	[1]

[a] Cs^+ present.

[b] Na^+ present.

References

[1] M. E. Jacox and D. E. Milligan, Chem. Phys. Lett. 28, 163 (1974).

FCO C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	CO stretch	1861.64	gas	DL	[3]
			1857vs	Ar	IR	[2]
			1855vs	CO	IR	[1]
	2	Bend	627.5m	Ar	IR	[2]
			626m	CO	IR	[1]
	3	CF stretch	1026.13	gas	DL	[3]
			1023vs	Ar	IR	[2]
			1018s	CO	IR	[1]

References

[1] D. E. Milligan, M. E. Jacox, A. M. Bass, J. J. Comeford, and D. E. Mann, J. Chem. Phys. 42, 3187 (1965).

[2] M. E. Jacox, J. Mol. Spectrosc. 80, 257 (1980).

[3] K. Nagai, C. Yamada, Y. Endo, and E. Hirota, J. Mol. Spectrosc. 90, 249 (1981).

ClCO C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	CO stretch	1877vs	Ar	IR	[1]
			1880vs	CO	IR	[1]
	2	Bend	281s	CO	IR	[1]
	3	CCl stretch	570s	Ar	IR	[1]
			570s	CO	IR	[1]

References

[1] M. E. Jacox and D. E. Milligan, J. Chem. Phys. 43, 866 (1965).

CF_2^+ $^2A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	650[a]	gas	PE	[1]
b_2	3	Asym. stretch	1588[b]	Ar	IR	[2]

[a] $\pm$ 40 cm^{-1}.

[b] Tentative assignment.

References

[1] J. M. Dyke, L. Golob, N. Jonathan, A. Morris, and M. Okuda, J. Chem. Soc., Faraday Trans. 2 70, 1828 (1974).

[2] L. Andrews and B. W. Keelan, J. Am. Chem. Soc. 101, 3500 (1979).

CCl_2^+ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	1195.40	Ar	IR	[1]-[3]

References

[1] L. Andrews and B. W. Keelan, J. Am. Chem. Soc. 101, 3500 (1979).

[2] B. W. Keelan and L. Andrews, J. Phys. Chem. 83, 2488 (1979).

[3] B. J. Kelsall and L. Andrews, J. Mol. Spectrosc. 97, 362 (1983).

$CClBr^+$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CCl stretch	1120.6	Ar	IR	[1][2]

References

[1] L. Andrews and B. W. Keelan, J. Am. Chem. Soc. 101, 3500 (1979).

[2] B. J. Kelsall and L. Andrews, J. Mol. Spectrosc. 97, 362 (1983).

CBr_2^+ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	1019.6	Ar	IR	[1]-[3]

References

[1] L. Andrews and B. W. Keelan, J. Am. Chem. Soc. 101, 3500 (1979).

[2] B. W. Keelan and L. Andrews, J. Phys. Chem. 83, 2488 (1979).

[3] B. J. Kelsall and L. Andrews, J. Mol. Spectrosc. 97, 362 (1983).

SNO C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	NO stretch	1523s[a]	Ar	IR	[1][2]
	3	NS stretch	790m	Ar	IR	[1][2]

[a] In Fermi resonance with $2\nu_3$.

References

[1] P. O. Tchir and R. D. Spratley, Can. J. Chem. 53, 2318 (1975).

[2] M. Hawkins and A. J. Downs, J. Phys. Chem. 88, 3042 (1984).

PO_2 $^2A_1$ C_{2v} Structure: UV [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	Bend	504[a]	gas	UV	[1]

[a] $\pm$ 4 cm^{-1}.

References

[1] R. D. Verma and C. F. McCarthy, Can. J. Phys. 61, 1149 (1983).

NSO C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′		SO stretch	1195	Ar	IR	[1]

References

[1] P. O. Tchir and R. D. Spratley, Can. J. Chem. 53, 2331 (1975).

SO_2^+ $^2A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1264[a]	gas	UV	[2]
	2	Bend	403[b]	gas	PE,UV	[1][2]

[a] $\pm$ 10 cm^{-1}.

[b] $\pm$ 20 cm^{-1}.

References

[1] J. H. D. Eland and C. J. Danby, Int. J. Mass Spectrom. Ion Phys. 1, 111 (1968).

[2] K. T. Wu and A. J. Yencha, Can. J. Phys. 55, 767 (1977).

CF_2 $^1A_1$ C_{2v} Structure: MW [4] UV [5][6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1225.08	gas	DL	[11]
			1220	Ne	IR	[8]
			1222vs	Ar	IR	[2][7]
	2	Bend	667	gas	UV	[1][6]
			668vw	Ar	IR,LF	[2][7] [10]
b_2	3	Asym. stretch	1114.44	gas	IR,DL	[3][9] [12]
			1104	Ne	IR	[8]
			1102vs	Ar	IR	[2][7]

References

[1] P. Venkateswarlu, Phys. Rev. 77, 676 (1950).

[2] D. E. Milligan, D. E. Mann, M. E. Jacox, and R. A. Mitsch, J. Chem. Phys. 41, 1199 (1964).

[3] K. C. Herr and G. C. Pimentel, Appl. Opt. 4, 25 (1965).

[4] F. X. Powell and D. R. Lide, Jr., J. Chem. Phys. 45, 1067 (1966).

[5] C. W. Mathews, J. Chem. Phys. 45, 1068 (1966).

[6] C. W. Mathews, Can. J. Phys. 45, 2355 (1967).

[7] D. E. Milligan and M. E. Jacox, J. Chem. Phys. 48, 2265 (1968).

[8] A. Snelson, High Temp. Sci. 2, 70 (1970).

[9] A. S. Lefohn and G. C. Pimentel, J. Chem. Phys. 55, 1213 (1971).

[10] V. E. Bondybey, J. Mol. Spectrosc. 63, 164 (1976).

[11] P. B. Davies, W. Lewis-Bevan, and D. K. Russell, J. Chem. Phys. 75, 5602 (1981).

[12] P. B. Davies, P. A. Hamilton, J. M. Elliott, and M. J. Rice, J. Mol. Spectrosc. 102, 193 (1983).

ClCF C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CF stretch	1158[a]	gas	LF	[4]
			1146vs	Ar	IR	[1]
	2	Bend	448[b]	gas	LF	[4]
			442	Ar	LF	[2][3]
	3	ClC stretch	750[b]	gas	LF	[4]
			742s	Ar	IR	[1]

[a] $\pm$ 10 cm^{-1}.

[b] $\pm$ 6 cm^{-1}.

References

[1] C. E. Smith, D. E. Milligan, and M. E. Jacox, J. Chem. Phys. 54, 2780 (1971).

[2] D. E. Tevault and L. Andrews, J. Mol. Spectrosc. 54, 54 (1975).

[3] V. E. Bondybey and J. H. English, J. Mol. Spectrosc. 68, 89 (1977).

[4] S. E. Bialkowski, D. S. King, and J. C. Stephenson, J. Chem. Phys. 71, 4010 (1979).

CFBr C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	CF stretch	1157vs	Ar	IR	[2]
	2	Bend	340[a]	Ar	LF	[1]
	3	CBr stretch	656s	Ar	IR	[2]

[a] $\pm$ 5 cm^{-1}.

References

[1] J. C. Miller and L. Andrews, J. Phys. Chem. 84, 401 (1980).

[2] F. T. Prochaska and L. Andrews, J. Chem. Phys. 73, 2651 (1980).

CFI C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	CF stretch	1133vs	Ar	IR	[1]
	3	CI stretch	573s	Ar	IR	[1]

References

[1] F. T. Prochaska and L. Andrews, J. Chem. Phys. 73, 2651 (1980).

CCl_2 C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	721w-m	Ar	IR,LF	[1]-[3] [5][6]
	2	Bend	333	Ar	LF	[4]-[6]
b_2	3	Asym. stretch	748vs	Ar	IR	[1]-[3]

References

[1] D. E. Milligan and M. E. Jacox, J. Chem. Phys. 47, 703 (1967).

[2] L. Andrews, J. Chem. Phys. 48, 979 (1968).

[3] M. E. Jacox and D. E. Milligan, J. Chem. Phys. 53, 2688 (1970).

[4] J. S. Shirk, J. Chem. Phys. 55, 3608 (1971).

[5] D. E. Tevault and L. Andrews, J. Mol. Spectrosc. 54, 110 (1975).

[6] V. E. Bondybey, J. Mol. Spectrosc. 64, 180 (1977).

CClBr C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CCl stretch	744	Ar	IR	[1][2]
	2	Bend	260	Ar	LF	[3][4]
	3	CBr stretch	611	Ar	IR	[1][2]

References

[1] L. Andrews and T. G. Carver, J. Chem. Phys. 49, 896 (1968).

[2] A. K. Maltsev, O. M. Nefedov, R. H. Hauge, J. L. Margrave, and D. Seyferth, J. Phys. Chem. 75, 3984 (1971).

[3] D. E. Tevault and L. Andrews, J. Am. Chem. Soc. 97, 1707 (1975).

[4] V. E. Bondybey and J. H. English, J. Mol. Spectrosc. 79, 416 (1980).

CBr_2 C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	595w	Ar	IR	[1][2]
	2	Bend	196	Ar	LF	[3][4]
b_2	3	Asym. stretch	641s	Ar	IR	[1][2]

References

[1] L. Andrews and T. G. Carver, J. Chem. Phys. 49, 896 (1968).

[2] E. E. Rogers, S. Abramowitz, M. E. Jacox, and D. E. Milligan, J. Chem. Phys. 52, 2198 (1970).

[3] D. E. Tevault and L. Andrews, J. Am. Chem. Soc. 97, 1707 (1975).

[4] V. E. Bondybey and J. H. English, J. Mol. Spectrosc. 79, 416 (1980).

SiF_2 $^1A_1$ C_{2v} Structure: MW [1][2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	855.01	gas	IR	[4][7]
			851s	Ne	IR	[6]
			843s	Ar	IR	[5][6]
	2	Bend	345	gas	MW,UV	[2][3]
			343	Ar	IR	[5]
b_2	3	Asym. stretch	870.40	gas	IR	[4][7]
			864.6s	Ne	IR	[6]
			855vs	Ar	IR	[5][6]

References

[1] V. M. Rao, R. F. Curl, Jr., P. L. Timms, and J. L. Margrave, J. Chem. Phys. 43, 2557 (1965).

[2] V. M. Rao and R. F. Curl, Jr., J. Chem. Phys. 45, 2032 (1966).

[3] V. M. Khanna, G. Besenbruch, and J. L. Margrave, J. Chem. Phys. 46, 2310 (1967).

[4] V. M. Khanna, R. Hauge, R. F. Curl, Jr., and J. L. Margrave, J. Chem. Phys. 47, 5031 (1967).

[5] D. E. Milligan and M. E. Jacox, J. Chem. Phys. 49, 4269 (1968).

[6] J. W. Hastie, R. H. Hauge, and J. L. Margrave, J. Am. Chem. Soc. 91, 2536 (1969).

[7] G. L. Caldow, C. M. Deeley, P. H. Turner, and I. M. Mills, Chem. Phys. Lett. 82, 434 (1981).

$SiCl_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	518.7	Ne	IR	[2]
			512.5s	Ar	IR	[1][2]
b_2	3	Asym. stretch	509.4	Ne	IR	[2]
			502vs	Ar	IR	[1][2]

References

[1] D. E. Milligan and M. E. Jacox, J. Chem. Phys. 49, 1938 (1968).

[2] G. Maass, R. H. Hauge, and J. L. Margrave, Z. Anorg. Allg. Chem. 392, 295 (1972).

$SiBr_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	402.6s	Ar	IR	[1]
b_2	3	Asym. stretch	399.5vs	Ar	IR	[1]

References

[1] G. Maass, R. H. Hauge, and J. L. Margrave, Z. Anorg. Allg. Chem. 392, 295 (1972).

NO_2^- C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	NO stretch	1244	Ar	IR	[1][2]

References

[1] D. E. Milligan, M. E. Jacox, and W. A. Guillory, J. Chem. Phys. 52, 3864 (1970).

[2] D. E. Milligan and M. E. Jacox, J. Chem. Phys. 55, 3404 (1971).

ClPO

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	PO stretch	1258vs	Ar	IR	[1]
	2	Bend	308wm	Ar	IR	[1]
	3	PCl stretch	489vs	Ar	IR	[1]

References

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

ClPS C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	PS stretch	716.1	Ar	IR,Ram	[1]
	2	Bend	229	Ar	Ram	[1]
	3	PCl stretch	462.4	Ar	IR	[1]

References

[1] H. Schnockel and M. Lakenbrink, Z. Anorg. Allg. Chem. 507, 70 (1983).

NF_2^+ $^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NF stretch	1250[a]	gas	PE	[1][2]

[a] ± 20 cm^{-1}.

References

[1] A. B. Cornford, D. C. Frost, F. G. Herring, and C. A. McDowell, J. Chem. Phys. 54, 1872 (1971).

[2] A. B. Cornford, D. C. Frost, F. G. Herring, and C. A. McDowell, J. Chem. Soc., Faraday Disc. 54, 56 (1972).

PF_2^+ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PF stretch	1000[a]	gas	PE	[1]

[a] ± 30 cm^{-1}.

References

[1] J. M. Dyke, N. Jonathan, and A. Morris, Int. Rev. Phys. Chem. 2, 3 (1982).

FON C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	2	Bend	735vs	Ar	IR	[1]-[3]
			725	N_2	IR	[1][2]
	3	OF stretch	492vs	Ar	IR	[1]-[3]
			480	N_2	IR	[1][2]

References

[1] R. R. Smardzewski and W. B. Fox, J. Am. Chem. Soc. 96, 304 (1974).

[2] R. R. Smardzewski and W. B. Fox, J. Chem. Phys. 60, 2104 (1974).

[3] M. E. Jacox, J. Phys. Chem. 87, 4940 (1983).

BrSN C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	SN stretch	1313m	Ar	IR	[1]
	2	Bend	226wm	Ar	IR	[1]
	3	SBr stretch	346s	Ar	IR	[1]

References

[1] S. C. Peake and A. J. Downs, J. Chem. Soc., Dalton Trans., 859 (1974).

NF_2 $^2B_1$ C_{2v} Structure: IR [1] MW [4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	1074.99	gas	IR,DL, LMR	[1][6] [7][8]
			1069m	Ar	IR	[3][5]
			1070	N_2	IR	[1][2]
	2	Bend	573w	N_2	IR	[2]
b_2	3	Asym. stretch	942.48	gas	IR,DL	[1][6] [9]
			932vs	Ar	IR	[3][5]
			931	N_2	IR	[1][2]

References

[1] M. D. Harmony, R. J. Myers, L. J. Schoen, D. R. Lide, Jr., and D. E. Mann, J. Chem. Phys. 35, 1129 (1961).

[2] M. D. Harmony and R. J. Myers, J. Chem. Phys. 37, 636 (1962).

[3] M. E. Jacox and D. E. Milligan, J. Chem. Phys. 46, 184 (1967).

[4] R. D. Brown, F. R. Burden, P. D. Godfrey, and I. R. Gillard, J. Mol. Spectrosc. 52, 301 (1974).

[5] M. E. Jacox, D. E. Milligan, W. A. Guillory, and J. J. Smith, J. Mol. Spectrosc. 52, 322 (1974).

[6] P. B. Davies, B. J. Handy, and D. K. Russell, Chem. Phys. Lett. 68, 395 (1979).

[7] K. Hakuta and H. Uehara, J. Chem. Phys. 74, 5995 (1981).

[8] P. B. Davies, P. A. Hamilton, W. Lewis-Bevan, and D. K. Russell, Proc. Roy. Soc. (London) A392, 445 (1984).

[9] P. B. Davies and P. A. Hamilton, Proc. Roy. Soc. (London) A393, 397 (1984).

NCl_2 C_{2v} Structure: IR [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	679	Ar	IR	[1]

References

[1] C. K. Kohlmiller and L. Andrews, Inorg. Chem. 21, 1519 (1982).

NBr_2 C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	604	Ar	IR	[1]

References

[1] C. K. Kohlmiller and L. Andrews, Inorg. Chem. 21, 1519 (1982).

PCl_2 C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	452	Ar	IR	[1]
b_2	3	Asym. stretch	525	Ar	IR	[1]

References

[1] L. Andrews and D. L. Frederick, J. Phys. Chem. 73, 2774 (1969).

PBr_2 C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	369	Ar	IR	[1]
b_2	3	Asym. stretch	410	Ar	IR	[1]

References

[1] L. Andrews and D. L. Frederick, J. Phys. Chem. 73, 2774 (1969).

O_3^- C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	982[a]	gas	PE	[6]
			1016[b]	Ar	Ram	[3][5]
			1011[c]	Ar	Ram	[3][5]
	2	Bend	550[d]	gas	PE	[6]
			600w[b]	Ar	IR	[4]
b_2	3	Asym. stretch	789s[b] 802s	Ar	IR	[2][4]
			802s[c]	Ar	IR	[1][2] [4]

[a] ± 30 cm^{-1}.

[b] Cs^+ present.

[c] Na^+ present.

[d] ± 50 cm^{-1}.

References

[1] M. E. Jacox and D. E. Milligan, Chem. Phys. Lett. 14, 518 (1972).

[2] M. E. Jacox and D. E. Milligan, J. Mol. Spectrosc. 43, 148 (1972).

[3] L. Andrews, J. Am. Chem. Soc. 95, 4487 (1973).

[4] R. C. Spiker, Jr., and L. Andrews, J. Chem. Phys. 59, 1851 (1973).

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[6] S. E. Novick, P. C. Engelking, P. L. Jones, J. H. Futrell, and W. C. Lineberger, J. Chem. Phys. 70, 2652 (1979).

SO_2^- C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	985m[a]	Ar	IR	[1]
			990[b]	Ar	IR	[1]
	2	Bend	495wm[a]	Ar	IR	[1]
			495[b]	Ar	IR	[1]
b_2	3	Asym. stretch	1042s[a]	Ar	IR	[1]
			1041[b]	Ar	IR	[1]

[a] Cs^+ present.

[b] Na^+ present.

References

[1] D. E. Milligan and M. E. Jacox, J. Chem. Phys. 55, 1003 (1971).

FO_2 C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	OO stretch	1490vs	Ar	IR	[1][3]
			1500vs	N_2	IR	[2]
	2	Bend	376m	N_2	IR	[2]
	3	OF stretch	579.32	gas	DL	[4]
			584s	Ar	IR	[1][3]
			586s	N_2	IR	[2]

References

[1] A. Arkell, J. Am. Chem. Soc. 87, 4057 (1965).

[2] R. D. Spratley, J. J. Turner, and G. C. Pimentel, J. Chem. Phys. 44, 2063 (1966).

[3] M. E. Jacox, J. Mol. Spectrosc. 84, 74 (1980).

[4] C. Yamada and E. Hirota, J. Chem. Phys. 80, 4694 (1984).

ClOO C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	OO stretch	1443[a]	gas	IR	[3]
			1441vs[b]	Ar	IR	[2]
			1438 1428	N_2	IR	[1]
	2	Bend	373m	Ar	IR	[2]
	3	ClO stretch	407s[b]	Ar	IR	[2]

[a] Absorption maximum; spectral slit width 13 cm^{-1}.

[b] Peaks at 1415 and 435 cm^{-1}, attributed in [2] to a structural isomer of ClOO, were attributed in [4] to the vibrationally unrelaxed molecule.

References

[1] M. M. Rochkind and G. C. Pimentel, J. Chem. Phys. 46, 4481 (1967).

[2] A. Arkell and I. Schwager, J. Am. Chem. Soc. 89, 5999 (1967).

[3] H. S. Johnston, E. D. Morris, Jr., and J. Van den Bogaerde, J. Am. Chem. Soc. 91, 7712 (1969).

[4] J. L. Gole, J. Phys. Chem. 84, 1333 (1980).

BrOO

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OO stretch	1487	Ar	IR	[1]

References

[1] D. E. Tevault and R. R. Smardzewski, J. Am. Chem. Soc. 100, 3955 (1978).

FSO C_s Structure: MW [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	SO stretch	1215[a]	gas	MW	[1]
	2	Bend	396[b]	gas	MW	[1]
	3	SF stretch	763[c]	gas	MW	[1]

[a] ± 33 cm^{-1} for 0.5 md/A uncertainty in SO stretching force constant.

[b] ± 1.3 cm^{-1} for 2.5 times standard error in least-squares fit to data.

[c] ± 12 cm^{-1} for 2.5 times standard error in least-squares fit to data.

References

[1] Y. Endo, S. Saito, and E. Hirota, J. Chem. Phys. 74, 1568 (1981).

SSCl C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	SS stretch	665	Ar	IR	[1]
	3	SCl stretch	404	Ar	IR	[1]

References

[1] G. Vahl and M. Feuerhahn, J. Chem. Res., Synop., 237 (1979).

SSBr C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	SS stretch	558	Ar	IR	[1]
	3	SBr stretch	346	Ar	IR	[1]

[1] G. Vahl and M. Feuerhahn, J. Chem. Res., Synop., 237 (1979).

SF_2^+ $^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SF stretch	935[a]	gas	PE	[1]

[a] ± 40 cm^{-1}.

References

[1] D. M. de Leeuw, R. Mooyman, and C. A. de Lange, Chem. Phys. 34, 287 (1978).

SBr_2^+ $^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SBr stretch	400[a]	gas	PE	[1]

[a] ± 50 cm^{-1}.

References

[1] D. M. de Leeuw, R. Mooyman, and C. A. de Lange, Chem. Phys. Lett. 61, 191 (1979).

SeF_2^+ $^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	780[a]	gas	PE	[1]

[a] ± 50 cm^{-1}.

References

[1] D. M. de Leeuw, R. Mooyman, and C. A. de Lange, Chem. Phys. 38, 21 (1979).

$SeCl_2^+$ $^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	450[a]	gas	PE	[1]

[a] ± 50 cm^{-1}.

References

[1] D. M. de Leeuw, R. Mooyman, and C. A. de Lange, Chem. Phys. 38, 21 (1979).

$O^{79}BrO$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	852	Ar	IR	[1]

References

[1] D. E. Tevault, N. Walker, R. R. Smardzewski, and W. B. Fox, J. Phys. Chem. 82, 2733 (1978).

BrOBr C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	526	Ar	IR	[1]

References

[1] D. E. Tevault, N. Walker, R. R. Smardzewski, and W. B. Fox, J. Phys. Chem. 82, 2733 (1978).

SF_2 C_{2v} Structure: MW [1][3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	838.53	gas	IR	[4]
			834	Ne	IR	[2]
			832vs	Ar	IR	[2]
			825	N_2	IR	[2]
	2	Bend	357[a]	gas	MW	[1]
			358	Ne	IR	[2]
			358m	Ar	IR	[2]
			358	N_2	IR	[2]
b_2	3	Asym. stretch	813.04	gas	IR	[4]
			807.5	Ne	IR	[2]
			804vs	Ar	IR	[2]
			795	N_2	IR	[5]

[a] $\pm$ 2 cm^{-1}.

References

[1] W. H. Kirchhoff, D. R. Johnson, and F. X. Powell, J. Mol. Spectrosc. 48, 157 (1973).

[2] A. Haas and H. Willner, Spectrochim. Acta 34A, 541 (1978).

[3] Y. Endo, S. Saito, E. Hirota, and T. Chikaraishi, J. Mol. Spectrosc. 77, 222 (1979).

[4] J.-C. Deroche, H. Burger, P. Schulz, and H. Willner, J. Mol. Spectrosc. 89, 269 (1981).

[5] H. Willner, Z. Anorg. Allg. Chem. 481, 117 (1981).

SBr_2 C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	405	Ar	IR	[1]
b_2	3	Asym. stretch	418	Ar	IR	[1]

References

[1] M. Feuerhahn and G. Vahl, Inorg. Nucl. Chem. Lett. 16, 5 (1980).

SI_2 C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	368	Ar	IR	[1]
b_2	3	Asym. stretch	376	Ar	IR	[1]

References

[1] M. Feuerhahn and G. Vahl, Inorg. Nucl. Chem. Lett. 16, 5 (1980).

$OClO^-$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	790[a]	Ar	IR	[1]
	2	Bend	418[a]	Ar	IR	[1]
b_2	3	Asym. stretch	823[a]	Ar	IR	[1]

[a] Cs^+ present.

References

[1] D. E. Tevault, F. K. Chi, and L. Andrews, J. Mol. Spectrosc. 51, 450 (1974).

FClO C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ClO stretch	1038s	Ar	IR	[1]
	2	Bend	315m	Ar	IR	[1]
	3	FCl stretch	593vs	Ar	IR	[1]

References

[1] L. Andrews, F. K. Chi, and A. Arkell, J. Am. Chem. Soc. 96, 1997 (1974).

ClClO C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	ClO stretch	962	Ar	IR,Ram	[3]
			963	N_2	IR	[1][2]
	2	Bend	239	Ar	IR,Ram	[3]
	3	ClCl stretch	375	Ar	IR,Ram	[3]
			377	N_2	IR	[1][2]

References

[1] M. M. Rochkind and G. C. Pimentel, J. Chem. Phys. 46, 4481 (1967).

[2] W. G. Alcock and G. C. Pimentel, J. Chem. Phys. 48, 2373 (1968).

[3] F. K. Chi and L. Andrews, J. Phys. Chem. 77, 3062 (1973).

BrBrO C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	BrO stretch	804	Ar	IR	[1]
	3	BrBr stretch	236	Ar	IR	[1]

References

[1] D. E. Tevault, N. Walker, R. R. Smardzewski, and W. B. Fox, J. Phys. Chem. 82, 2733 (1978).

ClF_2 C_{2v} Structure: MO [2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Sym. stretch	500	Ar	Ram	[3]
			500	N_2	Ram	[3]
b_2	3	Asym. stretch	574	Ar	IR	[1][3]
			578	N_2	IR	[1][3]

References

[1] G. Mamantov, E. J. Vasini, M. C. Moulton, D. G. Vickroy, and T. Maekawa, J. Chem. Phys. 54, 3419 (1971).

[2] S. R. Ungemach and H. F. Schaefer III, J. Am. Chem. Soc. 98, 1658 (1976).

[3] E. S. Prochaska and L. Andrews, Inorg. Chem. 16, 339 (1977).

ClClF C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	ClF stretch	559s	Ar	IR	[1]
	2	Bend	270w	Ar	IR	[1]
	3	ClCl stretch	464wm	Ar	IR	[1]

References

[1] E. S. Prochaska, L. Andrews, N. R. Smyrl, and G. Mamantov, Inorg. Chem. 17, 970 (1978).

BrF_2 C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	3	Asym. stretch	569	Ar	IR	[1]

References

[1] E. S. Prochaska, L. Andrews, N. R. Smyrl, and G. Mamantov, Inorg. Chem. 17, 970 (1978).

BrBrF C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	BrF stretch	507[a]	Ar	IR	[1]

[a] Tentative assignment.

References

[1] E. S. Prochaska, L. Andrews, N. R. Smyrl, and G. Mamantov, Inorg. Chem. 17, 970 (1978).

IIF C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	IF stretch	499[a]	Ar	IR	[1]

[a] Tentative assignment.

References

[1] E. S. Prochaska, L. Andrews, N. R. Smyrl, and G. Mamantov, Inorg. Chem. 17, 970 (1978).

F_3^- $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	461[a]	Ar	Ram	[1][2]
Σ_u^+	3	Asym. stretch	550[a]	Ar	IR	[1][2]

[a] K^+, Rb^+, or Cs^+ present.

References

[1] B. S. Ault and L. Andrews, J. Am. Chem. Soc. 98, 1591 (1976).

[2] B. S. Ault and L. Andrews, Inorg. Chem. 16, 2024 (1977).

$FClF^-$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	566[a]	Ar	IR	[2]
			565[b]	Ar	IR	[2]
			571[c]	Ar	IR	[1]
			589[d]	Ar	IR	[2]

[a] Cs^+ present.

[b] Rb^+ present.

[c] K^+ present.

[d] Na^+ present.

References

[1] E. S. Prochaska, B. S. Ault, and L. Andrews, Inorg. Chem. 16, 2021 (1977).

[2] B. S. Ault and L. Andrews, Inorg. Chem. 16, 2024 (1977).

$FFCl^-$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	FF stretch	365[a]	Ar	IR	[1][2]
			371[b]	Ar	IR	[1][2]
			391[c]	Ar	IR	[2]

[a] Cs^+ present.

[b] Rb^+ present.

[c] K^+ present.

References

[1] B. S. Ault and L. Andrews, Inorg. Chem. 16, 2024 (1977).

[2] J. H. Miller and L. Andrews, Inorg. Chem. 18, 988 (1979).

$FBrF^-$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	527[a]	Ar	IR	[1]
			524[b]	Ar	IR	[1]
			521[c]	Ar	IR	[1]
			543[d]	Ar	IR	[1]

[a] Cs^+ present.

[b] Rb^+ present.

[c] K^+ present.

[d] Na^+ present.

References

[1] J. H. Miller and L. Andrews, Inorg. Chem. 18, 988 (1979).

$FFBr^-$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	FF stretch	360[a]	Ar	IR	[1]
			366[b]	Ar	IR	[1]
			364[c]	Ar	IR	[1]

[a] Cs^+ present.

[b] Rb^+ present.

[c] K^+ present.

References

[1] J. H. Miller and L. Andrews, Inorg. Chem. 18, 988 (1979).

FIF^- $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	504[a]	Ar	IR	[1]
			503[b]	Ar	IR	[1]
			506[c]	Ar	IR	[1]
			520[d]	Ar	IR	[1]

[a] Cs^+ present.

[b] Rb^+ present.

[c] K^+ present.

[d] Na^+ present.

References

[1] J. H. Miller and L. Andrews, Inorg. Chem. 18, 988 (1979).

FFI^- $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	FF stretch	354[a]	Ar	IR	[1]
			356[b]	Ar	IR	[1]
			357[c]	Ar	IR	[1]

[a] Cs^+ present.

[b] Rb^+ present.

[c] K^+ present.

References

[1] J. H. Miller and L. Andrews, Inorg. Chem. 18, 988 (1979).

$ClFCl^-$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	474[a]	Ar	IR	[1]
			480[b]	Ar	IR	[1]
			486[c]	Ar	IR	[1]
			511[d]	Ar	IR	[1]

$ClFCl^-$---Footnote

[a] Cs^+ present.

[b] Rb^+ present.

[c] K^+ present.

[d] Na^+ present.

References

[1] B. S. Ault and L. Andrews, Inorg. Chem. 16, 2024 (1977).

$FClCl^-$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+			412[a]	Ar	IR,Ram	[1]
			409[b]	Ar	IR	[1]

[a] Cs^+ present.

[b] Rb^+ present.

References

[1] B. S. Ault and L. Andrews, Inorg. Chem. 16, 2024 (1977).

Cl_3^- $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	225[ae]	Ar	Ram	[2]
			253[b]	Ar	Ram	[2]
			258[c]	Ar	Ram	[2]
			276[d]	Ar	Ram	[2]
Σ_u^+	3	Asym. stretch	327[a]	Ar	IR,Ram	[2]
			340[b]	Ar	IR,Ram	[2]
			345[c]	Ar	IR,Ram	[2]
			375[d]	Ar	IR,Ram	[2]
			374[f]	Kr	IR	[1]

[a] Cs^+ present.

[b] Rb^+ present.

[c] K^+ present.

[d] Na^+ present.

[e] Tentative assignment.

[f] Attributed in [1] to the uncharged species. Reassigned by [3] to the anion.

References

[1] L. Y. Nelson and G. C. Pimentel, J. Chem. Phys. 47, 3671 (1967).

[2] B. S. Ault and L. Andrews, J. Chem. Phys. 64, 4853 (1976).

[3] C. A. Wight, B. S. Ault, and L. Andrews, J. Chem. Phys. 65, 1244 (1976).

$ClBrCl^-$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	311[a]	Ar	IR	[1]

[a] K^+ present.

References

[1] B. S. Ault and L. Andrews, J. Chem. Phys. 64, 4853 (1976).

$ClClBr^-$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	Stretch	273[a]	Ar	IR	[1]

[a] K^+ present.

References

[1] B. S. Ault and L. Andrews, J. Chem. Phys. 64, 4853 (1976).

$BrClBr^-$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	282[ab]	Ar	IR	[1]

[a] K^+ present.

[b] Tentative assignment.

References

[1] B. S. Ault and L. Andrews, J. Chem. Phys. 64, 4853 (1976).

$ClBrBr^-$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	Stretch	229[a]	Ar	IR	[1]

[a] K^+ present.

References

[1] B. S. Ault and L. Andrews, J. Chem. Phys. 64, 4853 (1976).

Br_3^- $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	154[ab]	Ar	Ram	[2]
			197[c]	Kr	Ram	[1]
			190[c]	Xe	Ram	[1]
Σ_u^+	3	Asym. stretch	214[a]	Ar	IR	[2]

[a] K^+ present.

[b] Tentative assignment.

[c] Assigned by [1] to the uncharged species. Arguments presented by [3] support reassignment to the anion.

References

[1] D. H. Boal and G. A. Ozin, J. Chem. Phys. 55, 3598 (1971).

[2] B. S. Ault and L. Andrews, J. Chem. Phys. 64, 4853 (1976).

[3] C. A. Wight, B. S. Ault, and L. Andrews, J. Chem. Phys. 65, 1244 (1976).

I_3^- $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	113[a]	Ar	Ram[b]	[1]

[a] Cs^+ present.

[b] Resonance Raman.

References

[1] L. Andrews, E. S. Prochaska, and A. Loewenschuss, Inorg. Chem. 19, 463 (1980).

KrF_2 $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	449	gas	Ram	[2]
			452	Kr	Ram	[3]
Π_u	2	Bend	233	gas	IR	[2]
			236m	Ar	IR	[1]
Σ_u^+	3	Asym. stretch	588	gas	IR	[2]
			580s	Ar	IR	[1]

References

[1] J. J. Turner and G. C. Pimentel, Science 180, 974 (1963).

[2] H. H. Claassen, G. L. Goodman, J. G. Malm, and F. Schreiner, J. Chem. Phys. 42, 1229 (1965).

[3] W. F. Howard, Jr., and L. Andrews, J. Am. Chem. Soc. 96, 7864 (1974).

XeF_2 $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	515	gas	IR[a]	[1][2]
			514.5	gas	Ram	[4]
			512	Ar	Ram	[5]
			512	Xe	Ram	[5]
Π_u	2	Bend	213.2s	gas	IR	[2]
			215	Ar	IR	[6]
Σ_u^+	3	Asym. stretch	555s	gas	IR	[1][2]
			547	Ar	IR	[3]

[a] From observation of $\nu_1 + \nu_3$.

References

[1] D. F. Smith, J. Chem. Phys. 38, 270 (1963).

[2] P. A. Agron, G. M. Begun, H. A. Levy, A. A. Mason, C. G. Jones, and D. F. Smith, Science 139, 842 (1963).

[3] J. J. Turner and G. C. Pimentel, in "Noble-Gas Compounds," H. H. Hyman, Ed., University of Chicago Press, Chicago, Ill., 1963, p. 101.

[4] P. Tsao, C. C. Cobb, and H. H. Claassen, J. Chem. Phys. 54, 5247 (1971).

[5] W. F. Howard, Jr., and L. Andrews, J. Am. Chem. Soc. 96, 7864 (1974).

[6] B. S. Ault, L. Andrews, D. W. Green, and G. T. Reedy, J. Chem. Phys. 66, 2786 (1977).

XeClF $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	Stretch	316wm	Xe	IR	[1]
			315.5	Xe	Ram	[1]
	3	Stretch	481s	Xe	IR	[1]
			480	Xe	Ram	[1]

References

[1] W. F. Howard, Jr., and L. Andrews, J. Am. Chem. Soc. 96, 7864 (1974).

$XeCl_2$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	Sym. stretch	255	Xe	Ram	[2]-[4]
Σ_u^+	3	Asym. stretch	313	Xe	IR	[1][3]

References

[1] L. Y. Nelson and G. C. Pimentel, Inorg. Chem. 6, 1758 (1967).

[2] D. Boal and G. A. Ozin, Spectrosc. Lett. 4, 43 (1971).

[3] W. F. Howard, Jr., and L. Andrews, J. Am. Chem. Soc. 96, 7864 (1974).

[4] I. R. Beattie, A. German, H. E. Blayden, and S. B. Brumbach, J. Chem. Soc., Dalton Trans. 1659 (1975).

6.4. Four-Atomic Trihydrides

$^{11}BH_3$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	1125w	Ar	IR	[1]
e′	3	BH stretch	2808w	Ar	IR	[1]
	4	Deformation	1604m	Ar	IR	[1]

$^{11}BD_3$

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]
	4	Deformation	1184sh	Ar	IR	[1]

References

[1] A. Kaldor and R. F. Porter, J. Am. Chem. Soc. 93, 2140 (1971).

CH_3^+ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	1380[a]	gas	UV[b],PE	[1][2]

CD_3^+

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	1070[c]	gas	UV[b],PE	[1][2]

[a] ± 20 cm^{-1}.

[b] Structure in Rydberg transitions of CH_3 and CD_3.

[c] ± 30 cm^{-1}.

References

[1] G. Herzberg, Proc. Roy. Soc. (London) A262, 291 (1961).

[2] J. Dyke, N. Jonathan, E. Lee, and A. Morris, J. Chem. Soc., Faraday Trans. II 72, 1385 (1976).

SiH_3^+ $^1A_1'$ D_{3h} Structure: [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	820[a]	gas	PE	[1]

[a] ± 40 cm^{-1}.

References

[1] J. M. Dyke, N. Jonathan, A. Morris, A. Ridha, and M. J. Winter, Chem. Phys. 81, 481 (1983).

CH_3 $^2A_2''$ D_{3h} Structure: [1][7]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	606.45	gas	IR,DL	[4][7]
			617vs	Ne	IR	[3]
			603[a]	Ar	IR	[2][6]
			611	N_2	IR	[2]
e′	3	CH stretch	3160.82	gas	LDF	[8]
			3162wm	Ne	IR	[3]
			3150	Ar	IR	[5]
	4	Deformation	1396w	Ne	IR	[3]
			1398[b]	Ar	IR	[6]

CD_3

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_2''	2	OPLA	463s	Ne	IR	[3]
			453[a]	Ar	IR	[2][6]
			463	N_2	IR	[2]
e′	3	CD stretch	2381w	Ne	IR	[3]
			2369	Ar	IR	[5]
	4	Deformation	1026vw	Ne	IR	[3]
			1029	Ar	IR	[5]

[a] Band center. Rotational structure assigned [6].

[b] $^RR(0_0)$ transition.

References

[1] G. Herzberg, Proc. Roy. Soc. (London) A262, 291 (1961).

[2] D. E. Milligan and M. E. Jacox, J. Chem. Phys. 47, 5146 (1967).

[3] A. Snelson, J. Phys. Chem. 74, 537 (1970).

[4] L. Y. Tan, A. M. Winer, and G. C. Pimentel, J. Chem. Phys. 57, 4028 (1972).

[5] J. Pacansky and J. Bargon, J. Am. Chem. Soc. 97, 6896 (1975).

[6] M. E. Jacox, J. Mol. Spectrosc. 66, 272 (1977).

[7] C. Yamada, E. Hirota, and K. Kawaguchi, J. Chem. Phys. 75, 5256 (1981).

[8] T. Amano, P. F. Bernath, C. Yamada, Y. Endo, and E. Hirota, J. Chem. Phys. 77, 5284 (1982).

SiH_3 C_{3v} Structure: ESR [1][2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SiH stretch	1999m	Ar	IR	[3]
		SiH stretch[a]	1974m	Ar	IR	[3]
		SiH stretch	1955m	Ar	IR	[3]
		Deformation	996wm	Ar	IR	[3]
		Deformation	926m	Ar	IR	[3]

[a] May result from Fermi resonance with first overtone of 996-cm^{-1} fundamental. Alternatively, may be contributed by SiH.

References

[1] R. L. Morehouse, J. J. Christiansen, and W. Gordy, J. Chem. Phys. 45, 1751 (1966).

[2] G. S. Jackel and W. Gordy, Phys. Rev. 176, 443 (1968).

[3] D. E. Milligan and M. E. Jacox, J. Chem. Phys. 52, 2594 (1970).

GeH_3 C_{3v} Structure: ESR [1][2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		GeH stretch	1839s	Ar	IR	[3]
		GeH stretch	1813ms	Ar	IR	[3]
		Deformation	928w	Ar	IR	[3]
		Deformation	850w	Ar	IR	[3]

GeD_3

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		GeD stretch	1360vs	Ar	IR	[3]
		GeD stretch	1356vs	Ar	IR	[3]
		Deformation	708m	Ar	IR	[3]
		Deformation	653m	Ar	IR	[3]

References

[1] R. L. Morehouse, J. J. Christiansen, and W. Gordy, J. Chem. Phys. 45, 1751 (1966).

[2] G. S. Jackel and W. Gordy, Phys. Rev. 176, 443 (1968).

[3] G. R. Smith and W. A. Guillory, J. Chem. Phys. 56, 1423 (1972).

H_3O^+ C_{3v} Structure: VMA [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	"Umbrella"	954.42[a]	gas	DL	[2]
e	3	OH stretch	3530.2[b]	gas	VMA	[1]
			3513.8[c]	gas	VMA	[1]

[a] $1^- - 0^+$ transition.

[b] Component arising from $\nu_2 = 0^+$.

[c] Component arising from $\nu_2 = 0^-$.

References

[1] M. H. Begemann, C. S. Gudeman, J. Pfaff, and R. Saykally, Phys. Rev. Lett. 51, 554 (1983).

[2] N. N. Haese and T. Oka, J. Chem. Phys. 80, 572 (1984).

6.5. Four-Atomic Dihydrides

$HN^{11}BH$ $C_{\infty v}$ 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	1785m	Ar	IR	[3]
Π	4	Bend	460m	Ar	IR	[3]

$DN^{11}BD$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	ND stretch	2836	Ar	IR	[3]
Σ^+	2	BD stretch	2730	Ar	IR	[3]
Σ^+	3	BN stretch	1734	Ar	IR	[3]
Π	4	Bend	360	Ar	IR	[3]

References

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

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

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

$H_2C{=}C{:}$ $^1A_1$ C_{2v}

(Vinylidene)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C=C stretch	1650[a]	gas	PE	[1]
	3	CH_2 "scissors"	1120[b]	gas	PE	[1]

$D_2C{=}C{:}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C=C stretch	1610[a]	gas	PE	[1]
	3	CD_2 "scissors"	840[b]	gas	PE	[1]

[a] $\pm$ 120 cm^{-1}.

[b] $\pm$ 100 cm^{-1}.

References

[1] S. M. Burnett, A. E. Stevens, C. S. Feigerle, and W. C. Lineberger, Chem. Phys. Lett. 100, 124 (1983).

$HCNH^+$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ	1	NH stretch	3482.84	gas	VMA	[1]
	2	CH stretch	3187.86	gas	VMA	[1]

References

[1] R. S. Altman, M. W. Crofton, and T. Oka, J. Chem. Phys. 80, 3911 (1984).

H_2CS^+

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CS stretch	1000[a]	gas	PE	[1]

[a] Uncertainty not given; estimated to be $\pm$ 50 cm^{-1}, a value typical for such measurements.

References

[1] H. W. Kroto and R. J. Suffolk, Chem. Phys. Lett. 15, 545 (1972).

t-$HNNH^+$ ^2A_g C_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g		NN stretch	~1850	gas	PE	[2]
		H deform.	1180[a]	gas	PE	[1][2]

t-$DNND^+$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g		D deform.	1020[a]	gas	PE	[1][2]

[a] $\pm$ 30 cm^{-1}.

References

[1] D. C. Frost, S. T. Lee, C. A. McDowell, and N. P. C. Westwood, Chem. Phys. Lett. 30, 26 (1975).

[2] D. C. Frost, S. T. Lee, C. A. McDowell, and N. P. C. Westwood, J. Chem. Phys. 64, 4719 (1976).

H_2CS $^1A_1$ C_{2v} Structure: MW [1][3][4] IR [2][8]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	2971.03	gas	IR	[2][8]
			2970w	Ar	IR	[5][10]
			2973w	N_2	IR	[5]
	2	CH_2 "scissors"	1457.3	gas	LF	[7]
			1447.0	gas	IR	[8]
			1447	Ar	IR	[10]
	3	CS stretch	1059.20	gas	LSS,IR	[6][8]
			1063w	Ar	IR	[5][10]
			1062w	N_2	IR	[5]
b_1	4	OPLA	990.19	gas	LSS,IR	[6][8]
			993s	Ar	IR	[5][10]
			995s	N_2	IR	[5]
b_2	5	CH stretch	3024.61	gas	IR	[2][8]
	6	CH_2 rock	991.01	gas	LSS,IR	[6][8]
			988m	Ar	IR	[5][10]

D_2CS

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD stretch	2158.5	gas	IR	[8]
			2155m	Ar	IR	[10]
	2	CD_2 "scissors"	1171.8	gas	IR	[8]
			1167m	N_2	IR	[10]
	3	CS stretch	936.13	gas	IR,LSS	[8][9]
			941vw	Ar	IR	[5][10]
			939wm	N_2	IR	[5]
b_1	4	OPLA	781.2	gas	IR	[8]
			783m	Ar	IR	[5][10]
			784s	N_2	IR	[5]
b_2	6	CD_2 rock	757.4	gas	IR	[8]

References

[1] D. R. Johnson, F. X. Powell, and W. H. Kirchhoff, J. Mol. Spectrosc. 39, 136 (1971).

[2] J. W. C. Johns and W. B. Olson, J. Mol. Spectrosc. 39, 479 (1971).

[3] Y. Beers, G. P. Klein, W. H. Kirchhoff, and D. R. Johnson, J. Mol. Spectrosc. 44, 553 (1972).

[4] D. R. Johnson, F. J. Lovas, and W. H. Kirchhoff, J. Phys. Chem. Ref. Data 1, 1011 (1972).

[5] M. E. Jacox and D. E. Milligan, J. Mol. Spectrosc. 58, 142 (1975).

[6] D. J. Bedwell and G. Duxbury, J. Mol. Spectrosc. 84, 531 (1980).

[7] D. J. Clouthier, C. M. L. Kerr, and D. A. Ramsay, Chem. Phys. 56, 73 (1981).

[8] P. H. Turner, L. Halonen, and I. M. Mills, J. Mol. Spectrosc. 88, 402 (1981).

[9] G. Duxbury, H. Kato, and M. L. Le Lerre, Disc. Faraday Soc. 71, 97 (1981).

[10] M. Torres, I. Safarik, A. Clement, and O. P. Strausz, Can. J. Chem. 60, 1187 (1982).

H_2CF^+ $^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF stretch	1450[a]	gas	PE	[1]

D_2CF^+

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF stretch	1530[a]	gas	PE	[1]

[a] $\pm$ 30 cm^{-1}.

References

[1] L. Andrews, J. M. Dyke, N. Jonathan, N. Keddar, A. Morris, and A. Ridha, J. Phys. Chem. 88, 2364 (1984).

H_2CCl^+ $^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCl stretch	1040[a]	gas	PE	[1][2]

[a] $\pm$ 30 cm^{-1}.

References

[1] L. Andrews, J. M. Dyke, N. Jonathan, N. Keddar, A. Morris, and A. Ridha, Chem. Phys. Lett. 97, 89 (1983).

[2] L. Andrews, J. M. Dyke, N. Jonathan, N. Keddar, and A. Morris, J. Am. Chem. Soc. 106, 299 (1984).

H_2CBr^+ $^1A_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CBr stretch	860[a]	gas	PE	[1][2]

D_2CBr^+

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_2 "scissors"	1130[a]	gas	PE	[2]
	3	CBr stretch	780[a]	gas	PE	[2]

[a] ± 30 cm^{-1}.

References

[1] L. Andrews, J. M. Dyke, N. Jonathan, N. Keddar, A. Morris, and A. Ridha, Chem. Phys. Lett. 97, 89 (1983).

[2] L. Andrews, J. M. Dyke, N. Jonathan, N. Keddar, and A. Morris, J. Phys. Chem. 88, 1950 (1984).

HSiOH C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	OH stretch	3650	Ar	IR	[1]
	2	SiH stretch	1882[a] 1847	Ar	IR	[1]
	3	HSiO bend	937	Ar	IR	[1]
	4	SiO stretch	851	Ar	IR	[1]
	5	SiOH bend	723	Ar	IR	[1]
a″	6	Torsion	595	Ar	IR	[1]

DSiOD

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	2	SiD stretch	1354	Ar	IR	[1]
	3	DSiO bend	715	Ar	IR	[1]
			701[b]	Ar	IR	[1]
	4	SiO stretch	847[b]	Ar	IR	[1]
			841	Ar	IR	[1]
	5	SiOD bend	521	Ar	IR	[1]
a″	6	Torsion	447	Ar	IR	[1]

[a] Fermi resonance splitting.

[b] Less stable rotamer, presumed to have the cis-structure.

References

[1] Z. K. Ismail, R. H. Hauge, L. Fredin, J. W. Kauffman, and J. L. Margrave, J. Chem. Phys. 77, 1617 (1982).

t-HNNH ^1A_g C_{2h} Structure: IR,UV [2][4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1	NH stretch	3128	N_2	Ram	[3]
	2	NH bend	1583	N_2	Ram	[3]
	3	N=N stretch	1529	N_2	Ram	[3]
a_u	4	Torsion	1250-1350	gas	IR	[4]
b_u	5	NH stretch	3120	gas	IR	[2][4]
	6	NH bend	1286	N_2	IR,Ram	[1][3]

t-DNND

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2	ND bend	1215	N_2	Ram	[3]
	3	N=N stretch	1539	N_2	Ram	[3]
b_u	5	ND stretch	2315	gas	IR	[4]
	6	ND bend	946	N_2	IR	[1][3]

References

[1] K. Rosengren and G. C. Pimentel, J. Chem. Phys. 43, 507 (1965).

[2] A. Trombetti, Can. J. Phys. 46, 1005 (1968).

[3] V. E. Bondybey and J. W. Nibler, J. Chem. Phys. 58, 2125 (1973).

[4] M. Carlotti, J. W. C. Johns, and A. Trombetti, Can. J. Phys. 52, 340 (1974).

H_2CF $^2B_1$ C_{2v} Structure: ESR[1] MW[5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CF stretch	1170.52	gas	DL	[6]
			1163m	Ar	IR	[2]-[4]
b_1	4	OPLA	300[a]	gas	MW	[5]

D_2CF

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CF stretch	1191m	Ar	IR	[2]-[4]
	3	CD_2 "scissors"	1013w	Ar	IR	[4]

[a] ± 30 cm^{-1}.

References

[1] R. W. Fessenden and R. H. Schuler, J. Chem. Phys. 43, 2704 (1965).

[2] M. E. Jacox and D. E. Milligan, J. Chem. Phys. 50, 3252 (1969).

[3] J. I. Raymond and L. Andrews, J. Phys. Chem. 75, 3235 (1971).

[4] M. E. Jacox, Chem. Phys. 59, 199 (1981).

[5] Y. Endo, C. Yamada, S. Saito, and E. Hirota, J. Chem. Phys. 79, 1605 (1983).

[6] C. Yamada and E. Hirota, Discussion of Molecular Structure, Chem. Soc. Japan, Tokyo (1982).

H_2CCl C_s Structure: ESR [3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′		CH_2 "scissors"	1356wm[a]	Ar	IR	[1]
		CCl stretch	827s	Ar	IR	[1][2]
		"Umbrella"	402s	Ar	IR	[1][2]

D_2CCl

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′		CD_2 "scissors"	1045m	Ar	IR	[1][2]
		CCl stretch	788m	Ar	IR	[1][2]
		"Umbrella"	291m	Ar	IR	[1][2]

[a] Absorption at 1390 cm^{-1} assigned to this fundamental in [2].

References

[1] M. E. Jacox and D. E. Milligan, J. Chem. Phys. 53, 2688 (1970).

[2] L. Andrews and D. W. Smith, J. Chem. Phys. 53, 2956 (1970).

[3] J. P. Michaut and J. Roncin, Chem. Phys. Lett. 12, 95 (1971).

H_2CBr

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_2 "scissors"	1355.7s	Ar	IR	[1][2]
		CH_2 rock	953w	Ar	IR	[1]
		CBr stretch	693.4s	Ar	IR	[1][2]
		"Umbrella"	368vs	Ar	IR	[1][2]

D_2CBr

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD_2 "scissors"	1016.4s	Ar	IR	[1][2]
		CD_2 rock	708w	Ar	IR	[1]
		CBr stretch	656.6m	Ar	IR	[1][2]
		"Umbrella"	263vs	Ar	IR	[1][2]

References

[1] D. W. Smith and L. Andrews, J. Chem. Phys. 55, 5295 (1971).

[2] L. Andrews, J. H. Miller, and E. S. Prochaska, J. Am. Chem. Soc. 101, 7158 (1979).

H_2CI

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_2 "scissors"	1331.5s	Ar	IR	[1]
		CI stretch	611wm	Ar	IR	[1]
		"Umbrella"	375s	Ar	IR	[1]

D_2CI

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD_2 "scissors"	994m	Ar	IR	[1]
		CI stretch	578w	Ar	IR	[1]
		"Umbrella"	271s	Ar	IR	[1]

References

[1] D. W. Smith and L. Andrews, J. Chem. Phys. 58, 5222 (1973).

H_2GeCl C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		GeH stretch	1856wm	Ar	IR	[1]
		GeH stretch	1810vs	Ar	IR	[1]
		GeH_2 "scissors"	734w	Ar	IR	[1]
		GeH_2 wag	715m	Ar	IR	[1]
		GeH_2 twist	685w	Ar	IR	[1]
		GeCl stretch	385s	Ar	IR	[1]

D_2GeCl

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	GeD stretch	1336w	Ar	IR	[1]
	GeD stretch	1304ms	Ar	IR	[1]
	GeD_2 "scissors"	533vw	Ar	IR	[1]
	GeD_2 wag	516w	Ar	IR	[1]
	GeD_2 twist	495vw	Ar	IR	[1]
	GeCl stretch	385m	Ar	IR	[1]

References

[1] R. J. Isabel and W. A. Guillory, J. Chem. Phys. 55, 1197 (1971).

H_2GeBr C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	GeH stretch	1859 ?	Ar	IR	[1]
	GeH stretch	1816s	Ar	IR	[1]
	GeH_2 wag	691m	Ar	IR	[1]
	GeH_2 twist	661wm	Ar	IR	[1]
	GeBr stretch	280s	Ar	IR	[1]

D_2GeBr

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	GeD stretch	1352s	Ar	IR	[1]
	GeD stretch	1339s	Ar	IR	[1]
	GeD_2 wag	498w	Ar	IR	[1]
	GeD_2 twist	472wm	Ar	IR	[1]
	GeBr stretch	279ms	Ar	IR	[1]

References

[1] R. J. Isabel and W. A. Guillory, J. Chem. Phys. 57, 1116 (1972).

HSOH

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	OH stretch	3425w	Ar	IR	[1]
	HOS bend	1177m	Ar	IR	[1]
	SO stretch	763s	Ar	IR	[1]
	Torsion	445m	Ar	IR	[1]

DSOD

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	OD stretch	2661wm	Ar	IR	[1]
	DOS bend	866m	Ar	IR	[1]
	SO stretch	775ms	Ar	IR	[1]
	DSO bend	737wm	Ar	IR	[1]
	Torsion	332wm	Ar	IR	[1]

References

[1] R. R. Smardzewski and M. C. Lin, J. Chem. Phys. 66, 3197 (1977).

6.6. Four-Atomic Monohydrides

HC_3

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C_3 a-stretch	1834	Ar	IR	[1]

DC_3

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C_3 a-stretch	1781	Ar	IR	[1]

References

[1] M. E. Jacox and D. E. Milligan, Chem. Phys. 4, 45 (1974).

HCCN

$^3\Sigma^-$ $C_{\infty v}$ Structure: ESR [1] MW [3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3229s	Ar	IR	[2]
	2	CCN a-stretch	1735s	Ar	IR	[2]
	3	CCN s-stretch	1178m	Ar	IR	[2]
Π	4	H deform.	458m	Ar	IR	[2]

DCCN

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2424ms	Ar	IR	[2]
	2	CCN a-stretch	1730s	Ar	IR	[2]
	3	CCN s-stretch	1127w	Ar	IR	[2]
Π	4	CCN bend	405wm	Ar	IR	[2]
	5	D deform.	318ms	Ar	IR	[2]

References

[1] R. A. Bernheim, R. J. Kempf, J. V. Gramas, and P. S. Skell, J. Chem. Phys. 43, 196 (1965).

[2] A. Dendramis and G. E. Leroi, J. Chem. Phys. 66, 4334 (1977).

[3] S. Saito, Y. Endo, and E. Hirota, J. Chem. Phys. 80, 1427 (1984).

HCNN

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3233wm	Ar	IR	[1]
			3229m	N_2	IR	[1]
		CNN a-stretch	1787s	Ar	IR	[1]
			1784s	Kr	IR	[1]
			1800s	N_2	IR	[1]
		H deform.	861vs	Ar	IR	[1]
			860vs	Kr	IR	[1]
			871m 863m	N_2	IR	[1]

DCNN

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CNN a-stretch	1771vs	Ar	IR	[1]
		D deform.	725vs	Ar	IR	[1]

References

[1] J. F. Ogilvie, Can. J. Chem. 46, 2472 (1968).

HOCN

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]
			3572	Ar	IR	[1]
			3506s	N_2	IR	[1]
	2	C≡N stretch	2294	Ne	IR	[5]
			2288	Ar	IR	[1]
			2294s	N_2	IR	[1]
	3	OH deform.	1227	Ne	IR	[5]
			1228	Ar	IR	[1]
			1241m	N_2	IR	[1]
	4	C-O stretch	1082	Ne	IR	[5]
			1080	Ar	IR	[1]
			1098s	N_2	IR	[1]
	5	OCN deform.	460wm	N_2	IR	[1]

DOCN

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	OD stretch	2635	Ar	IR	[1]
			2590sh	N_2	IR	[1]
	2	C≡N stretch	2285	Ar	IR	[1]
			2292s	N_2	IR	[1]
	3	C-O stretch	1078	Ar	IR	[1]
			1093m	N_2	IR	[1]
	4	OD deform.	949	Ar	IR	[1]
			957m	N_2	IR	[1]
	5	OCN deform.	437wm	N_2	IR	[1]

References

[1] M. E. Jacox and D. E. Milligan, J. Chem. Phys. 40, 2457 (1964).

[2] A. D. McLean, G. H. Loew, and D. S. Berkowitz, J. Mol. Spectrosc. 62, 184 (1977).

[3] D. Poppinger, L. Radom, and J. A. Pople, J. Am. Chem. Soc. 99, 7806 (1977).

[4] D. J. DeFrees, G. H. Loew, and A. D. McLean, Astrophys. J. 254, 405 (1982).

[5] V. E. Bondybey, J. H. English, C. W. Mathews, and R. J. Contolini, J. Mol. Spectrosc. 92, 431 (1982).

c-HOCO C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	OH stretch	3316wm	CO	IR	[1]
	2	C=O stretch	1797s	CO	IR	[1]
	3	HOC bend	1261s	CO	IR	[1]
	4	C-O stretch	1088s	CO	IR	[1]
	5	OCO bend	620m	CO	IR	[1]

c-DOCO

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	OD stretch	2456m	CO	IR	[1]
	2	C=O stretch	1798s	CO	IR	[1]
	3	C-O stretch + DOC bend	1148s	CO	IR	[1]
	5	OCO bend	563w	CO	IR	[1]
a"	6	Torsion	497wm	CO	IR	[1]

References

[1] D. E. Milligan and M. E. Jacox, J. Chem. Phys. 54, 927 (1971).

t-HOCO C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	OH stretch	3456vs	CO	IR	[1]
	2	C=O stretch	1833vs	CO	IR	[1]
	3	HOC bend	1261s	CO	IR	[1]
	4	C-O stretch	1077ms	CO	IR	[1]
	5	OCO bend	615m	CO	IR	[1]

t-DOCO

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

References

[1] D. E. Milligan and M. E. Jacox, J. Chem. Phys. 54, 927 (1971).

$HAlCl_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	AlH stretch	1968s	Ar	IR	[1]
	2	AlCl s-stretch	481s	Ar	IR	[1]
b_1	4	OPLA	472s	Ar	IR	[1]
b_2	5	AlCl a-stretch	579m	Ar	IR	[1]
	6	H deformation	654vs	Ar	IR	[1]

$DAlCl_2$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	AlD stretch	1430	Ar	IR	[1]
	2	AlCl s-stretch	478	Ar	IR	[1]
b_1	4	OPLA	355	Ar	IR	[1]
b_2	6	AlCl a-stretch	598	Ar	IR	[1]

References

[1] H. Schnockel, J. Mol. Struct. 50, 275 (1978).

HCOCl C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	CH stretch	2934w	gas	IR	[1]
	2	CO stretch	1784vs	gas	IR	[1]
	3	CH bend	1307m	gas	IR	[1]
	4	CCl stretch	739vs	gas	IR	[1]
	5	CCl bend	458vw	gas	IR	[1]
a″	6	OPLA	932vw	gas	IR	[1]

References

[1] I. C. Hisatsune and J. Heicklen, Can. J. Spectrosc. 18, 77 (1973).

HCF_2^+ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	5	CF_2 stretch	1608s 1605s	Ar	IR	[1]

DCF_2^+

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	5	CF_2 stretch	1599s 1596s	Ar Ar	IR IR	[1] [1]

References

[1] L. Andrews and F. T. Prochaska, J. Chem. Phys. 70, 4714 (1979).

$HCFCl^+$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′		CF stretch	1436m 1430m	Ar	IR	[1]
		CH deform.	1151wm	Ar	IR	[1]
		CCl stretch	920[a]	gas	PE	[2]

$DCFCl^+$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′		CF stretch	1414m 1406m	Ar	IR	[1]

[a] $\pm$ 40 cm^{-1}.

References

[1] F. T. Prochaska and L. Andrews, J. Chem. Phys. 73, 2651 (1980).

[2] L. Andrews, J. M. Dyke, N. Jonathan, N. Keddar, and A. Morris, J. Am. Chem. Soc. 106, 299 (1984).

$HCFBr^+$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′		CF stretch	1401s	Ar	IR	[1]
		CH deform.	1149m	Ar	IR	[1]

References

[1] F. T. Prochaska and L. Andrews, J. Chem. Phys. 73, 2651 (1980).

$HCFI^+$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′		CF stretch	1359m	Ar	IR	[1]

References

[1] F. T. Prochaska and L. Andrews, J. Chem. Phys. 73, 2651 (1980).

$HCCl_2^+$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	3032.8w	Ar	IR	[3]
	2	CCl stretch	860[a]	gas	PE	[4]
			845w	Ar	IR	[3]
b_2	5	H deformation	1291m	Ar	IR	[1]-[3]
	6	CCl stretch	1044s	Ar	IR	[1]-[3]

$DCCl_2^+$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CCl stretch	790[a]	gas	PE	[4]
b_2	5	CCl stretch	1122s	Ar	IR	[1][2]
	6	D deformation	864wm	Ar	IR	[1][2]

[a] ± 30 cm^{-1}.

References

[1] M. E. Jacox and D. E. Milligan, J. Chem. Phys. 54, 3935 (1971).

[2] M. E. Jacox, Chem. Phys. 12, 51 (1976).

[3] B. J. Kelsall and L. Andrews, J. Mol. Spectrosc. 97, 362 (1983).

[4] L. Andrews, J. M. Dyke, N. Jonathan, N. Keddar, and A. Morris, J. Chem. Phys. 79, 4650 (1983).

$HCClBr^+$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CCl stretch	994m	Ar	IR	[1]

$DCClBr^+$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1077s	Ar	IR	[1]

References

[1] L. Andrews, C. A. Wight, F. T. Prochaska, S. A. McDonald, and B. S. Ault, J. Mol. Spectrosc. 73, 120 (1978).

$HCBr_2^+$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	5	H deformation	1229m	Ar	IR	[1][2]
	6	CBr stretch	897vs	Ar	IR	[1]-[3]

$DCBr_2^+$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	5	D deformation	1015vs	Ar	IR	[1][2]
	6	CBr stretch	781s	Ar	IR	[1][2]

References

[1] L. Andrews, C. A. Wight, F. T. Prochaska, S. A. McDonald, and B. S. Ault, J. Mol. Spectrosc. 73, 120 (1978).

[2] L. Andrews, F. T. Prochaska, and B. S. Ault, J. Am. Chem. Soc. 101, 9 (1979).

[3] B. J. Kelsall and L. Andrews, J. Mol. Spectrosc. 97, 362 (1983).

c-HSNO

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	SH stretch	2566vw	Ar	IR	[2]
	2	NO stretch	1570vs	Ar	IR	[1][2]
	3	HSN bend	858.5m	Ar	IR	[2]
	4	SN stretch	503m[a]	Ar	IR	[1][2]
	5	SNO bend	307wm	Ar	IR	[2]
a″	6	Torsion	406.5w	Ar	IR	[2]

c-DSNO

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	2	NO stretch	1568vs	Ar	IR	[2]
	3	DNS bend	715	Ar	IR	[2]
	4	SN stretch	435	Ar	IR	[2]
	5	SNO bend	305.5	Ar	IR	[2]

[a] Assigned in [1] to the trans- rotamer.

References

[1] P. O. Tchir and R. D. Spratley, Can. J. Chem. 53, 2318 (1975).

[2] R. P. Muller, M. Nonella, P. Russegger, and J. R. Huber, Chem. Phys. 87, 351 (1984).

t-HSNO

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	SH stretch	2613vw 2607vw	Ar	IR	[2]
	2	NO stretch	1596vs	Ar	IR	[1][2]
	3	HSN bend	877.5m	Ar	IR	[1][2]
	4	SN stretch	543.5m	Ar	IR	[1][2]
	5	SNO bend	297m	Ar	IR	[1][2]
a"	6	Torsion	386.5w	Ar	IR	[2]

t-DSNO

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	NO stretch	1595vs	Ar	IR	[1][2]
	3	DSN bend	724m	Ar	IR	[1][2]
	4	SN stretch	485.5m	Ar	IR	[1][2]
	5	SNO bend	297m	Ar	IR	[1][2]

References

[1] P. O. Tchir and R. D. Spratley, Can. J. Chem. 53, 2318 (1975).

[2] R. P. Muller, M. Nonella, P. Russegger, and J. R. Huber, Chem. Phys. 87, 351 (1984).

c-HNSO [a] C_s Structure: MW [2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH stretch	3345w	gas	IR	[1]
			3308wm	Ar	IR	[3]
			3303	N_2	IR	[3]
	2	SO stretch	1261s	gas	IR	[1]
			1249vs	Ar	IR	[3]
			1252	N_2	IR	[3]
	3	NS stretch	1090w	gas	IR	[1]
			1083s	Ar	IR	[3]
			1094	N_2	IR	[3]
	4	HNS bend	911m	gas	IR	[1]
			900s	Ar	IR	[3]
			923	N_2	IR	[3]
	5	NSO bend	453m	gas	IR	[1]
			447s	Ar	IR	[3]
			455	N_2	IR	[3]
a"	6	Torsion	759s	gas	IR	[1]
			755vs	Ar	IR	[3]
			774	N_2	IR	[3]

c-DNSO

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	ND stretch	2480w	gas	IR	[1]
			2453	Ar	IR	[3]
	2	SO stretch	1257s	gas	IR	[1]
			1245	Ar	IR	[3]
	3	NS stretch	1055w	gas	IR	[1]
			1048	Ar	IR	[3]
	4	DNS bend	757m	gas	IR	[1]
			752	Ar	IR	[3]
	5	NSO bend	~410m	gas	IR	[1]
			400	Ar	IR	[3]
a"	6	Torsion	594s	gas	IR	[1]
			594	Ar	IR	[3]

[a] Stable rotamer.

References

[1] H. Richert, Z. Anorg. Allg. Chem. 309, 171 (1961).

[2] W. H. Kirchhoff, J. Am. Chem. Soc. 91, 2437 (1969).

[3] P. O. Tchir and R. D. Spratley, Can. J. Chem. 53, 2311 (1975).

t-HNSO

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	SO stretch	1382	Ar	IR	[1]
	3	NS stretch	986	Ar	IR	[1]
	4	HNS bend	881	Ar	IR	[1]
a"	6	Torsion	651	Ar	IR	[1]

t-DNSO

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	SO stretch	1380	Ar	IR	[1]
	3	NS stretch	951	Ar	IR	[1]

References

[1] P. O. Tchir and R. D. Spratley, Can. J. Chem. 53, 2331 (1975).

c-HOSN

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3520m	Ar	IR	[1]
		SN stretch	1321w	Ar	IR	[1]
		HOS bend	992w	Ar	IR	[1]
		SO stretch	674vs	Ar	IR	[1]
		Torsion	418m	Ar	IR	[1]
		OSN bend	374vw	Ar	IR	[1]

c-DOSN

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OD stretch	2597m	Ar	IR	[1]
		SN stretch	1319w	Ar	IR	[1]
		SO stretch	671vs	Ar	IR	[1]
		Torsion	325m	Ar	IR	[1]

References

[1] P. O. Tchir and R. D. Spratley, Can. J. Chem. 53, 2318 (1975).

HCF_2 C_s Structure: ESR [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CF s-stretch	1164s	Ar	IR	[2][3]
a"	5	HCF deform.	1317m	Ar	IR	[2][3]
	6	CF a-stretch	1173vs	Ar	IR	[2][3]

DCF_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CF s-stretch	1143m	Ar	IR	[2][3]
a"	5	CF a-stretch	1214s	Ar	IR	[2][3]
	6	DCF deform.	933wm	Ar	IR	[2][3]

References

[1] R. W. Fessenden and R. H. Schuler, J. Chem. Phys. 43, 2704 (1965).

[2] T. G. Carver and L. Andrews, J. Chem. Phys. 50, 5100 (1969).

[3] M. E. Jacox, J. Mol. Spectrosc. 81, 349 (1980).

HCFCl

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		H deform.	1283s	Ar	IR	[1]
		CF stretch	1151s	Ar	IR	[1]
		CCl stretch	757m	Ar	IR	[1]

DCFCl

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1154s	Ar	IR	[1]
		CD deform.	960m	Ar	IR	[1][2]

References

[1] F. T. Prochaska, B. W. Keelan, and L. Andrews, J. Mol. Spectrosc. 76, 142 (1979).

[2] F. T. Prochaska and L. Andrews, J. Chem. Phys. 73, 2651 (1980).

HCFBr

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		H deform.	1266m	Ar	IR	[1][2]
		CF stretch	1149s	Ar	IR	[1][2]
		CBr stretch	650wm[a]	Ar	IR	[1]

DCFBr

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1162s	Ar	IR	[1]
		D deform.	913m	Ar	IR	[1]

[a] Tentative assignment.

References

[1] F. T. Prochaska, B. W. Keelan, and L. Andrews, J. Mol. Spectrosc. 76, 142 (1979).

[2] F. T. Prochaska and L. Andrews, J. Chem. Phys. 73, 2651 (1980).

HCFI

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		H deform.	1256s	Ar	IR	[1][2]
		CF stretch	1138s	Ar	IR	[1][2]
		CI stretch	560m	Ar	IR	[1][2]

References

[1] F. T. Prochaska, B. W. Keelan, and L. Andrews, J. Mol. Spectrosc. 76, 142 (1979).

[2] F. T. Prochaska and L. Andrews, J. Chem. Phys. 73, 2651 (1980).

$HCCl_2$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a"	5	HCCl deform.	1226m	Ar	IR	[1]
	6	CCl a-stretch	902vs	Ar	IR	[1]

$DCCl_2$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a"	5	DCCl deform.	974vs	Ar	IR	[1][2]
	6	CCl a-stretch	814s	Ar	IR	[1][2]

References

[1] T. G. Carver and L. Andrews, J. Chem. Phys. 50, 4235 (1969).

[2] E. E. Rogers, S. Abramowitz, M. E. Jacox, and D. E. Milligan, J. Chem. Phys. 52, 2198 (1970).

HCClBr

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	H deformation	1196m	Ar	IR	[1]
	3	CCl stretch	866s	Ar	IR	[1]

References

[1] T. G. Carver and L. Andrews, J. Chem. Phys. 50, 4235 (1969).

$HCBr_2$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CBr s-stretch	633wm	Ar	IR	[1]
a"	5	HCBr deform.	1165s	Ar	IR	[1]-[4]
	6	CBr a-stretch	778vs	Ar	IR	[1]-[5]

$DCBr_2$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CBr s-stretch	616w	Ar	IR	[1]
a"	5	DCBr deform.	898vs	Ar	IR	[1][3][4]
	6	CBr a-stretch	725s	Ar	IR	[1][3][4]

References

[1] T. G. Carver and L. Andrews, J. Chem. Phys. 50, 4223 (1969).

[2] E. E. Rogers, S. Abramowitz, M. E. Jacox, and D. E. Milligan, J. Chem. Phys. 52, 2198 (1970).

[3] L. Andrews, C. A. Wight, F. T. Prochaska, S. A. McDonald, and B. S. Ault, J. Mol. Spectrosc. 73, 120 (1978).

[4] L. Andrews, F. T. Prochaska, and B. S. Ault, J. Am. Chem. Soc. 101, 9 (1979).

[5] B. J. Kelsall and L. Andrews, J. Mol. Spectrosc. 97, 362 (1983).

HCI_2 C_s (C_{2v} ?)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a"	5	HCI deform.	1106	Ar	IR	[1]
	6	CI stretch	716	Ar	IR	[1]

DCI_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a"	5	DCI deform.	850	Ar	IR	[1]
	6	CI stretch	653	Ar	IR	[1]

References

[1] D. W. Smith and L. Andrews, J. Phys. Chem. 76, 2718 (1972).

6.7. Four-Atomic Nonhydrides

C_4 $^3\Sigma_g^-$ $D_{\infty h}$ Structure: ESR [2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	Asym. stretch	2164	Ar	IR	[1][2]

References

[1] K. R. Thompson, R. L. DeKock, and W. Weltner, Jr., J. Am. Chem. Soc. 93, 4688 (1971).

[2] W. R. M. Graham, K. I. Dismuke, and W. Weltner, Jr., Astrophys. J. 204, 301 (1976).

CCCO

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Stretch	2244	Ar	IR	[1]

References

[1] R. L. DeKock and W. Weltner, Jr., J. Am. Chem. Soc. 93, 7106 (1971).

ClCCN

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2118s	Ar	IR	[1]
			2113s	Ar	IR	[1]
			1945s	Ar	IR	[1]
			1025m	Ar	IR	[1]
			996ms	Ar	IR	[1]

References

[1] D. E. Milligan, M. E. Jacox, and A. M. Bass, J. Chem. Phys. 43, 3149 (1965).

BrCCN

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			2102m	Ar	IR	[1]
			1923ms	Ar	IR	[1]
			1035vw	Ar	IR	[1]
			984vs	Ar	IR	[1]

References

[1] D. E. Milligan, M. E. Jacox, and A. M. Bass, J. Chem. Phys. 43, 3149 (1965).

FNCN

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C≡N stretch	2068s	Ar	IR	[1]
		NF stretch	874s	Ar	IR	[1]

References

[1] D. E. Milligan and M. E. Jacox, J. Chem. Phys. 48, 4811 (1968).

$FSCN^+$ $^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SF stretch	840[a]	gas	PE	[1]

[a] ± 50 cm^{-1}.

References

[1] G. Jonkers, O. Grabandt, R. Mooyman, and C. A. de Lange, J. Electron Spectrosc. Relat. Phenom. 26, 147 (1982).

$ClSCN^+$ $^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′		SCl stretch	570[a]	gas	PE	[1]

[a] ± 50 cm^{-1}.

References

[1] D. C. Frost, C. B. MacDonald, C. A. McDowell, and N. P. C. Westwood, J. Am. Chem. Soc. 103, 4423 (1981).

$BrSCN^+$ $^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′		SBr stretch	450[a]	gas	PE	[1]

[a] ± 50 cm^{-1}.

References

[1] D. C. Frost, C. B. MacDonald, C. A. McDowell, and N. P. C. Westwood, J. Am. Chem. Soc. 103, 4423 (1981).

$ClSeCN^+$ $^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′		SeCl stretch	440[a]	gas	PE	[1]

[a] ± 50 cm^{-1}.

References

[1] G. Jonkers, R. Mooyman, and C. A. de Lange, Mol. Phys. 43, 655 (1981).

$BrSeCN^+$ $^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′		SeBr stretch	360[a]	gas	PE	[1]

[a] ± 50 cm^{-1}.

References

[1] G. Jonkers, R. Mooyman, and C. A. de Lange, Mol. Phys. 43, 655 (1981).

C_2F_2 $D_{\infty h}$

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

References

[1] J. Heicklen and V. Knight, J. Phys. Chem. 69, 2484 (1965).

CO_3 C_{2v} Structure: IR [3]; MO [4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	C=O stretch	2053[a]	Ar	IR	[2]
			2045vs	CO_2	IR	[1][3]
	2	O...O stretch	1070	Ar	IR	[2]
			1073m	CO_2	IR	[1][3]
	3	C-O stretch	593m	CO_2	IR	[1][3]

CO_3---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	5	C-O stretch	975	Ar	IR	[2]
			972s	CO_2	IR	[1][3]
	6	O-C=O bend	564	Ar	IR	[2]
			568m	CO_2	IR	[1][3]

[a] Fermi resonance with overtone of 975-cm^{-1} fundamental leads to appearance of another very prominent absorption at 1894 cm^{-1} (1880 cm^{-1} in CO_2 matrix experiments).

References

[1] N. G. Moll, D. R. Clutter, and W. E. Thompson, J. Chem. Phys. 45, 4469 (1966).

[2] E. Weissberger, W. H. Breckenridge, and H. Taube, J. Chem. Phys. 47, 1764 (1967).

[3] M. E. Jacox and D. E. Milligan, J. Chem. Phys. 54, 919 (1971).

[4] J. R. Sabin and H. Kim, Chem. Phys. Lett. 11, 593 (1971).

$c\text{-}(NO)_2$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Asym. stretch	1776s	Ar	IR	[1]
			1785	N_2	IR	[2]
			1768s	CO_2	IR	[1]
		Sym. stretch	1866m	Ar	IR	[1]
			1870	N_2	IR	[2]
			1862m	CO_2	IR	[1]

References

[1] W. G. Fateley, H. A. Bent, and B. Crawford, Jr., J. Chem. Phys. 31, 204 (1959).

[2] W. A. Guillory and C. E. Hunter, J. Chem. Phys. 50, 3516 (1969).

$t\text{-}(NO)_2$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Asym. stretch	1764	N_2	IR	[2]
			1740	CO_2	IR	[1]

References

[1] W. G. Fateley, H. A. Bent, and B. Crawford, Jr., J. Chem. Phys. 31, 204 (1959).

[2] W. A. Guillory and C. E. Hunter, J. Chem. Phys. 50, 3516 (1969).

$F_2{}^{11}BO$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1		1369	gas	UV	[1]
	2		856.0	gas	UV	[1][2]
	3		491.0	gas	UV	[1][2]

References

[1] S. L. N. G. Krishnamachari and B. R. Vengsarkar, Proc. Ind. Acad. Sci. 61, 172 (1965).

[2] C. W. Mathews and K. K. Innes, J. Mol. Spectrosc. 15, 199 (1965).

$^{11}BCl_3^+$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e′	3	BCl stretch	1090	Ar	IR	[1]

References

[1] J. H. Miller and L. Andrews, J. Am. Chem. Soc. 102, 4900 (1980).

$^{11}BBr_3^+$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e′	3	BBr stretch	930	Ar	IR	[1]

References

[1] J. H. Miller and L. Andrews, J. Am. Chem. Soc. 102, 4900 (1980).

CO_3^- $^2B_1$ C_{2v} Structure: MO [2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	OCO s-stretch	1314[ab]	Ar	IR	[1]
			1308[ac]	Ar	IR	[1]
			1308[ad]	Ar	IR	[1]
b_2	5	OCO a-stretch	1480[ab]	Ar	IR	[1]
			1494[ac]	Ar	IR	[1]
			1513[ad]	Ar	IR	[1]

[a] Assignment given for structure obtained in ab initio calculation of [2]. D_{3h} structure cannot be excluded on the basis of the infrared observations; NO_3^-, known to have a D_{3h} structure, exhibits a similar splitting for its NO-stretching fundamentals in an argon matrix, due to the electric field of the cation.

[b] Cs^+ present.

[c] K^+ present.

[d] Na^+ present.

References

[1] M. E. Jacox and D. E. Milligan, J. Mol. Spectrosc. 52, 363 (1974).

[2] S. P. So, J. Chem. Soc., Faraday Trans. 2 72, 646 (1976).

F_2CN $^2B_2$ C_{2v} Structure: UV [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	C=N stretch	1734vs[a] 1771vs	Ar	IR	[2]
	2	CF stretch	955ms	Ar	IR	[2]
b_1	4	OPLA	660m	Ar	IR	[2]
b_2	5	CF stretch	1257vs	Ar	IR	[2]
	6	CF_2 rock	497ms	N_2	IR	[2]

[a] Strong Fermi resonance interaction with $(\nu_5 + \nu_6)$ (A_1).

References

[1] R. N. Dixon, G. Duxbury, R. C. Mitchell, and J. P. Simons, Proc. Roy. Soc. (London) A300, 405 (1967).

[2] M. E. Jacox and D. E. Milligan, J. Chem. Phys. 48, 4040 (1968).

NO_3 $^2A_2'$ D_{3h} Structure: DL [3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1	Sym. stretch	1050	gas	LF	[1][2]
e'	3	NO stretch	1492.39	gas	LF,DL	[1]-[3]
	4	Deformation	360	gas	LF	[1][2]

References

[1] H. H. Nelson, L. Pasternack, and J. R. McDonald, J. Phys. Chem. 87, 1286 (1983).

[2] T. Ishiwata, I. Fujiwara, Y. Naruge, K. Obi, and I. Tanaka, J. Phys. Chem. 87, 1349 (1983).

[3] T. Ishiwata, I. Tanaka, K. Kawaguchi, and E. Hirota, XVI Internat. Symp. on Free Radicals, Lauzelle-Ottignies, Belgium (1983).

FCO_2^- C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CO stretch	1316[a]	Ar	IR	[1]
	2	CF stretch	883[a]	Ar	IR	[1]
b_2	4	CO stretch	1749[a]	Ar	IR	[1]

[a] Cs^+ in adjacent site.

References

[1] B. S. Ault, Inorg. Chem. 21, 756 (1982).

Cl_2CSe C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CSe stretch	991vs	Ne	IR	[1]
			984vs	Ar	IR,Ram	[1]
	2	CCl_2 s-stretch	437m	Ne	IR	[1]
			434m	Ar	IR,Ram	[1]
	3	CCl_2 deform.	260m	Ar	Ram	[1]
b_2	5	CCl_2 a-stretch	821vs	Ne	IR	[1]
			809vs	Ar	IR	[1]
	6	SeCCl deform.	248w	Ar	Ram	[1]

References

[1] A. Darmadi, A. Haas, H. Willner, and H. Schnockel, Z. Naturforsch. 86b, 1261 (1981).

CF_3^+ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	3	CF stretch	1667	Ar	IR	[1]

References

[1] F. T. Prochaska and L. Andrews, J. Am. Chem. Soc. 100, 2102 (1978).

CF_2Cl^+ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF stretch	1507s	Ar	IR	[1]-[3]
b_2	5	CF stretch	1406vs	Ar	IR	[1]-[3]

References

[1] M. E. Jacox, Chem. Phys. Lett. 54, 176 (1978).

[2] F. T. Prochaska and L. Andrews, J. Am. Chem. Soc. 100, 2102 (1978).

[3] F. T. Prochaska and L. Andrews, J. Chem. Phys. 68, 5577 (1978).

CF_2Br^+ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF stretch	1480m	Ar	IR	[1]-[3]
b_2	5	CF stretch	1362s	Ar	IR	[1]-[3]

References

[1] M. E. Jacox, Chem. Phys. Lett. 54, 176 (1978).

[2] F. T. Prochaska and L. Andrews, J. Am. Chem. Soc. 100, 2102 (1978).

[3] F. T. Prochaska and L. Andrews, J. Phys. Chem. 82, 1731 (1978).

CF_2I^+ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF stretch	1433	Ar	IR	[1]
b_2	5	CF stretch	1321	Ar	IR	[1]

References

[1] F. T. Prochaska and L. Andrews, J. Am. Chem. Soc. 100, 2102 (1978).

$CFCl_2^+$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1352vs	Ar	IR	[1]
		CCl a-stretch	1142vs	Ar	IR	[1]

References

[1] F. T. Prochaska and L. Andrews, J. Chem. Phys. 68, 5568 (1978).

$CFBr_2^+$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1322vs	Ar	IR	[1]
			1311vs	Ar	IR	[1][2]
		CBr stretch	991vs	Ar	IR	[1][2]

References

[1] F. T. Prochaska and L. Andrews, J. Phys. Chem. 82, 1731 (1978).

[2] B. W. Keelan and L. Andrews, J. Phys. Chem. 83, 2488 (1979).

CFI_2^+ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1270s	Ar	IR	[1]
		CI a-stretch	914m	Ar	IR	[1]

References

[1] B. W. Keelan and L. Andrews, J. Phys. Chem. 83, 2488 (1979).

CCl_3^+ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e′	3	CCl stretch	1037	Ar	IR	[1]-[3]

References

[1] M. E. Jacox and D. E. Milligan, J. Chem. Phys. 54, 3935 (1971).

[2] M. E. Jacox, Chem. Phys. 12, 51 (1976).

[3] F. T. Prochaska and L. Andrews, J. Chem. Phys. 67, 1091 (1977).

CCl_2Br^+ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1020	Ar	IR	[1]
			954	Ar	IR	[1]

References

[1] L. Andrews, C. A. Wight, F. T. Prochaska, S. A. McDonald, and B. S. Ault, J. Mol. Spectrosc. 73, 120 (1978).

$CClBr_2^+$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			976	Ar	IR	[1][2]
			892	Ar	IR	[1][2]

References

[1] L. Andrews, J. M. Grzybowski, and R. O. Allen, J. Phys. Chem. 79, 904 (1975).

[2] L. Andrews, C. A. Wight, F. T. Prochaska, S. A. McDonald, and B. S. Ault, J. Mol. Spectrosc. 73, 120 (1978).

CBr_3^+ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e′		CBr stretch	874	Ar	IR	[1]-[3]

References

[1] L. Andrews, J. M. Grzybowski, and R. O. Allen, J. Phys. Chem. 79, 904 (1975).

[2] F. T. Prochaska and L. Andrews, J. Chem. Phys. 67, 1091 (1977).

[3] L. Andrews, C. A. Wight, F. T. Prochaska, S. A. McDonald, and B. S. Ault, J. Mol. Spectrosc. 73, 120 (1978).

F_2SiO C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Si=O stretch	1309vs	Ar	IR	[1]
	2	SiF s-stretch	835m	Ar	IR	[1]
	3	SiF_2 deform.	423wm	Ar	IR	[1]
b_1	4	OPLA	344s	Ar	IR	[1]
b_2	5	SiF a-stretch	996s	Ar	IR	[1]
	6	SiF_2 rock	333m	Ar	IR	[1]

References

[1] H. Schnockel, J. Mol. Struct. 65, 115 (1980).

Cl_2SiO C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	Si=O stretch	1240s	Ar	IR	[1]
	2	SiCl s-stretch	501m	Ar	IR	[1]
b_1	4	OPLA	280ms	Ar	IR	[1]
b_2	5	SiCl a-stretch	638vs	Ar	IR	[1]
	6	$SiCl_2$ rock	269m	Ar	IR	[1]

References

[1] H. Schnockel, Z. Anorg. Allg. Chem. 460, 37 (1980).

$SiCl_3^+$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SiCl stretch	742	Ar	IR	[1]

References

[1] J. H. Miller and L. Andrews, J. Mol. Struct. 77, 65 (1981).

FONO

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		NO_2 a-stretch	1716s	N_2	IR	[1]
		NO_2 s-stretch	1200m	N_2	IR	[1]
		FON bend	702wm	N_2	IR	[1]
		Torsion	412m	N_2	IR	[1]

References

[1] R. R. Smardzewski and W. B. Fox, J. Chem. Phys. 60, 2980 (1974).

ClONO 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]
		ClO stretch	856m	Ar	IR	[1]
		ONO bend	390ms	Ar	IR	[1]
a"		Torsion	398m	Ar	IR	[1]

References

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

[2] H. Niki, P. D. Maker, C. M. Savage, and L. P. Breitenbach, Chem. Phys. Lett. 59, 78 (1978).

OClNO

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		N=O stretch	1752ms	Ar	IR	[1]

References

[1] D. E. Tevault and R. R. Smardzewski, J. Chem. Phys. 37, 3777 (1977).

$BrNO_2$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NO_2 s-stretch	1289s	Ar	IR	[1][2]
	2	NO_2 deform.	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	1660m[a]	Ar	IR	[2]
	6	NO_2 wag	402w[b]	Ar	IR	[2]

[a] Partially obscured by nearby N_2O_4 absorption.

[b] This fundamental assigned to a moderately intense 360-cm^{-1} absorption by [1].

References

[1] M. Feuerhahn, R. Minkwitz, and U. Engelhardt, J. Mol. Spectrosc. 77, 429 (1979).

[2] D. E. Tevault, J. Phys. Chem. 83, 2217 (1979).

BrONO

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		N=O stretch	1725vs[a]	Ar	IR	[1][2]
			837s	Ar	IR	[2]
			588vs[a]	Ar	IR	[1][2]
			392m	Ar	IR	[2]

[a] Attributed by [1] to $Br-NO_2$.

References

[1] M. Feuerhahn, R. Minkwitz, and U. Engelhardt, J. Mol. Spectrosc. 77, 429 (1979).

[2] D. E. Tevault, J. Phys. Chem. 83, 2217 (1979).

INO_2 C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	NO_2 s-stretch	1279s	Ar	IR	[1]
	2	NO_2 deform.	569vs	Ar	IR	[1]
	3	NI stretch	468w	Ar	IR	[1]
b_1	4	OPLA	650w	Ar	IR	[1]
b_2	5	NO_2 a-stretch	1700s	Ar	IR	[1]
	6	NO_2 rock	305m	Ar	IR	[1]

References

[1] M. Feuerhahn, R. Minkwitz, and U. Engelhardt, J. Mol. Spectrosc. 77, 429 (1979).

S_4

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			680	Ar	IR	[1]
			681s	Kr	IR	[1]
			680	Xe	IR	[1]
			660	Ar	IR	[1]
			660s	Kr	IR	[1]
			660	Xe	IR	[1]
			636s	Kr	IR	[1]

S_4---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			483wm	Kr	IR	[1]
			320m	Kr	IR	[1]
			270wm	Kr	IR	[1]

References

[1] B. Meyer and T. Stroyer-Hansen, J. Phys. Chem. 76, 3968 (1972).

CF_3 C_{3v} Structure: ESR [1]; IR [6]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CF stretch	1090[a]	gas	IR	[2]
			1083	Ne	IR	[5]
			1087s	Ar	IR	[3][4]
	2	"Umbrella"	701[b]	gas	IR	[2]
			700	Ne	IR	[5]
			703m	Ar	IR	[3][4]
e	3	CF stretch	1260.16	gas	IR	[2][6]
			1252	Ne	IR	[5]
			1251vs	Ar	IR	[3][4]
	4	Deformation	508	Ne	IR	[5]
			512w	Ar	IR	[4]

[a] $\pm$ 2 cm^{-1}.

[b] $\pm$ 3 cm^{-1}.

References

[1] R. W. Fessenden and R. H. Schuler, J. Chem. Phys. 43, 2704 (1965).

[2] G. A. Carlson and G. C. Pimentel, J. Chem. Phys. 44, 4053 (1966).

[3] D. E. Milligan, M. E. Jacox, and J. J. Comeford, J. Chem. Phys. 44, 4058 (1966).

[4] D. E. Milligan and M. E. Jacox, J. Chem. Phys. 48, 2265 (1968).

[5] A. Snelson, High Temp. Sci. 2, 70 (1970).

[6] C. Yamada and E. Hirota, J. Chem. Phys. 78, 1703 (1983).

CF_2Cl C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CF stretch	1148vs	Ar	IR	[1][2]
	2	CCl stretch	761s	Ar	IR	[1][2]
	3	CF_2 "scissors"	599m	Ar	IR	[1][2]
a"	5	CF stretch	1208vs	Ar	IR	[1][2]

References

[1] D. E. Milligan, M. E. Jacox, J. H. McAuley, and C. E. Smith, J. Mol. Spectrosc. 45, 377 (1973).

[2] F. T. Prochaska and L. Andrews, J. Chem. Phys. 68, 5577 (1978).

CF_2Br C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1198	Ar	IR	[1][2]
		CF stretch	1138	Ar	IR	[1][2]
		CBr stretch	684	Ar	IR	[1][2]

References

[1] M. E. Jacox, Chem. Phys. Lett. 53, 192 (1978).

[2] F. T. Prochaska and L. Andrews, J. Am. Chem. Soc. 100, 2102 (1978).

CF_2I C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1126	Ar	IR	[1]
		CI stretch	627	Ar	IR	[1]

References

[1] F. T. Prochaska and L. Andrews, J. Am. Chem. Soc. 100, 2102 (1978).

$CFCl_2$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CF stretch	1143vs	Ar	IR	[1][2]
	2	CCl stretch	747m	Ar	IR	[1][2]
a"	5	CCl stretch	919vs	Ar	IR	[1][2]

References

[1] D. E. Milligan, M. E. Jacox, J. H. McAuley, and C. E. Smith, J. Mol. Spectrosc. 45, 377 (1973).

[2] F. T. Prochaska and L. Andrews, J. Chem. Phys. 68, 5568 (1978).

$CFBr_2$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1136vs	Ar	IR	[1][2]
			782s	Ar	IR	[1]

References

[1] F. T. Prochaska and L. Andrews, J. Phys. Chem. 82, 1731 (1978).

[2] B. W. Keelan and L. Andrews, J. Phys. Chem. 83, 2488 (1979).

CFI_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1149vs	Ar	IR	[1]
			735ms	Ar	IR	[1]

References

[1] B. W. Keelan and L. Andrews, J. Phys. Chem. 83, 2488 (1979).

CCl_3 C_{3v} Structure: ESR [5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	CCl stretch	898vs	Ar	IR	[1]-[4] [6]

References

[1] L. Andrews, J. Phys. Chem. 71, 2761 (1967).

[2] L. Andrews, J. Chem. Phys. 48, 972 (1968).

[3] J. H. Current and J. K. Burdett, J. Phys. Chem. 73, 3504 (1979).

[4] E. E. Rogers, S. Abramowitz, M. E. Jacox, and D. E. Milligan, J. Chem. Phys. 52, 2198 (1970).

[5] C. Hesse, N. Leray, and J. Roncin, Mol. Phys. 22, 137 (1971).

[6] A. K. Maltsev, R. G. Mikaelian, O. M. Nefedov, R. H. Hauge, and J. L. Margrave, Proc. Natl. Acad. Sci. (U. S. A.) 68, 3238 (1971).

CCl_2Br C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CCl stretch	888vs	Ar	IR	[1]-[3]
		CCl stretch	835vs	Ar	IR	[1]-[3]

References

[1] L. Andrews, J. Chem. Phys. 48, 972 (1968).

[2] J. H. Current and J. K. Burdett, J. Phys. Chem. 73, 3504 (1969).

[3] A. K. Maltsev, O. M. Nefedov, R. H. Hauge, J. L. Margrave, and D. Seyferth, J. Phys. Chem. 75, 3984 (1971).

CCl_2I

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CCl stretch	871	Ar	IR	[1]
		CCl stretch	810	Ar	IR	[1]

References

[1] L. Andrews, J. Chem. Phys. 48, 972 (1968).

$CClBr_2$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CCl stretch	856vs	Ar	IR	[1][2]
		CBr stretch	783vs	Ar	IR	[1][2]

References

[1] L. Andrews, J. Chem. Phys. 48, 972 (1968).

[2] A. K. Maltsev, O. M. Nefedov, R. H. Hauge, J. L. Margrave, and D. Seyferth, J. Phys. Chem. 75, 3984 (1971).

CBr_3

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	CBr stretch	773vs	Ar	IR	[1]-[3]

References

[1] L. Andrews, J. Chem. Phys. 48, 972 (1968).

[2] L. Andrews and T. G. Carver, J. Chem. Phys. 49, 896 (1968).

[3] E. E. Rogers, S. Abramowitz, M. E. Jacox, and D. E. Milligan, J. Chem. Phys. 52, 2198 (1970).

CI_3

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	3	CI stretch	693	Ar	IR	[1]

References

[1] D. W. Smith and L. Andrews, J. Phys. Chem. 76, 2718 (1972).

SiF_3 C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiF stretch	830[a]	gas	UV	[3]
			832s	Ar	IR	[2]
	2	"Umbrella"	427[b]	gas	UV	[3]
			406s	Ar	IR	[2]
e	3	SiF stretch	937[b]	gas	UV	[3]
			954vs	Ar	IR	[2]
	4	Deformation	290wm[c]	Ar	IR	[2]

[a] $\pm$ 10 cm^{-1}.

[b] $\pm$ 5 cm^{-1}.

[c] Ref. [3] reports a value of 345 $\pm$ 5 cm^{-1} for this fundamental. However, the Deslandres table from which this value is obtained would correspond to a doubly forbidden transition of SiF_3, and the data in it agree within the experimental error with those reported by [1] for SiF_2, a likely product in such discharge experiments.

References

[1] V. M. Khanna, G. Besenbruch, and J. L. Margrave, J. Chem. Phys. 46, 2310 (1967).

[2] D. E. Milligan, M. E. Jacox, and W. A. Guillory, J. Chem. Phys. 49, 5330 (1968).

[3] J. L-F. Wang, C. N. Krishnan, and J. L. Margrave, J. Mol. Spectrosc. 48, 346 (1973).

$SiCl_3$ C_{3v} Structure: ESR [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SiCl stretch	470m	Ar	IR	[2][3]
e	3	SiCl stretch	582vs	Ar	IR	[2][3]

References

[1] N. Leray and J. Roncin, J. Chem. Phys. 42, 800 (1965).

[2] M. E. Jacox and D. E. Milligan, J. Chem. Phys. 49, 3130 (1968).

[3] J. H. Miller and L. Andrews, J. Mol. Struct. 77, 65 (1981).

$t\text{-}O_4^-$ Structure: MO [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		O=O a-stretch	1001[a]	Ar	IR	[4]
			992[b]	Ar	IR	[3]
			993[c]	Ar	IR	[3]
			1001[d] 991	Ar	IR	[2][4]
		O_2–O_2 stretch	287[a]	Ar	Ram	[5]
			298[b]	Ar	Ram	[5]

[a] Cs^+ present.

[b] Rb^+ present.

[c] K^+ present.

[d] Na^+ present.

References

[1] D. C. Conway, J. Chem. Phys. 50, 3864 (1969).

[2] L. Andrews, J. Phys. Chem. 73, 3922 (1969).

[3] L. Andrews, J. Chem. Phys. 54, 4935 (1971).

[4] M. E. Jacox and D. E. Milligan, Chem. Phys. Lett. 14, 518 (1972).

[5] R. R. Smardzewski and L. Andrews, J. Phys. Chem. 77, 801 (1973).

CF_2Br^-

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1219m[a]	Ar	IR	[1]
			1099s[a]	Ar	IR	[1]

[a] Tentative assignment.

References

[1] F. T. Prochaska and L. Andrews, J. Phys. Chem. 82, 1731 (1978).

FSO_2^-

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	SO_2 s-stretch	1100m[a]	Ar	IR	[1]
	2		598m[a]	Ar	IR	[1]
	3		572m[a]	Ar	IR	[1]
	4		360w[a]	Ar	IR	[1]
	5	SO_2 a-stretch	1178m[a]	Ar	IR	[1]

[a] Cs^+ present.

References

[1] K. Garber and B. S. Ault, Inorg. Chem. 22, 2509 (1983).

$(ClO)_2$ (Structure I)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ClO stretch	947	Ar	IR,Ram	[3][5]
			945	N_2	IR	[1][3]

$(ClO)_2$ (Structure II)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ClO stretch	985	Ar	IR	[5]
			982	N_2	IR	[1]

$(ClO)_2$ (Structure III)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		ClO stretch	995	Ar	IR	[2][4] [5]
			993	N_2	IR	[1]

References

[1] M. M. Rochkind and G. C. Pimentel, J. Chem. Phys. 46, 4481 (1967).

[2] A. Arkell and I. Schwager, J. Am. Chem. Soc. 89, 5999 (1967).

[3] W. G. Alcock and G. C. Pimentel, J. Chem. Phys. 48, 2373 (1968).

[4] L. Andrews and J. I. Raymond, J. Chem. Phys. 55, 3087 (1971).

[5] F. K. Chi and L. Andrews, J. Phys. Chem. 77, 3062 (1973).

$SSCl_2$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′		SS stretch	699	Ar	IR	[1][2]
			696	N_2	IR	[1]
		SCl_2 s-stretch	403	Ar	IR	[1][2]
			403	N_2	IR	[1]
a"		SCl_2 stretch	377	Ar	IR	[1][2]
			378	N_2	IR	[1][2]

References

[1] B. M. Chadwick, J. M. Grzybowski, and D. A. Long, J. Mol. Struct. 48, 139 (1978).

[2] M. Feuerhahn and G. Vahl, Chem. Phys. Lett. 65, 322 (1979).

$SSBr_2$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′		SS stretch	693	Ar	IR	[1]
		SBr_2 stretch	317	Ar	IR	[1]
a"		SBr_2 stretch	311	Ar	IR	[1]

References

[1] M. Feuerhahn and G. Vahl, Chem. Phys. Lett. 65, 322 (1979).

SF_3 C_{2v} Structure: ESR [1][4]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SF_2 a-stretch	682	Ar	IR	[2][3]

References

[1] A. J. Colussi, J. R. Morton, K. F. Preston, and R. W. Fessenden, J. Chem. Phys. 61, 1247 (1974).

[2] R. R. Smardzewski and W. B. Fox, J. Fluorine Chem. 7, 353 (1976).

[3] R. R. Smardzewski and W. B. Fox, J. Chem. Phys. 67, 2309 (1977).

[4] J. R. Morton, K. F. Preston, and S. J. Strach, J. Chem. Phys. 69, 1392 (1978).

Cl_2F_2 C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	5	FClF stretch	636	Ar	IR	[1]

References

[1] E. S. Prochaska, L. Andrews, N. R. Smyrl, and G. Mamantov, Inorg. Chem. 17, 970 (1978).

Br_2F_2 C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	5	FBrF stretch	555	Ar	IR	[1]

References

[1] E. S. Prochaska, L. Andrews, N. R. Smyrl, and G. Mamantov, Inorg. Chem. 17, 970 (1978).

I_2F_2 C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	5	FIF stretch	526	Ar	IR	[1]

References

[1] E. S. Prochaska, L. Andrews, N. R. Smyrl, and G. Mamantov, Inorg. Chem. 17, 970 (1978).

6.8. NH_4^+ and Five-Atomic Trihydrides

NH_4^+ T_d Structure: VMA [1][2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
f_2	3	NH stretch	3343.14	gas	VMA	[1]-[3]

References

[1] M. Crofton and T. Oka, J. Chem. Phys. 79, 3157 (1983).

[2] E. Schaeffer, M. H. Begemann, C. S. Gudeman, and R. J. Saykally, J. Chem. Phys. 79, 3159 (1983).

[3] E. Schafer, R. J. Saykally, and A. G. Robiette, J. Chem. Phys. 80, 3969 (1984).

CH_2NH C_s Structure: MW [2][3][5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	NH stretch	3264	gas	IR	[9]
	2	CH stretch	3038	gas	IR	[9]
			3036wm	Ar	IR	[1][4]
	3	CH stretch	2915	gas	IR	[9]
			2926m	Ar	IR	[1][4]
	4	C=N stretch	1638.30	gas	LSS,IR	[6][7] [9]
			1641s	Ar	IR	[1][4]
	5	CH_2 "scissors"	1452.04	gas	IR	[7]-[9]
			1453s	Ar	IR	[1][4]
	6	HCNH deform.	1344.27	gas	IR	[7]-[9]
			1348vs	Ar	IR	[1][4]
	7	HCNH deform.	1055[a]	gas	IR	[9]
			1059s	Ar	IR	[1][4]
a"	8	Torsion	1131	gas	IR	[9]
			1123vs	Ar	IR	[1][4]
	9	H_2CN OPLA	1059	gas	IR	[9]
			1063m	Ar	IR	[1][4]

CD_2ND

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	2	CD stretch	2269m	Ar	IR	[1][4]
	3	CD stretch	2184m	Ar	IR	[1][4]
	4	C=N stretch	1577ms	Ar	IR	[1][4]
	5	DCND deform.	1089m	Ar	IR	[1][4]
	6	CD_2 "scissors"	1067w	Ar	IR	[1][4]
	7	DCND deform.	770s	Ar	IR	[1][4]

CD_2ND---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a"	9	Torsion	821s	Ar	IR	[1][4]

[a] Tentative assignment.

References

[1] D. E. Milligan, J. Chem. Phys. 35, 1491 (1961).

[2] D. R. Johnson and F. J. Lovas, Chem. Phys. Lett. 15, 65 (1972).

[3] W. H. Kirchhoff, D. R. Johnson, and F. J. Lovas, J. Phys. Chem. Ref. Data 2, 1 (1973).

[4] M. E. Jacox and D. E. Milligan, J. Mol. Spectrosc. 56, 333 (1975).

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[6] M. Allegrini, J. W. C. Johns, and A. R. W. McKellar, J. Chem. Phys. 70, 2829 (1979).

[7] G. Duxbury, H. Kato, and M. L. Le Lerre, Discuss. Faraday Soc. 71, 97 (1981).

[8] G. Duxbury and M. L. Le Lerre, J. Mol. Spectrosc. 92, 326 (1982).

[9] Y. Hamada, K. Hashiguchi, M. Tsuboi, Y. Koga, and S. Kondo, J. Mol. Spectrosc. 105, 70 (1984).

CH_3O ^2E C_{3v} Structure: LMR [1][5]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 "umbrella"	1325[a]	gas	PE	[2]
			1380[b]	gas	LF	[4]
	3	CO stretch	1015	gas	LF,UV	[3][4] [6]

CD_3O

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_3 "umbrella"	1020[a]	gas	PE	[2]
			1168	gas	LF	[4]
	3	CO stretch	1010	gas	LF	[4]
e	6	D_3-C-O def.	936	gas	LF	[4]

[a] $\pm$ 30 cm^{-1}.

[b] $\pm$ 20 cm^{-1}.

References

[1] H. E. Radford and D. K. Russell, J Chem. Phys. 66, 2222 (1977).

[2] P. C. Engelking, G. B. Ellison, and W. C. Lineberger, J. Chem. Phys. 69, 1826 (1978).

[3] G. Inoue, H. Akimoto, and M. Okuda, Chem. Phys. Lett. 63, 213 (1979).

[4] G. Inoue, H. Akimoto, and M. Okuda, J. Chem. Phys. 72, 1769 (1980).

[5] D. K. Russell and H. E. Radford, J. Chem. Phys. 72, 2750 (1980).

[6] T. Ebata, H. Yanagishita, K. Obi, and I. Tanaka, Chem. Phys. 69, 27 (1982).

CH_2OH

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OH stretch	3650m	Ar	IR	[1][2]
			3637m	N_2	IR	[1]
	4	CH_2 "scissors"	1459w	Ar	IR	[2]
	5	OH deform.	1334m	Ar	IR	[1][2]
	6	CO stretch	1183vs	Ar	IR	[1][2]
			1183s	N_2	IR	[1]
	7	HCOH deform.	1048s	Ar	IR	[1][2]
			1056m	N_2	IR	[1]
	9	Torsion	420m	Ar	IR	[1][2]
			482m	N_2	IR	[1]

CD_2OD

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	OD stretch	2694wm	Ar	IR	[2]
			2682m	N_2	IR	[1]
	4	CO stretch	1223m	Ar	IR	[2]
			1222m	N_2	IR	[1]
	5		1041m	Ar	IR	[2]
	7		765wm	Ar	IR	[2]

References

[1] M. E. Jacox and D. E. Milligan, J. Mol. Spectrosc. 47, 148 (1973).

[2] M. E. Jacox, Chem. Phys. 59, 213 (1981).

CH_3S C_{3v} Structure: MO [3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 "umbrella"	1360[a]	gas	PD	[3]
			1040[b]	gas	PE	[2]
	3	CS stretch	670[c]	gas	UV	[1]
			680[d]	gas	PE	[2]
			770[e]	gas	PD	[3]

CD_3S

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_3 "umbrella"	1100[e]	gas	PD	[3]
	3	CS stretch	660[f]	gas	PD	[3]
			620m?	Ar	IR	[4]
e	5	DCS deform.	780[g]	gas	PD	[3]
			815w?	Ar	IR	[4]

[a] $\pm$ 70 cm^{-1}.

[b] $\pm$ 80 cm^{-1}.

[c] $\pm$ 75 cm^{-1}.

[d] $\pm$ 40 cm^{-1}.

[e] $\pm$ 50 cm^{-1}.

[f] $\pm$ 60 cm^{-1}.

[g] $(2\nu_5)/2$; $2\nu_5 = 1560 \pm 50$ cm^{-1}.

References

[1] K. Ohbayashi, H. Akimoto, and I. Tanaka, Chem. Phys. Lett. 52, 47 (1977).

[2] R. C. Engelking, G. B. Ellison, and W. C. Lineberger, J. Chem. Phys. 69, 1826 (1978).

[3] B. K. Janousek and J. I. Brauman, J. Chem. Phys. 72, 694 (1980).

[4] M. E. Jacox, Can. J. Chem. 61, 1036 (1983).

CH_2SH

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		H_2CS "umbrella"	425s	Ar	IR	[1][2]

CD_2SD

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		D_2CS "umbrella"	322[a]	Ar	IR	[2]

CH_2SH---Footnote

[a] ± 5 cm^{-1}.

References

[1] M. E. Jacox and D. E. Milligan, J. Mol. Spectrosc. 58, 142 (1975).

[2] M. E. Jacox, Can. J. Chem. 61, 1036 (1983).

CH_3O^-

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CH_3 "umbrella"	1075[a]	gas	PE	[1]

CD_3O^-

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	CD_3 "umbrella"	915[a]	gas	PE	[1]

[a] ± 100 cm^{-1}.

References

[1] P. C. Engelking, G. B. Ellison, and W. C. Lineberger, J. Chem. Phys. 69, 1826 (1978).

CH_3S^- C_{3v} Structure: MO [2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	CS stretch	625[a]	gas	PE	[1]

[a] ± 80 cm^{-1}.

References

[1] P. C. Engelking, G. B. Ellison, and W. C. Lineberger, J. Chem. Phys. 69, 1826 (1978).

[2] B. K. Janousek and J. I. Brauman, J. Chem. Phys. 72, 694 (1980).

6.9. Five-Atomic Dihydrides

C_3H_2 $^3\Sigma$ $D_{\infty h}$ Structure: ESR [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	CH stretch	3285	Kr	IR	[2]
	4	C_3 a-stretch	2140	Kr	IR	[2]
Π_u	6	C_3 deform.	402wm	Ar	IR	[3]
			408	Kr	IR	[2]
	7	HCC deform.	246s	Ar	IR	[3]
			258	Kr	IR	[2]

C_3D_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_u^+	3	CD stretch	2472m	Ar	IR	[3]
			2482	Kr	IR	[2]
	4	C_3 a-stretch	2065?	Kr	IR	[2]
Π_u	6	C_3 deform.	392	Kr	IR	[2]
	7	DCC deform.	171m	Ar	IR	[3]

References

[1] R. A. Bernheim, R. J. Kempf, J. V. Gramas, and P. S. Skell, J. Chem. Phys. 43, 196 (1965).

[2] F. K. Chi and G. E. Leroi, private communication.

[3] M. E. Jacox and D. E. Milligan, Chem. Phys. 4, 45 (1974).

H_2CCS^+

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CS stretch	1450[a]	gas	PE	[1]
		CC stretch	700[a]	gas	PE	[1]

[a] ± 80 cm^{-1}.

References

[1] H. Bock, B. Solouki, G. Bert, and P. Rosmus, J. Am. Chem. Soc. 99, 1663 (1977).

HN=C=NH C_2

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	NCN s-stretch	1275[a]	Ar	IR	[1]
	Torsion	886vs	Ar	IR	[1]
	NCN deform.	537m	Ar	IR	[1]
b	NCN a-stretch	2097s	Ar	IR	[1]

DN=C=ND

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	ND stretch	2545s[b]	Ar	IR	[1]
	Torsion	752s	Ar	IR	[1]
	NCN deform.	471m	Ar	IR	[1]
b	ND stretch	2545s[b]	Ar	IR	[1]
	NCN a-stretch	2107vs	Ar	IR	[1]

[a] Calculated from combination with torsion at 2169 cm^{-1}.

[b] Both ND-stretching frequencies presumed equal.

References

[1] S. T. King and J. H. Strope, J. Chem. Phys. 54, 1289 (1971).

$H_2C=C=S$ C_{2v} Structure: MW [2]-[4]

(Thioketene)

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CH_2 stretch	3010w	Ar	IR	[1][5]
		1840m	Ar	IR	[5]
	C=C stretch	1755vs	Ar	IR	[1][5]
		1410w	Ar	IR	[5]
	C=S stretch	1322m	Ar	IR	[1][5]
	CH_2 rock	692s	Ar	IR	[1][5]
	CCS bend	400vw	Ar	IR	[1]

$D_2C=C=S$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CD_2 stretch	2240s	Ar	IR	[1]
	C=C stretch	1735vs	Ar	IR	[1]
	CD_2 deform.	860w	Ar	IR	[1]
	CD_2 rock	560s	Ar	IR	[1]

References

[1] A. Krantz and J. Laureni, J. Am. Chem. Soc. 96, 6768 (1974).

[2] K. Georgiou, H. W. Kroto, and B. M. Landsberg, J. Chem. Soc., Chem. Commun., 739 (1974).

[3] B. Bak, O. J. Nielsen, H. Svanholt, A. Holm, N. H. Toubro, A. Krantz, and J. Laureni, Acta Chem. Scand. A33, 161 (1979).

[4] K. Georgiou, H. W. Kroto, and B. M. Landsberg, J. Mol. Spectrosc. 77, 365 (1979).

[5] A. Krantz and J. Laureni, J. Am. Chem. Soc. 103, 486 (1981).

HC≡CSH

(Ethynyl Mercaptan)

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CH stretch	3315s	Ar	IR	[1][2]
	SH stretch	2575vw	Ar	IR	[2]
	C≡C stretch	2065w	Ar	IR	[1][2]
		1112m	Ar	IR	[2]
		959w	Ar	IR	[2]
	CCH bend (⊥ plane)	558w	Ar	IR	[1][2]

DC≡CSD

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CD stretch	2580s	Ar	IR	[1]
	C≡C stretch	1925vw	Ar	IR	[1]
	SD stretch	1835vw	Ar	IR	[1]
	CCD bend (⊥ plane)	430m	Ar	IR	[1]

References

[1] A. Krantz and J. Laureni, J. Am. Chem. Soc. 96, 6768 (1974).

[2] A. Krantz and J. Laureni, J. Am. Chem. Soc. 103, 486 (1981).

C_2H_2S C_{2v}

(Thiirene)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3207w	Ar	IR	[2]-[4]
			3202	N_2	IR	[6]
		CH stretch	3169m 3166m	Ar	IR	[1]-[4]
			3161	N_2	IR	[6]
		C=C stretch	1663w	Ar	IR	[1]-[4]
			1660	N_2	IR	[6]
			912m	Ar	IR	[1]-[4]
			910	N_2	IR	[6]
			657m[a]	Ar	IR	[3][4]
			563m	Ar	IR	[1]-[4]
			570	N_2	IR	[6]

C_2D_2S

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD stretch	2485w	Ar	IR	[2][4] [6]
		CD stretch	2355m	Ar	IR	[4]
		C=C stretch	1567w	Ar	IR	[2][4] [6]
			873w	Ar	IR	[2]
			716s	Ar	IR	[4][6]
			681m	Ar	IR	[4]
			423m	Ar	IR	[2][4] [6]

[a] Tentative. See [5] and [6].

References

[1] J. Laureni, A. Krantz, and R. A. Hajdu, J. Am. Chem. Soc. 98, 7872 (1976).

[2] A. Krantz and J. Laureni, J. Am. Chem. Soc. 99, 4842 (1977).

[3] M. Torres, A. Clement, J. E. Bertie, H. E. Gunning, and O. P. Strausz, J. Org. Chem. 43, 2490 (1978).

[4] M. Torres, I. Safarik, A. Clement, J. E. Bertie, and O. P. Strausz, Nouv. J. Chim. 3, 365 (1979).

[5] A. Krantz and J. Laureni, J. Org. Chem. 44, 2730 (1979).

[6] A. Krantz and J. Laureni, J. Am. Chem. Soc. 103, 486 (1981).

t-CHF=CH C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	C=C stretch	1623vs	Ar	IR	[1]
	4	HCF "scissors"	1211wm	Ar	IR	[1]
	5	CF stretch	1066vs	Ar	IR	[1]
	6	C=CH deform.	678s	Ar	IR	[1]
	7	C=CF deform.	462m	Ar	IR	[1]
a"	8	HFC=C OPLA	785s	Ar	IR	[1]
	9	Torsion	631vs	Ar	IR	[1]

t-DCF=CD

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	C=C stretch	1564s	Ar	IR	[1]
	4	CF stretch	1070m	Ar	IR	[1]
a"	8	DFC=C OPLA	624m	Ar	IR	[1]
	9	Torsion	485m	Ar	IR	[1]

References

[1] M. E. Jacox, Chem. Phys. 53, 307 (1980).

H_2CSO 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	3013w	Ar	IR	[3]
	2	CH_2 s-stretch	2960m	Ar	IR	[3]
	3	CH_2 "scissors"	1395w	Ar	IR	[3]
	4	CSO a-stretch	1357s	Ar	IR	[3]
	5	CSO s-stretch	1170	gas	IR	[1]
			1165vs	Ar	IR	[3]
	6	CH_2 rock	1055m	Ar	IR	[3]
	7	CSO bend	394m	Ar	IR	[3]
a"	8	Torsion	972m	Ar	IR	[3]
	9	H_2CS OPLA	760	gas	IR	[1]
			767vs	Ar	IR	[3]

References

[1] E. Block, R. E. Penn, R. J. Olsen, and P. F. Sherwin, J. Am. Chem. Soc. 98, 1264 (1976).

[2] R. E. Penn and R. J. Olsen, J. Mol. Spectrosc. 61, 21 (1976).

[3] D. E. Powers, C. A. Arrington, W. C. Harris, E. Block, and V. F. Kalasinsky, J. Phys. Chem. 83, 1890 (1979).

$CH_2F_2^+$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CH stretch	2744m	Ar	IR	[1]
b_1	6	CH stretch	2854wm	Ar	IR	[1]
b_2	8	CH_2 wag	1408s	Ar	IR	[1]
	9	CF stretch	1255vs	Ar	IR	[1]

$CD_2F_2^+$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	CD stretch	2062m	Ar	IR	[1]
b_1	7		980w	Ar	IR	[1]
b_2	8	CD_2 wag	1063s	Ar	IR	[1]
	9	CF stretch	1262vs	Ar	IR	[1]

References

[1] L. Andrews and F. T. Prochaska, J. Chem. Phys. 70, 4714 (1979).

CH_2FCl^+

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_2 stretch	2902m	Ar	IR	[1]
		CCl stretch	874s	Ar	IR	[1]

CD_2FCl^+

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD_2 stretch	2162m[a]	Ar	IR	[1]
		CCl stretch	843vs	Ar	IR	[1]

[a] Tentative assignment.

References

[1] F. T. Prochaska and L. Andrews, J. Chem. Phys. 73, 2651 (1980).

CH_2FBr^+

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_2 stretch	2913m	Ar	IR	[1]
		CBr stretch	735s	Ar	IR	[1]

References

[1] F. T. Prochaska and L. Andrews, J. Chem. Phys. 73, 2651 (1980).

CH_2FI^+

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_2 stretch	2914m	Ar	IR	[1]
		CI stretch	653m	Ar	IR	[1]

References

[1] F. T. Prochaska and L. Andrews, J. Chem. Phys. 73, 2651 (1980).

$CH_2Cl_2^+$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	8	CH_2 wag	1193s	Ar	IR	[1][2]
	9	CCl_2 stretch	764s	Ar	IR	[1][2]

$CD_2Cl_2^+$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	8	CD_2 wag	1083m	Ar	IR	[2]
	9	CCl_2 stretch	603s	Ar	IR	[1][2]

References

[1] L. Andrews, F. T. Prochaska, and B. S. Ault, J. Am. Chem. Soc. 101, 9 (1979).

[2] B. J. Kelsall and L. Andrews, J. Mol. Spectrosc. 97, 362 (1983).

$CH_2Br_2^+$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	8	CH_2 wag	1129m	Ar	IR	[1]
			695m	Ar	IR	[1]
	9		684s	Ar	IR	[1][2]

$CD_2Br_2^+$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_2	9		546s	Ar	IR	[1][2]

References

[1] L. Andrews, F. T. Prochaska, and B. S. Ault, J. Am. Chem. Soc. 101, 9 (1979).

[2] B. J. Kelsall and L. Andrews, J. Mol. Spectrosc. 97, 362 (1983).

6.10. Five-Atomic Monohydrides

C_4H $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	3	C≡C a-stretch	2060	Ar	IR	[1]
	5	HCC bend	735	Ar	IR	[1]

C_4D

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	3	C≡C a-stretch	2050	Ar	IR	[1]
	5	DCC bend	586	Ar	IR	[1]

References

[1] K. I. Dismuke, W. R. M. Graham, and W. Weltner, Jr., J. Mol. Spectrosc. 57, 127 (1975).

HC(O)OO

(Formylperoxy)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C=O stretch	1790.2	O_2	IR	[1]
		C-O stretch	1089.9	O_2	IR	[1]

References

[1] T-L. Tso, M. Diem, and E. K. C. Lee, Chem. Phys. Lett. 91, 339 (1982).

$HOSO_2$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3540wm	Ar	IR	[1]
		SO_2 a-stretch	1309m	Ar	IR	[1]
		SO_2 s-stretch	1097m	Ar	IR	[1]
		OH deform.	760m	Ar	IR	[1]

References

[1] S. Hashimoto, G. Inoue, and H. Akimoto, Chem. Phys. Lett. 107, 198 (1984).

6.11. Five-Atomic Nonhydrides

$C(CN)_2$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CN a-stretch	1756m	Ar	IR	[1]
		C_3 a-stretch	1158w	Ar	IR	[1]
		CCN deform.	392w	Ar	IR	[1]

References

[1] W. H. Smith and G. E. Leroi, Spectrochim. Acta 25A, 1917 (1969).

$Si(CO)_2$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1928	Ar	IR	[1]

References

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

Cl_2CCO^+ $^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		CO stretch	2200[a]	gas	PE	[1]
		CC stretch	1100[a]	gas	PE	[1]
		CCl_2 deform.	330[a]	gas	PE	[1]

[a] $\pm$ 40 cm^{-1}.

References

[1] D. Colbourne, D. C. Frost, C. A. McDowell, and N. P. C. Westwood, J. Chem. Soc., Chem. Commun., 250 (1980).

Cl_2CCO C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C=O stretch	2155s	Ar	IR	[1]
		C=C stretch	1290w	Ar	IR	[1]
		CCl stretch	935m	Ar	IR	[1]
		CCl stretch	770w	Ar	IR	[1]

References

[1] M. Torres, J. Ribo, A. Clement, and O. P. Strausz, Nouv. J. Chim. 5, 351 (1981).

O_2N-NO C_s Structure: MW [2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	N=O stretch	1832	gas	IR	[1][5]
			1840m	N_2	IR	[4]
			1867vs	O_2	IR	[2]
			1861	NO	IR,Ram	[6]
	2	NO_2 a-stretch	1652	gas	IR	[5]
			1630vs	N_2	IR	[4]
			1596s	O_2	IR	[2]
			1593	NO	IR,Ram	[6]
	3	NO_2 s-stretch	1305	gas	IR	[1][5]
			1302s	N_2	IR	[4]
			1303	O_2	IR	[2]
			1298	NO	IR,Ram	[6]
	4	NO_2 deform.	773	gas	IR	[1][5]
			776wm	N_2	IR	[4]
			788	O_2	IR	[2]
			787	NO	IR,Ram	[6]
	5	NO_2 rock	414	gas	IR	[5]
			420w	N_2	IR	[4]
			405	NO	Ram	[6]
	6	N-N stretch	241	gas	IR	[5]
			266	NO	Ram	[6]
	7	NO_2 wag	205	NO	Ram	[6]
a"	8	NNO_2 OPLA	627	NO	Ram	[6]
	9	Torsion	63	gas	IR	[5]
			70	NO	Ram	[6]

References

[1] L. D'Or and P. Tarte, Bull. Soc. Roy. Sci. Liege 22, 276 (1953).

[2] W. G. Fateley, H. A. Bent, and B. Crawford, Jr., J. Chem. Phys. 31, 204 (1959).

[3] A. H. Brittain, A. P. Cox, and R. L. Kuczkowski, Trans. Faraday Soc. 65, 1963 (1969).

[4] E. L. Varetti and G. C. Pimentel, J. Chem. Phys. 55, 3813 (1971).

[5] C. H. Bibart and G. E. Ewing, J. Chem. Phys. 61, 1293 (1974).

[6] E. M. Nour, L.-H. Chen, and J. Laane, J. Phys. Chem. 87, 1113 (1983).

O=N-O-N=O C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	N=O s-stretch	1740	NO	Ram	[2]
	2	N-O s-stretch	969w	N_2	IR	[1]
			973m	NO	IR,Ram	[2]
	3	NON bend	387m	N_2	IR	[1]
			395	NO	Ram	[2]
	4	Sym. O=NO bend	366s	N_2	IR	[1]
a_2	5	Torsion	140	NO	Ram	[2]
b_1	6	Torsion	105[a]	NO	Ram	[2]
b_2	7	N=O a-stretch	1690s	N_2	IR	[1]
			1687vs	NO	IR	[2]
			1661w	N_2	IR	[1]
	8	N-O a-stretch	877vw	N_2	IR	[1]
			865vw	NO	IR	[2]
	9	Asym. O=NO bend	704vw	N_2	IR	[1]
			705vw	NO	IR	[2]

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

References

[1] E. L. Varetti and G. C. Pimentel, J. Chem. Phys. 55, 3813 (1971).

[2] E. M. Nour, L.-H. Chen, and J. Laane, J. Phys. Chem. 87, 1113 (1983).

SO_4

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		S=O stretch	1434s	Ar	IR	[1]
		S=O stretch	1267s	Ar	IR	[1]
		O-O stretch	925wm	Ar	IR	[1]
			777wm	Ar	IR	[1]
			611m	Ar	IR	[1]
			498sh	Ar	IR	[1]
			490sh	Ar	IR	[1]

References

[1] R. Kugel and H. Taube, J. Phys. Chem. 79, 2130 (1975).

CF_3Cl^+

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1299vs	Ar	IR	[1][2]
		CCl stretch	734wm	Ar	IR	[1][2]
		Deformation	460ms 451m	Ar	IR	[1][2]
		Deformation	416m	Ar	IR	[1][2]

References

[1] F. T. Prochaska and L. Andrews, J. Am. Chem. Soc. 100, 2102 (1978).

[2] F. T. Prochaska and L. Andrews, J. Chem. Phys. 68, 5577 (1978).

CF_3Br^+

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1293s	Ar	IR	[1][2]
		CF stretch	1255vs	Ar	IR	[1][2]
			469s	Ar	IR	[1][2]

References

[1] F. T. Prochaska and L. Andrews, J. Am. Chem. Soc. 100, 2102 (1978).

[2] F. T. Prochaska and L. Andrews, J. Phys. Chem. 82, 1731 (1978).

CF_3I^+

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CF stretch	1229vs	Ar	IR	[1]
			677m	Ar	IR	[1]
			497s	Ar	IR	[1]

References

[1] F. T. Prochaska and L. Andrews, J. Am. Chem. Soc. 100, 2102 (1978).

$CF_2Cl_2^+$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CF_2 a-stretch	1234vs	Ar	IR	[1]
	CCl_2 a-stretch	1067m	Ar	IR	[1]
	CF_2 bend	609wm	Ar	IR	[1]
	FCCl deform.	424m	Ar	IR	[1]
	FCCl deform.	406m	Ar	IR	[1]

References

[1] F. T. Prochaska and L. Andrews, J. Chem. Phys. 68, 5577 (1978).

$CF_2Br_2^+$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CF_2 stretch	1244s	Ar	IR	[1]
		873m	Ar	IR	[1]
		868m	Ar	IR	[1]
		428wm	Ar	IR	[1]
		406wm	Ar	IR	[1]

References

[1] F. T. Prochaska and L. Andrews, J. Phys. Chem. 82, 1731 (1978).

$CFCl_3^+$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CF stretch	1214vs	Ar	IR	[1]
	CCl a-stretch	1041s	Ar	IR	[1]
	CCl s-stretch	585m	Ar	IR	[1]
	Deformation	432m	Ar	IR	[1]
	Deformation	324wm[a]	Ar	IR	[1]

[a] Tentative assignment.

References

[1] F. T. Prochaska and L. Andrews, J. Chem. Phys. 68, 5568 (1978).

$CFBr_3^+$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CF stretch	1167vs 1160vs	Ar	IR	[1]
		853vs	Ar	IR	[1]
		423s	Ar	IR	[1]
		399s	Ar	IR	[1]
		316m	Ar	IR	[1]

References

[1] F. T. Prochaska and L. Andrews, J. Phys. Chem. 82, 1731 (1978).

CCl_4^+

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CCl_2 a-stretch	927s	Ar	IR	[1]
	$C\cdot\cdot Cl_2$ stretch[a]	374wm	Ar	IR	[1]

[a] Molecule possesses less than tetrahedral symmetry.

References

[1] F. T. Prochaska and L. Andrews, J. Chem. Phys. 67, 1091 (1977).

CBr_4^+

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CBr stretch	778	Ar	IR	[1]
	$C\cdot\cdot Br_2$ stretch[a]	326	Ar	IR	[1]

[a] Molecule possesses less than tetrahedral symmetry.

References

[1] F. T. Prochaska and L. Andrews, J. Chem. Phys. 67, 1091 (1977).

FSO_3 $^2A_2$ C_{3v} Structure: UV [1][3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	SO stretch	1055.5	gas	UV	[2]
			1053vs	Ar	IR	[4]
	2	SF stretch	839.3	gas	UV	[2]
			833vs	Ar	IR	[4]
	3	SO deform.	533.5	gas	UV	[2]
			531m	Ar	IR	[4]
e	4	SO stretch	1177.5	gas	UV	[2]
			1177m	Ar	IR	[4]
	5	SO deform.	604.1	gas	UV	[2]
			601vw	Ar	IR	[4]
	6	SF wag	369.4	gas	UV	[2]
			366vw	Ar	IR	[4]

References

[1] G. W. King, D. P. Santry, and C. H. Warren, J. Mol. Spectrosc. 32, 108 (1969).

[2] G. W. King and C. H. Warren, J. Mol. Spectrosc. 32, 121 (1969).

[3] G. W. King and C. H. Warren, J. Mol. Spectrosc. 32, 138 (1969).

[4] E. M. Suzuki, J. W. Nibler, K. A. Oakes, and D. Eggers, Jr., J. Mol. Spectrosc. 58, 201 (1975).

$^{11}BF_4^-$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BF stretch	1197vs[a]	Ar	IR	[1]
		BF stretch	1014[a]	Ar	IR	[1]
		Deformation	524[a]	Ar	IR	[1]

[a] Cs^+ present.

References

[1] R. L. Hunt and B. S. Ault, Spectrochim. Acta 37A, 63 (1981).

$^{11}BF_3Cl^-$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BF stretch	1210[a]	Ar	IR	[1]
		BCl stretch	840[a]	Ar	IR	[1]

[a] Cs^+ present.

References

[1] R. L. Hunt and B. S. Ault, Spectrochim. Acta 37A, 63 (1981).

$^{11}BCl_4^-$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		BCl stretch	766[a]	Ar	IR	[1]
		BCl stretch	642[a]	Ar	IR	[1]

[a] Cs^+ present.

References

[1] R. L. Hunt and B. S. Ault, Spectrochim. Acta 37A, 63 (1981).

CF_3O^-

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CO stretch	1514[a]	Ar	IR	[1]
		CF stretch	1039[a]	Ar	IR	[1]
		CF stretch	919[a]	Ar	IR	[1]
		CF stretch	808[a]	Ar	IR	[1]
		OCF deform.	555[a]	Ar	IR	[1]

[a] Cs^+ present.

References

[1] B. S. Ault, J. Phys. Chem. 84, 3448 (1980).

CF_3Cl^-

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			938s	Ar	IR	[1][2]
			933s	Ar	IR	[1][2]
			666m	Ar	IR	[1][2]

References

[1] F. T. Prochaska and L. Andrews, J. Am. Chem. Soc. 100, 2102 (1978).

[2] F. T. Prochaska and L. Andrews, J. Chem. Phys. 68, 5577 (1978).

CF_3Br^-

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CF stretch	918s	Ar	IR	[1][2]
		914s	Ar	IR	[1][2]
	CF_3 deform.	662m	Ar	IR	[1][2]

References

[1] F. T. Prochaska and L. Andrews, J. Am. Chem. Soc. 100, 2102 (1978).

[2] F. T. Prochaska and L. Andrews, J. Phys. Chem. 82, 1731 (1978).

CF_3I^-

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CF stretch	893m	Ar	IR	[1]
	CF_3 deform.	660wm	Ar	IR	[1]

References

[1] F. T. Prochaska and L. Andrews, J. Am. Chem. Soc. 100, 2102 (1978).

$CF_2Cl_2^-$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CF_2 a-stretch	1029m	Ar	IR	[1]
		626m	Ar	IR	[1]
		564vs	Ar	IR	[1]

References

[1] F. T. Prochaska and L. Andrews, J. Chem. Phys. 68, 5577 (1978).

CF_2ClBr^-

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CF_2 a-stretch	1013	Ar	IR	[1]
		622	Ar	IR	[1]
		564	Ar	IR	[1]

References

[1] F. T. Prochaska and L. Andrews, J. Chem. Phys. 68, 5577 (1978).

$CF_2Br_2^-$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		1001s[a]	Ar	IR	[1]
		554vs[a]	Ar	IR	[1]

[a] Tentative assignment.

References

[1] F. T. Prochaska and L. Andrews, J. Phys. Chem. 82, 1731 (1978).

$CFCl_3^-$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CF stretch	1056ms	Ar	IR	[1]
	CCl stretch	776m	Ar	IR	[1]
		486s	Ar	IR	[1]
		440ms	Ar	IR	[1]

References

[1] F. T. Prochaska and L. Andrews, J. Chem. Phys. 68, 5568 (1978).

$CFBr_3^-$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CF stretch	1029m	Ar	IR	[1]
		1019m	Ar	IR	[1]
	CBr stretch	626m	Ar	IR	[1]
	Deformation	465s	Ar	IR	[1]

References

[1] F. T. Prochaska and L. Andrews, J. Phys. Chem. 82, 1731 (1978).

PF_4^- C_{2v} ?

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PF eq. stretch	789[a]	Ar	IR	[1]
	2	PF ax. stretch	621[a]	Ar	IR	[1]
b_1	6	PF stretch	710[a]	Ar	IR	[1]
b_2	8	PF eq. stretch	780[a]	Ar	IR	[1]

[a] Cs^+ in adjacent site.

References

[1] P. Wermer and B. S. Ault, Inorg. Chem. 20, 970 (1981).

$PClF_3^-$ C_{2v} ?

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	PF eq. stretch	780[a]	Ar	IR	[1]
	2	PF ax. stretch	621[a]	Ar	IR	[1]
b_2	8	PF eq. stretch	767[a]	Ar	IR	[1]

[a] Cs^+ in adjacent site.

References

[1] P. Wermer and B. S. Ault, Inorg. Chem. 20, 970 (1981).

SOF_3^- C_s ?

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SO stretch	1264m[a]	Ar	IR	[1]
		SF stretch	695[a]	Ar	IR	[1]
		SF stretch	667[a]	Ar	IR	[1]
		SF stretch	623[a]	Ar	IR	[1]

[a] Cs^+ present.

References

[1] K. Garber and B. S. Ault, Inorg. Chem. 22, 2509 (1983).

6.12. Six-Atomic Molecules

$CH_2{=}SiH_2^+$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_2 deform.	1010[a]	gas	PE	[1]
		Si=C stretch + SiH_2 deform.	840[a]	gas	PE	[1]
		Si=C stretch + SiH_2 deform.	620[a]	gas	PE	[1]
		Torsion	~200	gas	PE	[1]

$CH_2{=}SiD_2^+$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Si=C stretch + SiD_2 deform.	770[a]	gas	PE	[1]
		Si=C stretch + SiD_2 deform.	550[a]	gas	PE	[1]
		Torsion	~120	gas	PE	[1]

[a] $\pm$ 40 cm^{-1}.

References

[1] P. Rosmus, H. Bock, B. Solouki, G. Maier, and G. Mihm, Angew. Chem. 93, 616 (1981); Angew. Chem. Int. Ed. Engl. 20, 598 (1981).

$CH_2{=}SiH_2$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SiH stretch	2239m	Ar	IR	[1][2]
			2235m	N_2	IR	[2]
		SiH stretch	2219m	Ar	IR	[1][2]
			2214m	N_2	IR	[2]
			1350w	Ar	IR	[2]
			1350w	N_2	IR	[2]
			985w	Ar	IR	[1][2]
			985w	N_2	IR	[1][2]
			927w	Ar	IR	[1][2]
			927w	N_2	IR	[2]
			817s	Ar	IR	[1][2]
			817s	N_2	IR	[2]
			741s	Ar	IR	[1][2]
			747s	N_2	IR	[2]

$CH_2=SiD_2$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	SiD stretch	1635m	Ar	IR	[1]
	SiD stretch	1600m	Ar	IR	[1]
		952w	Ar	IR	[1]
		759s	Ar	IR	[1]
		719s	Ar	IR	[1]
		396w	Ar	IR	[1]

References

[1] G. Maier, G. Mihm, and H. P. Reisenauer, Angew. Chem. 93, 615 (1981); Angew. Chem. Int. Ed. Engl. 20, 597 (1981).

[2] H. P. Reisenauer, G. Mihm, and G. Maier, Angew. Chem. 94, 864 (1982); Angew. Chem. Int. Ed. Engl. 21, 854 (1982).

CH_3SiH

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		2004m	Ar	IR	[1]
		1986w	N_2	IR	[1]
		1978w	N_2	IR	[1]
		1971m	N_2	IR	[1]
		1935w	Ar	IR	[1]

References

[1] H. P. Reisenauer, G. Mihm, and G. Maier, Angew. Chem. 94, 864 (1982); Angew. Chem. Int. Ed. Engl. 21, 854 (1982).

CH_2CCH

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CH stretch	3310m	Ar	IR	[1]
	H deformation	687m	Ar	IR	[1]
		548wm	Ar	IR	[1]
	C_3 deformation	483m	Ar	IR	[1]

CD_2CCD

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CD stretch	2548m	Ar	IR	[1]
	D deformation	553m	Ar	IR	[1]

References

[1] M. E. Jacox and D. E. Milligan, Chem. Phys. 4, 45 (1974).

CH_3CP^+

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	C≡P stretch	1420[a]	gas	PE	[1]

[a] $\pm$ 50 cm^{-1}.

References

[1] N. P. C. Westwood, H. W. Kroto, J. F. Nixon, and N. P. C. Simmons, J. Chem. Soc., Dalton Trans., 1405 (1979).

$CH_2=C=NH$ C_s Structure: MO [2]

Vib. No. sym.		Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CCN a-stretch	2040vs	Ar	IR	[1][3]
	5	CCN s-stretch; NH deform.	1124wm	Ar	IR	[1][3]
	6	NH deform.	1000 s	Ar	IR	[1][3]
	7	H_2CC OPLA	690m	Ar	IR	[1][3]
a"	11	Torsion	872m	Ar	IR	[1][3]

$CD_2=C=ND$

Vib. No. sym.		Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	3	CCN a-stretch	1998vs	Ar	IR	[1][3]
	5	CD_2 "scissors"	921m	Ar	IR	[1][3]
	6	ND deform.	800s	Ar	IR	[1][3]
a"	11	Torsion	648m	Ar	IR	[1][3]

References

[1] M. E. Jacox and D. E. Milligan, J. Am. Chem. Soc. 85, 278 (1963).

[2] A. C. Hopkinson, M. H. Lien, K. Yates, P. G. Mezey, and I. G. Csizmadia, J. Chem. Phys. 67, 517 (1977).

[3] M. E. Jacox, Chem. Phys. 43, 157 (1979).

CH_3CO C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CO stretch[a]	1875m	Ar[b]	IR	[2]
		1842m	Ar[b]	IR	[1][2]
	CH_3 deform.	1420wm	Ar[b]	IR	[2]
	CH_3 deform.	1329wm	Ar[b]	IR	[1][2]

CD_3CO

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CO stretch	1855m	Ar[b]	IR	[2]

[a] Fermi resonance with overtone or combination band.

[b] In [1], LiCl trapped in nearby site; in [2], HF trapped in nearby site.

References

[1] J. S. Shirk, Ph.D. Thesis, Univ. of California, Berkeley (1966); J. S. Shirk and G. C. Pimentel, J. Am. Chem. Soc. 90, 3349 (1968).

[2] M. E. Jacox, Chem. Phys. 69, 407 (1982).

CH_2CHO C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	CH_2 "scissors"	1558m	Ar[a]	IR	[2]
	C=O stretch	1540	gas	LF	[1][3]
		1542m[b] 1525m	Ar[a]	IR	[2]
	OCH deform.	1375m	Ar[a]	IR	[2]
	CC stretch	1143	gas	LF,PE	[1][3] [4]
	CCO bend	496[c]	gas	LF,PE	[1][3] [4]
a"	Torsion	765ms	Ar[a]	IR	[2]
		723m	Ar[a]	IR	[2]
		692ms	Ar[a]	IR	[2]

CD_2CDO

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	C=O stretch	1540	gas	LF	[1]
		1513ms	Ar[a]	IR	[2]
		1223w	Ar[a]	IR	[2]
	CC stretch	1050	gas	LF	[1]
	CCO bend	445[c]	gas	LF	[1]

[a] HF trapped in nearby site.

[b] Fermi resonance with overtone of 765-cm^{-1} fundamental.

[c] Ref. [1] attributed a band displaced by approximately 950 cm^{-1} in fluorescence spectrum of CH_2CHO, with a counterpart near 800 cm^{-1} in the fluorescence spectrum of CD_2CDO, to a H-deformation fundamental of a" symmetry. However, measurements of [3] for CH_2CHO support reassignment to the first overtone of the CCO bend, which has a rather large anharmonic constant.

References

[1] G. Inoue and H. Akimoto, J. Chem. Phys. 74, 425 (1981).

[2] M. E. Jacox, Chem. Phys. 69, 407 (1982).

[3] L. F. DiMauro, M. Heaven, and T. A. Miller, 39th Symposium on Molecular Spectroscopy, Columbus, Ohio, June 1984.

[4] W. C. Lineberger, private communication.

CH_2CHO^-

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CCO bend	525[a]	gas	PE	[1]

[a] $\pm$ 5 cm^{-1}.

References

[1] W. C. Lineberger, private communication.

CH_2=SiHCl

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	SiH stretch	2230w	Ar	IR	[1]
		2230w	N_2	IR	[1]

CH_2=SiHCl---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			984m	Ar	IR	[1]
			980m	N_2	IR	[1]
			843s	Ar	IR	[1]
			840s	N_2	IR	[1]
			699w	Ar	IR	[1]
			544m	Ar	IR	[1]
			537w	Ar	IR	[1]

References

[1] H. P. Reisenauer, G. Mihm, and G. Maier, Angew. Chem. 94, 864 (1982); Angew. Chem. Int. Ed. Engl. 21, 854 (1982).

CH_3SiCl

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1223m	Ar	IR	[1]
			485m	Ar	IR	[1]
			480w	Ar	IR	[1]

References

[1] H. P. Reisenauer, G. Mihm, and G. Maier, Angew. Chem. 94, 864 (1982); Angew. Chem. Int. Ed. Engl. 21, 854 (1982).

CH_3NO C_s Structure: MW [3]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'		CH_3 a-stretch	2991wm	Ar	IR	[2]
		CH_3 s-stretch	2901wm	Ar	IR	[2]
		N=O stretch	1564	gas	IR	[1]
			1549s	Ar	IR	[2]
		CH_3 a-deform.	1410s	Ar	IR	[2]
		CH_3 s-deform.	1348s	Ar	IR	[2]
		CH_3 rock	967w	Ar	IR	[2]
		C-N stretch	842	gas	IR	[1]
			870m	Ar	IR	[2]
		CNO bend	574wm	Ar	IR	[2]
a"		CH_3 a-stretch	2955w	Ar	IR	[2]
		CH_3 a-deform.	1410s	Ar	IR	[2]
		CH_3 rock	916wm	Ar	IR	[2]

References

[1] W. Luttke, Z. Elektrochem. 61, 302 (1957).

[2] A. J. Barnes, H. E. Hallam, S. Waring, and J. R. Armstrong, J. Chem. Soc., Faraday Trans. 2 72, 1 (1976).

[3] P. H. Turner and A. P. Cox, J. Chem. Soc., Faraday Trans. 2 74, 533 (1978).

$C_4H_2^+$ $^2\Pi_g$ $D_{\infty h}$ Structure: UV [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CH s-stretch	3136.9	gas	UV	[1]
			3143	Ne	LF	[2]
	2	C≡C s-stretch	2176.6	gas	UV	[1]
			2177	Ne	LF	[2]
	3	C-C stretch	860.6	gas	UV	[1]
			865	Ne	LF	[2]
Π_g	7	Deformation	485.8[a]	gas	UV	[1]
			486[a]	Ne	LF	[2]

$C_4D_2^+$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	1	CD s-stretch	2531.1	gas	UV	[1]
			2534	Ne	LF	[2]
	2	C≡C s-stretch	2066.3	gas	UV	[1]
			2067	Ne	LF	[2]
	3	C-C stretch	825.6	gas	UV	[1]
			829	Ne	LF	[2]
Π_g	7	Deformation	469.8[a]	gas	UV	[1]
			466[a]	Ne	LF	[2]

[a] $\frac{1}{2}(2\nu_7)$.

References

[1] J. H. Callomon, Can. J. Phys. 34, 1046 (1956).

[2] V. E. Bondybey and J. H. English, J. Chem. Phys. 71, 777 (1979).

CHOCHS

(Thioglyoxal)

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		2885w	Ar	IR	[1]
		2860m	Ar	IR	[1]
		2825w	Ar	IR	[1]
	C=O stretch	1700s	Ar	IR	[1]
		1698s	Ar	IR	[1]
		1368w	Ar	IR	[1]
		1268m	Ar	IR	[1]
		1095m	Ar	IR	[1]
	C=S stretch ?	1023s	Ar	IR	[1]
		788m	Ar	IR	[1]
		483m	Ar	IR	[1]

References

[1] M. Torres, A. Clement, and O. P. Strausz, Nouv. J. Chim. 7, 269 (1983).

HS-CH=C=S C_s

(Thiolthioketene)

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CH stretch	3040w	Ar	IR	[1]
	C=S stretch	1750s	Ar	IR	[1]
		945w	Ar	IR	[1]
		935w	Ar	IR	[1]
		735w	Ar	IR	[1]
		695w	Ar	IR	[1]

References

[1] M. Torres, A. Clement, O. P. Strausz, A. C. Weedon, and P. de Mayo, Nouv. J. Chim. 6, 401 (1982).

c-CHF=CHF$^+$ $^2B_1$ (C_{2v})

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1 2	C=C stretch	1600[a]	gas	EF	[1]
3	CH deformation	1330[a]	gas	EF	[1]
4	CF stretch	1030[a]	gas	EF	[1]
5	CF deformation	250[a]	gas	EF	[1]

[a] ± 10 cm^{-1}.

References

[1] J. P. Maier, O. Marthaler, and G. Bieri, Chem. Phys. 44, 131 (1979).

CH_2NO_2

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CH_2 a-stretch	3200wm	Ar[a]	IR	[1]
	CH_2 s-stretch	3055w	Ar[a]	IR	[1]
		1484vs	Ar[a]	IR	[1]
	NO_2 a-stretch	1461vs	Ar[a]	IR	[1]
		1419wm	Ar[a]	IR	[1]
		1307sh	Ar[a]	IR	[1]
	NO_2 s-stretch	1297s	Ar[a]	IR	[1]
		1209wm	Ar[a]	IR	[1]
		1095s	Ar[a]	IR	[1]
		1060w	Ar[a]	IR	[1]
		986wm	Ar[a]	IR	[1]
		719s	Ar[a]	IR	[1]
		693m	Ar[a]	IR	[1]
		606s	Ar[a]	IR	[1]

CD_2NO_2

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	NO_2 a-stretch	1460vs	Ar[a]	IR	[1]
		1307m	Ar[a]	IR	[1]
	NO_2 s-stretch	1296vs	Ar[a]	IR	[1]
		905m	Ar[a]	IR	[1]
		694m	Ar[a]	IR	[1]
		436m 432m	Ar[a]	IR	[1]

[a] HF trapped in adjacent site.

References

[1] M. E. Jacox, J. Phys. Chem. 87, 3126 (1983).

$CH_2=SiCl_2$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		1008m	Ar	IR	[1]
		732s	Ar	IR	[1]
		593m	Ar	IR	[1]

References

[1] G. Maier, G. Mihm, and H. P. Reisenauer, Angew. Chem. 93, 615 (1981); Angew. Chem. Int. Ed. Engl. 20, 597 (1981).

$(SCN)_2^+$ ^2A C_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C-S stretch?	920[a]	gas	PE	[1]

[a] ± 80 cm^{-1}.

References

[1] D. C. Frost, C. Kirby, W. M. Lau, C. B. MacDonald, C. A. McDowell, and N. P. C. Westwood, Chem. Phys. Lett. 69, 1 (1980).

N_2O_4 V_h Structure: ED [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	1		1383[a]	Ne	Ram	[7]
			1383	Ar	Ram	[5]
			1387[a]	Xe	Ram	[7]
	2		807[a]	Ne	Ram	[7]
			813	Ar	Ram	[5]
			815[a]	Xe	Ram	[7]
	3		265[a]	Ne	Ram	[7]
			262	Ar	Ram	[5]
			257[a]	Xe	Ram	[7]
a_u	4		79	gas	IR[b]	[6]
b_{1g}	5		1718[a]	Xe	Ram	[7]
	6		498[a]	Ne	Ram	[7]
			485[a]	Xe	Ram	[7]
b_{1u}	7		425	gas	IR	[6]
b_{2g}	8		657[a]	Xe	Ram	[7]
b_{2u}	9		1758	gas	IR	[6]
			1750s	Ar	IR	[3]
			1761	N_2	IR	[4]
			1750	O_2	IR	[3]
			1735s	Ar	IR	[2][3]
			1737	N_2	IR	[4]
			1735	O_2	IR	[3]

N_2O_4---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{3u}	11		1264	gas	IR	[2][6]
			1257s	Ar	IR	[2][3]
			1261	N_2	IR	[4]
			1261	O_2	IR	[3]
	12		751	gas	IR	[6]
			755sh	Ar	IR	[3]
			755	O_2	IR	[3]
			746sh	Ar	IR	[3]
			751	N_2	IR	[4]
			746	O_2	IR	[3]

[a] ± 3 cm^{-1}.

[b] From analysis of sequence bands near 540 cm^{-1}.

References

[1] D. W. Smith and K. Hedberg, J. Chem. Phys. 25, 1282 (1956).

[2] W. G. Fateley, H. A. Bent, and B. Crawford, Jr., J. Chem. Phys. 31, 204 (1959).

[3] R. V. St. Louis and B. Crawford, Jr., J. Chem. Phys. 42, 857 (1965).

[4] E. L. Varetti and G. C. Pimentel, J. Chem. Phys. 55, 3813 (1971).

[5] D. E. Tevault and L. Andrews, Spectrochim. Acta 30A, 969 (1974).

[6] C. H. Bibart and G. E. Ewing, J. Chem. Phys. 61, 1284 (1974).

[7] F. Bolduan and H. J. Jodl, Chem. Phys. Lett. 85, 283 (1982).

N_2O_4 V_d ?

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1717	Ar	IR	[1][2]
			1718	O_2	IR	[1][2]
			1282	Ar	IR	[1]
			1282	O_2	IR	[1]
			752	Ar	IR	[1]
			752	O_2	IR	[1]

References

[1] W. G. Fateley, H. A. Bent, and B. Crawford, Jr., J. Chem. Phys. 31, 204 (1959).

[2] R. V. St. Louis and B. Crawford, Jr., J. Chem. Phys. 42, 857 (1965).

ONO–NO_2 (Structure D)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		N=O stretch	1806[a]	Ne	Ram	[5]
			1829	Ar	IR	[1][2]
			1861	N_2	IR	[3]
			1829	O_2	IR	[1][2] [4]
		NO_2 a-stretch	1635[a]	Ne	Ram	[5]
			1645	Ar	IR	[1][2]
			1646[a]	Xe	Ram	[5]
			1628	N_2	IR	[3]
			1645	O_2	IR	[1][2] [4]
		NO_2 s-stretch	1295[a]	Ne	Ram	[5]
			1290	Ar	IR	[1][2]
			1299[a]	Xe	Ram	[5]
			1279	N_2	IR	[3]
			1291	O_2	IR	[1][2] [4]
		N-O stretch	905	O_2	IR	[2]
		NO_2 bend	783[a]	Ne	Ram	[5]
			787	Ar	IR	[1][2]
			788[a]	Xe	Ram	[5]
			792	N_2	IR	[3]
			783	O_2	IR	[1][2] [4]
		O=N-O bend	622[a]	Ne	Ram	[5]
			626[a]	Xe	Ram	[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]

[a] ± 3 cm^{-1}.

References

[1] W. G. Fateley, H. A. Bent, and B. Crawford, Jr., J. Chem. Phys. 31, 204 (1959).

[2] R. V. St. Louis and B. Crawford, Jr., J. Chem. Phys. 42, 857 (1965).

[3] E. L. Varetti and G. C. Pimentel, J. Chem. Phys. 55, 3813 (1971).

[4] G. R. Smith and W. A. Guillory, J. Mol. Spectrosc. 68, 223 (1977).

[5] F. Bolduan and H. J. Jodl, Chem. Phys. Lett. 85, 283 (1982).

ONO–NO_2 (Structure D′)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		N=O stretch	1873[a]	Ne	Ram	[2]
			1899 1889	O_2	IR	[1]
		NO_2 a-stretch	1584	O_2	IR	[1]
		NO_2 s-stretch	1290	O_2	IR	[1]
		N-O stretch	949[a]	Ne	Ram	[2]
			953[a]	Xe	Ram	[2]
			916	O_2	IR	[1]
		NO_2 bend	794	O_2	IR	[1]
		O=N-O bend	660	O_2	IR	[1]
		NO_2 rock or wag	524	O_2	IR	[1]

[a] ± 3 cm^{-1}.

References

[1] R. V. St. Louis and B. Crawford, Jr., J. Chem. Phys. 42, 857 (1965).

[2] F. Bolduan and H. J. Jodl, Chem. Phys. Lett. 85, 283 (1982).

CF_3O_2 C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	CF_3 stretch	1303vs	Ar	IR	[2]
	2	FCF_2 stretch	1260vs	Ar	IR	[2]
	3	O-O stretch	1092m	Ar	IR	[1][2]
	4	C-O stretch	870w	Ar	IR	[2]
	5	CF_3 deform.	692m	Ar	IR	[2]
	6	FCF_2 deform.	597w	Ar	IR	[2]
	7	COO bend	448vw	Ar	IR	[2]
a″	9	FCF_2 stretch	1172s	Ar	IR	[1][2]
	10	FCF_2 deform.	580w	Ar	IR	[2]
	11	CF_3 rock	286vw	Ar	IR	[2]

References

[1] R. R. Smardzewski, R. A. DeMarco, and W. B. Fox, J. Chem. Phys. 63, 1083 (1975).

[2] R. Butler and A. Snelson, J. Phys. Chem. 83, 3243 (1979).

CF_3ClF C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CF stretch	1235s	Ar	IR	[1]
	CF stretch	1224s	Ar	IR	[1]
	CF stretch	1073vs	Ar	IR	[1]
	ClF stretch	633m	Ar	IR	[1]

References

[1] M. E. Jacox, Chem. Phys. 51, 69 (1980).

CF_3BrF C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CF stretch	1251s	Ar	IR	[1]
	CF stretch	1225s	Ar	IR	[1]
	CF stretch	1051vs	Ar	IR	[1]
	BrF stretch	588wm	Ar	IR	[1]
	CF_3 deform.	454wm	Ar	IR	[1]

References

[1] M. E. Jacox, Chem. Phys. 51, 69 (1980).

CF_3IF C_s

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CF stretch	1223s	Ar	IR	[1]
	CF stretch	1197s	Ar	IR	[1]
	CF stretch	1052vs	Ar	IR	[1]
	IF stretch + CF_3 deform.	432m	Ar	IR	[1]

References

[1] M. E. Jacox, Chem. Phys. 51, 69 (1980).

SiF_5^-

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	Ax. SiF stretch	932vs[a]	Ar	IR	[1]
	Eq. SiF stretch	855s[a]	Ar	IR	[1]
	Br. SiF stretch	812vs[a]	Ar	IR	[1]
	Deform.	480s[a]	Ar	IR	[1]
	Deform.	457wm[a]	Ar	IR	[1]
	Deform.	444wm[a]	Ar	IR	[1]

[a] Cs^+ present.

References

[1] B. S. Ault, Inorg. Chem. 18, 3339 (1979).

SiF_4Cl^-

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	Ax. SiF stretch	932[a]	Ar	IR	[1]
	Eq. SiF stretch	902[a]	Ar	IR	[1]
	Eq. SiF stretch	879[a]	Ar	IR	[1]
	Br. SiF stretch	802[a]	Ar	IR	[1]
	Eq. SiCl str.	579[a]	Ar	IR	[1]

[a] Cs^+ present.

References

[1] B. S. Ault, Inorg. Chem. 18, 3339 (1979).

$SiF_3Cl_2^-$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	Ax. SiF stretch	928[a]	Ar	IR	[1]
	Br. SiF stretch	787[a]	Ar	IR	[1]
	Eq. SiCl str.	567[a]	Ar	IR	[1]

[a] Cs^+ present.

References

[1] B. S. Ault, Inorg. Chem. 18, 3339 (1979).

$SiF_2Cl_3^-$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Ax. SiF stretch	925[a]	Ar	IR	[1]
		Br. SiF stretch	779[a]	Ar	IR	[1]
		Eq. SiCl str.	563[a]	Ar	IR	[1]

[a] Cs^+ present.

References

[1] B. S. Ault, Inorg. Chem. 18, 3339 (1979).

$SiFCl_4^-$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		Br. SiF stretch	769[a]	Ar	IR	[1]
		Eq. SiCl str.	558[a]	Ar	IR	[1]
		Ax. SiCl str.	499[a]	Ar	IR	[1]

[a] Cs^+ present.

References

[1] B. S. Ault, Inorg. Chem. 18, 3339 (1979).

$SO_2F_3^-$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SO_2 a-stretch	1408w[a]	Ar	IR	[1]
		SO_2 s-stretch	1130m[a]	Ar	IR	[1]
		SF_2 a-stretch	925m[a]	Ar	IR	[1]
		SF eq. stretch	810m[a]	Ar	IR	[1]
		SF_2 s-stretch	649m[a]	Ar	IR	[1]

[a] Cs^+ present.

References

[1] K. Garber and B. S. Ault, Inorg. Chem. 22, 2509 (1983).

XeO_3F_2 D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1		806.7	Ar	Ram	[1]
	2		567.4	Ar	Ram	[1]
a_2''	3		631.7	Ne	IR	[1]
	4		375.4	Ne	IR	[1]
e'	5		895.8	Ne	IR	[1]
			892	Ar	Ram	[1]
	6		320.8	Ne	IR	[1]
			316	Ar	Ram	[1]
	7		190	Ar	Ram	[1]
e"	8		361	Ar	Ram	[1]

References

[1] H. H. Claassen and J. L. Huston, J. Chem. Phys. 55, 1505 (1971).

SF_5 C_{4v} Structure: ESR [1][2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e	7	SF stretch	812vs	Ar	IR	[3][4]
	8	SF stretch	552m	Ar	IR	[3][4]

References

[1] R. W. Fessenden and R. H. Schuler, J. Chem. Phys. 45, 1845 (1966).

[2] J. R. Morton and K. F. Preston, Chem. Phys. Lett. 18, 98 (1973).

[3] R. R. Smardzewski and W. B. Fox, J. Fluorine Chem. 7, 456 (1976).

[4] R. R. Smardzewski and W. B. Fox, J. Chem. Phys. 67, 2309 (1977).

SF_5^-

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SF stretch	796m	Ar	IR	[2]
		SF stretch	596s[a]	Ar	IR	[1][2]
			470w	Ar	IR	[2]

[a] This absorption was attributed to SF_6^- by [1]. Reassignment to SF_5^- is dictated by the close correspondence, discussed in [2], of these three absorptions to peaks observed for solid $CsSF_5$.

References

[1] J. E. Barefield, II, and W. A. Guillory, J. Phys. Chem. 81, 634 (1977).

[2] R. R. Smardzewski and W. B. Fox, J. Chem. Phys. 67, 2309 (1977).

6.13. Seven-Atomic Molecules

$C_2H_5^+$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CCH_2 OPLA	400[a]	gas	PE	[1][2]

[a] $\pm$ 30 cm^{-1}.

References

[1] J. M. Dyke, N. Jonathan, and A. Morris, Int. Rev. Phys. Chem. 2, 3 (1982).

[2] J. M. Dyke, A. R. Ellis, N. Keddar, and A. Morris, J. Phys. Chem. 88, 2565 (1984).

C_2H_5 C_s Structure: MO [2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′		CH_2 s-stretch	3033m	Ar	IR	[1]-[3]
		CH_3 s-stretch	2920m	Ar	IR	[2][3]
		2-CH stretch	2842s	Ar	IR	[1]-[3]
		CH_2 deform.	1440m	Ar	IR	[1]-[3]
		CH_3 deform.	1366m	Ar	IR	[1]-[3]
		CC stretch	1138w	Ar	IR	[2][3]
		CCH_2 "umbrella"	540vs	Ar	IR	[1]-[3]
a"		CH_2 a-stretch	3112s	Ar	IR	[1]-[3]
		CH_3 a-stretch	2987s	Ar	IR	[1]-[3]
		CH_3 deform.	1440m	Ar	IR	[1]-[3]
		H deform.	1175m	Ar	IR	[2][3]

C_2D_5

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′		CD_2 s-stretch	2199m	Ar	IR	[2][3]
		CD_3 s-stretch	2094m	Ar	IR	[2][3]
		2-CD stretch	2048m	Ar	IR	[2][3]
		CD_3 deform.	1070m	Ar	IR	[2][3]
		CD_3 deform.	1035m	Ar	IR	[2][3]
		CCD_2 "umbrella"	398vs	Ar	IR	[2][3]
a"		CD_2 a-stretch	2249m	Ar	IR	[2][3]
		CD_3 a-stretch	2170s	Ar	IR	[2][3]
		CD_3 deform.	1041m	Ar	IR	[2][3]

References

[1] J. Pacansky, G. P. Gardini, and J. Bargon, J. Am. Chem. Soc. 98, 2665 (1976).

[2] J. Pacansky and M. Dupuis, J. Am. Chem. Soc. 104, 415 (1982).

[3] J. Pacansky and B. Schrader, J. Chem. Phys. 78, 1033 (1983).

CH_3CHS^+

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CS stretch	950[a]	gas	PE	[1]

[a] ± 50 cm^{-1}.

References

[1] H. W. Kroto, B. M. Landsberg, R. J. Suffolk, and A. Vodden, Chem. Phys. Lett. 29, 265 (1974).

CH_2=CHOH C_s Structure: MW [1][3]

(Vinyl Alcohol)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	OH stretch	3620s	Ar	IR	[2][4]
	5	C=C stretch[a]	1662vs 1622s	Ar	IR	[2][4]
	7		1326w	Ar	IR	[4]
	8		1300m	Ar	IR	[4]
	9	CO stretch + OH deform.	1121s[b] 1079vs	Ar	IR	[2][4]
	10		943w	Ar	IR	[4]
	11		486w	Ar	IR	[4]
a"	12		960w	Ar	IR	[4]
	13	H_2C=C OPLA	814s	Ar	IR	[2][4]
	14		698vw	Ar	IR	[4]
	15	Torsion	413s	Ar	IR	[2][4]

CD_2=CDOD

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′		OD stretch	2677	Ar	IR	[2]
		C=C stretch	1590 1584	Ar	IR	[2]
		CO stretch + OD deform.	926 922	Ar	IR	[2]
a"		D_2C=C OPLA	651	Ar	IR	[2]
		Torsion	310	Ar	IR	[2]

Vinyl Alcohol---Footnotes

[a] Fermi resonance between ν_5 and $2\nu_{13}$.

[b] Fermi resonance between ν_9 and $(\nu_{14} + \nu_{15})$.

References

[1] S. Saito, Chem. Phys. Lett. 42, 399 (1976).

[2] M. Hawkins and L. Andrews, J. Am. Chem. Soc. 105, 2523 (1983).

[3] M. Rodler and A. Bauder, J. Am. Chem. Soc. 106, 4025 (1984).

[4] M. Rodler, C. E. Blom, and A. Bauder, J. Am. Chem. Soc. 106, 4029 (1984).

FCH_2CH_2 C_s Structure: MO [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		2-CH_2 stretch	2860m	Ar	IR	[2]
			1372wm	Ar	IR	[2]
		CF stretch	1047s	Ar	IR	[2]
		CCF deform.	427wm	Ar	IR	[2]

FCD_2CD_2

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		2-CD_2 stretch	2090wm	Ar	IR	[2]
		CF stretch + CD_2 "scissors"	1211s	Ar	IR	[2]
			1091m	Ar	IR	[2]
			1059wm	Ar	IR	[2]
		CF stretch + CD_2 "scissors"	969s	Ar	IR	[2]
		CCF deform.	424w	Ar	IR	[2]

References

[1] S. Kato and K. Morokuma, J. Chem. Phys. 72, 206 (1980).

[2] M. E. Jacox, Chem. Phys. 58, 289 (1981).

CH_3OCCl

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	2963	Ar	IR	[1]
			1449m	Ar	IR	[1]
		COC a-stretch	1300s	Ar	IR	[1]
			1286m	Ar	IR	[1]
			1280sh	Ar	IR	[1]

CH_3OCCl---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1135vs	Ar	IR	[1]
			950s	Ar	IR	[1]
			842wm	Ar	IR	[1]
			777s	Ar	IR	[1]
			698s	Ar	IR	[1]
			402m	Ar	IR	[1]

CD_3OCCl

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD stretch	2178	Ar	IR	[1]
			1370w	Ar	IR	[1]
		COC a-stretch	1330	Ar	IR	[1]
			1324	Ar	IR	[1]
			1073	Ar	IR	[1]
			1053	Ar	IR	[1]
			926	Ar	IR	[1]
			807	Ar	IR	[1]
			755	Ar	IR	[1]
			680	Ar	IR	[1]
			386	Ar	IR	[1]

References

[1] R. S. Sheridan and M. A. Kasselmayer, J. Am. Chem. Soc. 106, 436 (1984).

$c\text{-}CH_2(NO)OH$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	OH stretch	3477m	Ar	IR	[1]-[3]
	2	CH stretch	2906w	Ar	IR	[2]
	3	N=O stretch	1559wm	Ar	IR	[1][2]
	4	CH_2 "scissors"	1439m	Ar	IR	[2]
	5	COH bend	1355m	Ar	IR	[2][3]
	6	CH_2 wag	1250wm	Ar	IR	[2]
	7	C-O stretch	1130vs	Ar	IR	[1]-[3]
	8	CNO bend + CN stretch	792m	Ar	IR	[2]
	9	Skel. deform.	755wm	Ar	IR	[2]
	10	Skel. deform.	334w	Ar	IR	[2]

$c\text{-}CH_2(NO)OH$---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a"	11	CH stretch	2916w	Ar	IR	[2]
	12	CH_2 twist	1202vw	Ar	IR	[2]
	13	CH_2 rock	888w	Ar	IR	[2]
	14	OH torsion	346wm	Ar	IR	[2]
	15	NO torsion	191wm	Ar	IR	[2]

$c\text{-}CD_2(NO)OD$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	OD stretch	2571s	Ar	IR	[1]-[3]
	2	CD stretch	2125vw	Ar	IR	[2]
	3	N=O stretch	1558vs	Ar	IR	[2]
	4	C-O stretch	1191vs	Ar	IR	[2][3]
	5	CD_2 wag	1094m	Ar	IR	[2]
	6	CD_2 "scissors"	1009m	Ar	IR	[2]
	7	COD bend	929s	Ar	IR	[2][3]
	8	CNO bend	765m	Ar	IR	[2]
	9	CN stretch + OCN "scissors"	738m	Ar	IR	[2]
	10	OCN "scissors"	352w	Ar	IR	[2]
a"	12	CD_2 twist	878w	Ar	IR	[2]
	13	CD_2 rock	702m	Ar	IR	[2]
	14	OD torsion	285wm	Ar	IR	[2]

References

[1] R. P. Muller and J. R. Huber, J. Phys. Chem. 87, 2460 (1983).

[2] R. P. Muller, J. R. Huber, and H. Hollenstein, J. Mol. Spectrosc. 104, 209 (1984).

[3] M. E. Jacox, J. Phys. Chem. 88, 3373 (1984).

$t\text{-}CH_2(NO)OH$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	1	OH stretch	3638m	Ar	IR	[1]-[3]
	2	CH stretch	2906w	Ar	IR	[2]
	3	N=O stretch	1555s	Ar	IR	[1][2]
	4	CH_2 "scissors"	1432wm	Ar	IR	[2]
	5	COH bend	1352m	Ar	IR	[2][3]
	6	CH_2 wag	1181w	Ar	IR	[2]
	7	C-O stretch	1107vs	Ar	IR	[1]-[3]
	8	CN stretch	847w	Ar	IR	[2]

t-$CH_2(NO)OH$---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	9	Skel. deform.	542vw	Ar	IR	[2]
	10	OCN "scissors"	386m	Ar	IR	[2]
a"	11	CH stretch	2916w	Ar	IR	[2]
	13	CH_2 rock	865w	Ar	IR	[2]
	14	OH torsion	220m	Ar	IR	[2]

t-$CD_2(NO)OD$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	OD stretch	2687s	Ar	IR	[1]-[3]
	3	N=O stretch	1555s	Ar	IR	[2]
	4	C-O stretch	1173vs	Ar	IR	[2][3]
	5	CD_2 "scissors"	1028w	Ar	IR	[2][3]
	6	COD bend	984m	Ar	IR	[2][3]
	7	CD_2 wag	906w	Ar	IR	[2]
	8	CN stretch + COD bend	816wm	Ar	IR	[2][3]
	9	CN stretch + CNO bend	522w	Ar	IR	[2]
	10	OCN "scissors"	369m	Ar	IR	[2]
a"	11	CD stretch	2170w	Ar	IR	[2]
	13	CD_2 rock	692wm	Ar	IR	[2][3]
	14	NO torsion	173m	Ar	IR	[2]

References

[1] R. P. Muller and J. R. Huber, J. Phys. Chem. 87, 2460 (1983).

[2] R. P. Muller, J. R. Huber, and H. Hollenstein, J. Mol. Spectrosc. 104, 209 (1984).

[3] M. E. Jacox, J. Phys. Chem. 88, 3373 (1984).

$C_2H_2O_3$ C_s Structure: MW [1]

(Formic Acid Anhydride)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CH stretch	2987vw	Ar	IR	[2]
	2	CH stretch	2967w	Ar	IR	[2]
	3	C=O stretch	1822wm	gas	IR	[3]
			1812m	Ar	IR	[2][4]
	4	C=O stretch	1767s	gas	IR	[3]
			1762s	Ar	IR	[2][4]
	5	H deformation	1381w	Ar	IR	[2]
	6	H deformation	1359vw	Ar	IR	[2]

$C_2H_2O_3$---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	7	C-O stretch + skel. deform.	1105s	gas	IR	[3]
			1090s	Ar	IR	[2][4]
	8	C-O stretch	998m	gas	IR	[3]
			998m	Ar	IR	[2][4]
	9	C-O stretch	776w	Ar	IR	[2]
	10	O-C=O bend	540w	Ar	IR	[2][4]
	11	C-O-C bend	260w	Ar	IR	[2]
a"	12	H deformation	1067vw	Ar	IR	[2]
	14	Torsion	227m	Ar	IR	[2]

$C_2D_2O_3$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CD stretch	2260w	Ar	IR	[2]
	2	CD stretch	2241w	Ar	IR	[2]
	3	C=O stretch	1774m	Ar	IR	[2]
	4	C=O stretch	1744s[a]	Ar	IR	[2]
	5	C-O stretch + CD, OC=O deform.	1101s	Ar	IR	[2]
	6	C-O stretch + CD, OC=O deform.	1056s	Ar	IR	[2]
	8	C-O stretch	944m	Ar	IR	[2]
	9	C-O stretch + skel. deform.	743w	Ar	IR	[2]
	10	O-C=O bend	532w	Ar	IR	[2]
	11	C-O-C bend	250w	Ar	IR	[2]
a"	13	D deformation	865vw	Ar	IR	[2]
	14	Torsion	205w	Ar	IR	[2]

[a] Fermi resonance with overtone of 865-cm^{-1} fundamental leads to appearance of a strong absorption at 1700 cm^{-1}.

References

[1] S. Vaccani, U. Roos, A. Bauder, and H. H. Gunthard, Chem. Phys. 19, 51 (1977).

[2] H. Kuhne, T.-K. Ha, R. Meyer, and H. H. Gunthard, J. Mol. Spectrosc. 77, 251 (1979).

[3] H. Niki, P. D. Maker, C. M. Savage, and L. P. Breitenbach, J. Phys. Chem. 85, 1024 (1981).

[4] M. Hawkins, C. K. Kohlmiller, and L. Andrews, J. Phys. Chem. 86, 3154 (1982).

$O_2N-O-NO_2$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	NO_2 a-stretch	1720	gas	IR	[1]
		1745	N_2	IR	[2]
		1752	CO_2	IR	[1]
		1704	N_2	IR	[2]
		1700	CO_2	IR	[1]
	NO_2 s-stretch	1240	gas	IR	[1]
		1305	N_2	IR	[2]
		1316	CO_2	IR	[1]
		1247	N_2	IR	[2]
		1248	CO_2	IR	[1]
	NO_2 bend	730	gas	IR	[1]
		739	N_2	IR	[2]
		737	CO_2	IR	[1]
		719	CO_2	IR	[1]

References

[1] W. G. Fateley, H. A. Bent, and B. Crawford, Jr., J. Chem. Phys. 31, 204 (1959).

[2] E. L. Varetti and G. C. Pimentel, J. Chem. Phys. 55, 3813 (1971).

C_2F_5

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.[a]
a'	CF_3 a-stretch	1273vs	Ar	IR	[1][3]
	CF_3 s-stretch	1227s	Ar	IR	[1][3]
	CF_2 s-stretch	1117s	Ar	IR	[1][3]
	C-C stretch	956vw	Ar	IR	[1][3]
	CF_3 s-deform.	703m	Ar	IR	[1][3]
	CF_2 s-deform.	694vw	Ar	IR	[1]
	CF_3 a-deform.	514w	Ar	IR	[1][3]
	CF_2 wag	366vw	Ar	IR	[1]
	CF_3 rock	211vw	Ar	IR	[1]
a"	CF_3 a-stretch	1398w	Ar	IR	[1][3]
	CF_2 a-stretch	1184vs	Ar	IR	[1][3]
	CF_3 a-deform.	604w	Ar	IR	[1][3]
	CF_2 twist	419vw	Ar	IR	[1][3]
	CF_3 rock	227vw	Ar	IR	[1]

[a] Revised assignment offered by [2], based on more detailed study of infrared and Raman spectrum of C_2F_5I.

References

[1] R. Butler and A. Snelson, J. Fluorine Chem. 15, 89 (1980).

[2] D. A. C. Compton and D. M. Rayner, J. Phys. Chem. 86, 1628 (1982).

[3] M. E. Jacox, J. Phys. Chem. 88, 445 (1984).

6.14. Eight-Atomic Molecules

$CH_2CHCH_2^+$

(Allyl Cation)

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

[a] ± 40 cm^{-1}.

References

[1] F. A. Houle and J. L. Beauchamp, J. Am. Chem. Soc. 100, 3290 (1978).

CH_2CHCH_2 C_{2v}

(Allyl)

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CH stretch	3107m	Ar	IR	[1][2]
	CH stretch	3051w	Ar	IR	[1][2]
	CH stretch	3040w	Ar	IR	[1]
	CH stretch	3019m	Ar	IR	[1][2]
		1602m	Ar	IR	[1]
		1477m	Ar	IR	[1][2]
		1463m	Ar	IR	[1][2]
		1403vw	Ar	IR	[2]
		1388s	Ar	IR	[1][2]
		1317vw	Ar	IR	[1]
		1283w	Ar	IR	[1][2]
		1242w	Ar	IR	[1][2]
		1182w	Ar	IR	[1]
		983s	Ar	IR	[1][2]
		972m	Ar	IR	[1]
		810w	Ar	IR	[2]
		801vs	Ar	IR	[1][2]
		510s	Ar	IR	[1][2]

References

[1] A. K. Mal'tsev, V. A. Korolov, and O. M. Nefedov, Izv. Akad. Nauk SSSR, Ser. Khim., 2415 (1982); Bull. Acad. Sci. USSR, Chem. Ser., 31, 2131 (1982).

[2] G. Maier, H. P. Reisenauer, B. Rohde, and K. Dehnicke, Chem. Ber. 16, 732 (1983).

C_2H_5O

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CH_2 wag	1370	gas	LF	[1]
	C-O stretch	1067	gas	LF,UV	[1][2]
	C-C stretch	875[a]	gas	LF	[1]
	CCO bend	442	gas	LF	[1]

[a] Assignment to overtone of CCO bend cannot be excluded.

References

[1] G. Inoue, M. Okuda, and H. Akimoto, J. Chem. Phys. 75, 2060 (1981).

[2] T. Ebata, H. Yanagishita, K. Obi, and I. Tanaka, Chem. Phys. 69, 27 (1982).

C_4H_4 D_{2h} Structure: IR [3][4]

(Cyclobutadiene)

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CH stretch	3040?	Ar	IR	[1]
b_{1u}	C=C stretch	1523vw	Ar	IR	[4]
b_{2u}		1240s	Ar	IR	[1]-[4]
		723wm	Ar	IR	[4]
b_{3u}		573vs	Ar	IR	[1]-[4]

C_4D_4

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b_{1u}	C=C stretch	1456w	Ar	IR	[4]
b_{2u}		1043wm	Ar	IR	[4]
		609wm	Ar	IR	[4]
b_{3u}		421vs	Ar	IR	[4]

References

[1] O. L. Chapman, C. L. McIntosh, and J. Pacansky, J. Am. Chem. Soc. 95, 614 (1973).

[2] C. Y. Lin and A. Krantz, J. Chem. Soc., Chem. Commun. 1111 (1972).

[3] G. Maier, H.-G. Hartan, and T. Sayrac, Angew. Chem. 88, 252 (1976); Angew. Chem., Int. Ed. Engl. 15, 226 (1976).

[4] S. Masamune, F. A. Souto-Bachiller, T. Machiguchi, and J. E. Bertie, J. Am. Chem. Soc. 100, 4889 (1978).

CH_3C_2HS

(Methylthiirene)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3203w	Ar	IR	[1][2]
		CH stretch	2930vw	Ar	IR	[1][2]
			1440m	Ar	IR	[1][2]
			1429m	Ar	IR	[1][2]
			1036m	Ar	IR	[1][2]
			897m	Ar	IR	[1][2]
			650w	Ar	IR	[1][2]

References

[1] A. Krantz and J. Laureni, J. Am. Chem. Soc. 99, 4842 (1977).

[2] A. Krantz and J. Laureni, J. Am. Chem. Soc. 103, 486 (1981).

$C_6H_2^+$ $^2\Pi_g$ $D_{\infty h}$

(Triacetylene Cation)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	2	C_6 stretch	2180[a]	gas	EF	[1]
	3	C_6 stretch	1900[a]	gas	EF	[1]
	4		640[a]	gas	EF	[1]

[a] $\pm$ 5 cm^{-1}.

References

[1] M. Allan, E. Kloster-Jensen, and J. P. Maier, Chem. Phys. 17, 11 (1976).

CF_3C_2HS

(Trifluoromethylthiirene)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH stretch	3210w	Ar	IR	[1]
			1240s	Ar	IR	[1]
			1190s	Ar	IR	[1]
			1180s	Ar	IR	[1]
			720w	Ar	IR	[1]

References

[1] M. Torres, A. Clement, J. E. Bertie, H. E. Gunning, and O. P. Strausz, J. Org. Chem. 43, 2490 (1978).

6.15. Hydrocarbons with More Than Eight Atoms

$i\text{-}C_3H_7^+$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		970[a]	gas	PE	[1]
		730[a]	gas	PE	[1]

[a] ± 40 cm^{-1}.

References

[1] F. A. Houle and J. L. Beauchamp, J. Am. Chem. Soc. 101, 4067 (1979).

$n\text{-}C_3H_7$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CH stretch	3100	Ar	IR	[1]
	CH stretch	3018	Ar	IR	[1]
	2-CH stretch	2812	Ar	IR	[1]
	RCH_2· deform.	530vs	Ar	IR	[1]

References

[1] J. Pacansky, D. E. Horne, G. P. Gardini, and J. Bargon, J. Phys. Chem. 81, 2149 (1977).

$i\text{-}C_3H_7$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CH stretch	3069sh 3058	Ar	IR	[1]
	CH_3 stretch	2920	Ar	IR	[1]
	CH_3 stretch	2850	Ar	IR	[1]
	CH_3 stretch	2830	Ar	IR	[1]
	CH_3 deform.	1468	Ar	IR	[1]
	CH_3 deform.	1440	Ar	IR	[1]
	CH_3 deform.	1388	Ar	IR	[1]
	CH_3 deform.	1378	Ar	IR	[1]
	$HC(CH_3)_2$ OPLA	382s 366s	Ar	IR	[1]

References

[1] J. Pacansky and H. Coufal, J. Chem. Phys. 62, 3298 (1980).

$t\text{-}C_4H_9^+$ C_{3h}[a]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	C-C s-stretch[b]	760[c]	gas	PE	[1][2]
	C_4 OPLA[b]	460[c]	gas	PE	[1]-[3]

[a] Probable symmetry of carbon skeleton; see [2].

[b] Presumes C_{3v} structure for $t\text{-}C_4H_9$.

[c] ± 30 cm^{-1}.

References

[1] T. Koenig, T. Balle, and W. Snell, J. Am. Chem. Soc. 97, 662 (1975).

[2] J. Dyke, N. Jonathan, E. Lee, A. Morris, and M. Winter, Phys. Scr. 16, 197 (1977).

[3] F. A. Houle and J. L. Beauchamp, J. Am. Chem. Soc. 101, 4067 (1979).

$n\text{-}C_4H_9$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	$1\text{-}CH_2$ stretch	3105	Ar	IR	[1][2]
	$1\text{-}CH_2$ stretch	3024	Ar	IR	[1][2]
		2886	Ar	IR	[2]
	$2\text{-}CH_2$ stretch	2835	Ar	IR	[2]
	$2\text{-}CH_2$ stretch	2809	Ar	IR	[1][2]
		1471	Ar	IR	[2]
		1463	Ar	IR	[2]
	$2\text{-}CH_2$ deform.	1425	Ar	IR	[2]
		1183	Ar	IR	[2]
		1098	Ar	IR	[2]
	$(C_3H_7)CH_2$ OPLA	520s	Ar	IR	[1]

References

[1] J. Pacansky, D. E. Horne, G. P. Gardini, and J. Bargon, J. Phys. Chem. 81, 2149 (1977).

[2] J. Pacansky and A. Gutierrez, J. Phys. Chem. 87, 3074 (1983).

$(CH_3)_2CHCH_2$·

(Isobutyl)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		1-CH stretch	3023	Ar	IR	[1]
		1-CH stretch	3115	Ar	IR	[1]
		2-CH stretch	2820	Ar	IR	[1]
		$(C_3H_7)CH_2$ OPLA	557s 546s	Ar	IR	[1]

References

[1] J. Pacansky, D. W. Brown, and J. S. Chang, J. Phys. Chem. 85, 2562 (1981).

$t\text{-}C_4H_9$ C_{3v} Structure: IR [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH a-stretch	2931	Ar	IR	[1]
		CH s-stretch	2833[a]	gas	IR	[2]
			2825vs	Ar	IR	[1]
		CH_3 a-deform.	1455	Ar	IR	[1]
		CH_3 s-deform.	1370	Ar	IR	[1]
		CH_3 rock	1279	Ar	IR	[1]
		CH_3 rock	1252	Ar	IR	[1]
		CH_3 rock	1189	Ar	IR	[1]
		CH_3 rock	1126	Ar	IR	[1]
		CC a-stretch	992	Ar	IR	[1]
		CC s-stretch	733	Ar	IR	[1]
		C_3 a-bend	541	Ar	IR	[1]

[a] Time-resolved infrared spectral photography (TRISP); resolution 3 cm^{-1}.

References

[1] J. Pacansky and J. S. Chang, J. Chem. Phys. 74, 5539 (1981).

[2] D. S. Bethune, J. R. Lankard, P. P. Sorokin, A. J. Schell-Sorokin, R. M. Plecenik, and Ph. Avouris, J. Chem. Phys. 75, 2231 (1981).

$C_5H_4^+$ ^2E C_{3v}

(Methyldiacetylene Cation)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	C≡C stretch	2212	gas	EF	[1][2]
	4	C≡C stretch	1921	gas	EF	[2]
	6	C-C a-stretch	1203	gas	EF	[1][2]
	7	C-C s-stretch	685[a] 691	gas	EF	[1][2]
e	13	Skel. deform.	313[ab] 324	gas	EF	[2]

$C_5D_4^+$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3	C≡C stretch	2186	gas	EF	[1][2]
	4	C≡C stretch	1884	gas	EF	[2]
	5	CD_3 deform.	1020[a]	gas	EF	[1][2]
	6	C-C a-stretch	1219	gas	EF	[1][2]
	7	C-C s-stretch	634[a]	gas	EF	[1][2]
e	13	Skel. deform.	283[ab] 292	gas	EF	[2]

[a] Uncorrected for Fermi resonance.

[b] $\frac{1}{2}(2\nu_{13})$.

References

[1] J. P. Maier, O. Marthaler, and E. Kloster-Jensen, J. Chem. Phys. 72, 701 (1980).

[2] S. Leutwyler, D. Klapstein, and J. P. Maier, Chem. Phys. 78, 151 (1983).

C_5H_4:

(Cyclopentadienylidine)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1345w	N_2	IR	[1]
			1335m	N_2	IR	[1]
			1101w	N_2	IR	[1]
			1074w	N_2	IR	[1]
			922w	N_2	IR	[1]
			703s	N_2	IR	[1]
			577w	N_2	IR	[1]

References

[1] M. S. Baird, I. R. Dunkin, N. Hacker, M. Poliakoff, and J. J. Turner, J. Am. Chem. Soc 103, 5190 (1981).

C_5H_5 $^2E_1''$ D_{5h} Structure: ESR [1]; UV [2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	2	C-C stretch	880	gas	PD,LF	[3][4]
e_2'	10	C-C stretch	1690[ab]	gas	PD	[3]
	11	CH in-plane deform.	1170[a]	gas	PD	[3]
	13	In-plane ring deform.	475	gas	LF	[4]
e_2''	14	Out-of-plane ring deform.	380	gas	LF	[4]

[a] ± 40 cm^{-1}.

[b] Alternatively, may be contributed by $2\nu_2$.

References

[1] G. R. Liebling and H. M. McConnell, J. Chem. Phys. 42, 3931 (1965).

[2] R. Engleman, Jr., and D. A. Ramsay, Can. J. Phys. 48, 964 (1970).

[3] P. C. Engelking and W. C. Lineberger, J. Chem. Phys. 67, 1412 (1977).

[4] H. H. Nelson, L. Pasternack, and J. R. McDonald, Chem. Phys. 74, 227 (1983).

$n\text{-}C_5H_{11}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		1-CH_2 stretch	3103	Ar	IR	[1]
		1-CH_2 stretch	3025	Ar	IR	[1]
		2-CH_2 stretch	2838	Ar	IR	[1]
		2-CH_2 stretch	2802	Ar	IR	[1]
		2-CH_2 deform.	1425	Ar	IR	[1]
			1181	Ar	IR	[1]
			1096	Ar	IR	[1]
		$(C_4H_9)CCH_2$ OPLA	519s	Ar	IR	[1]

References

[1] J. Pacansky and A. Gutierrez, J. Phys. Chem. 87, 3074 (1983).

$(CH_3)_3CCH_2$.

(Neopentyl)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		1-CH stretch	3105	Ar	IR	[1]
		1-CH stretch	3020	Ar	IR	[1]
		$(C_4H_9)CCH_2$ OPLA	565vs 555vs	Ar	IR	[1]

References

[1] J. Pacansky, D. W. Brown, and J. S. Chang, J. Phys. Chem. 85, 2562 (1981).

C_6H_4

(Benzyne)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C=C stretch	1627ms	Ar	IR	[1]
		C=C stretch	1607m	Ar	IR	[1]
		CH deform.	1451m	Ar	IR	[1]
			1053m	Ar	IR	[1]
			1038m	Ar	IR	[1]
			849s	Ar	IR	[1]
			736vs	Ar	IR	[1]
			469vs	Ar	IR	[1]

References

[1] O. L. Chapman, K. Mattes, C. L. McIntosh, J. Pacansky, G. V. Calder, and G. Orr, J. Am. Chem. Soc. 95, 6134 (1973).

C_6H_5 C_{2v}

(Phenyl)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C_6 deform.	707s	Ar	IR	[1]-[3]

C_6D_5

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C_6 deform.	519s	Ar	IR	[1][3]

References

[1] J. Pacansky and J. Bargon, J. Am. Chem. Soc. 97, 6896 (1975).

[2] J. Pacansky, G. P. Gardini, and J. Bargon, J. Am. Chem. Soc. 98, 2665 (1976).

[3] M. E. Jacox, J. Phys. Chem. 86, 670 (1982).

$CH_3(C{\equiv}C)_2CH_3^+$ ^2E_g (D_{3d})

(Dimethyldiacetylene Cation)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	2	C≡C stretch	2247	gas	PS,EF	[1][2][6]
			2246	Ne	LF	[3]
	4	C-C stretch	1323	gas	EF	[2][6]
			1322	Ne	LF	[3]
	5	C-C stretch	555	gas	PS,EF, LF	[2][4][5][6]
			558	Ne	LF	[3]
e_u	14	Skel. deform.	327[a]	gas	EF	[6]
e_g	20	Skel. deform.	237[a]	gas	EF	[6]

$CD_3(C{\equiv}C)_2CD_3^+$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	2	C≡C stretch	2248	gas	EF	[5][6]
	4	C-C stretch	1335	gas	EF	[5][6]
	5	C-C stretch	509	gas	EF	[5][6]
e_g	20	Skel. deform.	217[a]	gas	EF	[6]

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

References

[1] F. Brogli, E. Heilbronner, V. Hornung, and E. Kloster-Jensen, Helv. Chim. Acta 56, 2171 (1973).

[2] M. Allan, J. P. Maier, O. Marthaler, and E. Kloster-Jensen, Chem. Phys. 29, 331 (1978).

[3] V. E. Bondybey, J. H. English, and T. A. Miller, J. Chem. Phys. 70, 1765 (1979).

[4] T. A. Miller, V. E. Bondybey, and B. R. Zegarski, J. Chem. Phys. 70, 4982 (1979).

[5] J. P. Maier, O. Marthaler, and E. Kloster-Jensen, J. Chem. Phys. 72, 701 (1980).

[6] D. Klapstein, R. Kuhn, S. Leutwyler, and J. P. Maier, Chem. Phys. 78, 167 (1983).

$C_6H_8^+$ ^2A_u C_{2h}

(trans-1,3,5-Hexatriene Cation)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	5	C=C stretch	1610[a]	gas	EF	[1]
			1622	Ne	LF	[2]
	6	C=C stretch	1513	Ne	LF	[2]
	7	CH deform.	1376	Ne	LF	[2]
	8	CH deform.	1293	Ne	LF	[2]
	9	CH deform. + C-C stretch	1239	Ne	LF	[2]
	10	CH deform. + C-C stretch	1115	Ne	LF	[2]
	11	CH deform. + C-C stretch	951	Ne	LF	[2]
	12	Skel. deform.	442	Ne	LF	[2]
	13	Skel. deform.	350[a]	gas	EF	[1]
			350	Ne	LF	[2]

[a] ± 10 cm^{-1}.

References

[1] M. Allan and J. P. Maier, Chem. Phys. Lett. 43, 94 (1976).

[2] V. E. Bondybey, J. H. English, and T. A. Miller, J. Mol. Spectrosc. 80, 200 (1980).

C_7H_6

(Phenylmethylene)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			3080ms[a]	Ar	IR	[1]
			1505m[b]	Ar	IR	[1]
			1460m[b]	Ar	IR	[1]
			1430m[b]	Ar	IR	[1]
			1390m[b]	Ar	IR	[1]
			1210wm[b]	Ar	IR	[1]
			1020m[b]	Ar	IR	[1]
			945wm[b]	Ar	IR	[1]
			885m[b]	Ar	IR	[1]
			740vs[b]	Ar	IR	[1]
			670vs[b]	Ar	IR	[1]
			550wm[b]	Ar	IR	[1]
			445s[b]	Ar	IR	[1]

[a] ± 10 cm^{-1}.

[b] ± 5 cm^{-1}.

References

[1] P. R. West, O. L. Chapman, and J.-P. LeRoux, J. Am. Chem. Soc. 104, 1779 (1982).

C_7H_6

(Cyclohepta-1,2,4,6-Tetraene)

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		3040s[a]	Ar	IR	[1]
		3010s[a]	Ar	IR	[1]
		1824m	Ar	IR	[1]
		1816sh	Ar	IR	[1]
		1500wm[b]	Ar	IR	[1]
		1425wm[b]	Ar	IR	[1]
		1380vs[b]	Ar	IR	[1]
		1365wm[b]	Ar	IR	[1]
		1270m[b]	Ar	IR	[1]
		1190m[b]	Ar	IR	[1]
		965m[b]	Ar	IR	[1]
		915m[b]	Ar	IR	[1]
		770vs[b]	Ar	IR	[1]
		690s[b]	Ar	IR	[1]
		680vs[b]	Ar	IR	[1]
		580ms[b]	Ar	IR	[1]
		410m[b]	Ar	IR	[1]

[a] ± 10 cm^{-1}.

[b] ± 5 cm^{-1}.

References

[1] P. R. West, O. L. Chapman, and J.-P. LeRoux, J. Am. Chem. Soc. 104, 1779 (1982).

$C_6H_5CH_2^+$

(Benzyl Cation)

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

$C_6H_5CD_2^+$

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

[a] ± 40 cm^{-1}.

References

[1] F. A. Houle and J. L. Beauchamp, J. Am. Chem. Soc. 100, 3290 (1978).

$C_7H_7^+$ $^1A_1$ D_{7h}

(Tropylium)

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	Ring stretch	1424[a]	gas	PE	[1]

[a] ± 100 cm^{-1}.

References

[1] T. Koenig and J. C. Chang, J. Am. Chem. Soc. 100, 2240 (1978).

$C_6H_5CH_2$ $^2B_1$ C_{2v}

(Benzyl)

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1 8a	CC stretch	1606	gas	UV	[1][2]
19a	CC stretch	1430	gas	UV	[1][2]
		1423	Ar	LF	[3]
7a	C-CH_2 stretch	1269	gas	UV	[1][2]
9a	CH deform.	1181	gas	UV	[1][2]
1	CC stretch	983	gas	UV	[1][2]
		982	Ar	LF	[3]
12a	CC deform.	814	gas	UV	[1][2]
6a	CC deform.	522	gas	UV	[1][2]
		520	Ar	LF	[3]
a_2 10a	CH deform.	861	gas	UV	[2]
16a	CC deform.	393	gas	UV	[2]
b_1 16b	CC deform.	430	gas	UV	[2]
b_2 8b	CC stretch	1546	gas	UV	[1][2]
		1530	Ar	LF	[3]
9b	CH deform.	1156	gas	UV	[1][2]
15	CH deform.	1089	gas	UV	[1][2]
6b	CC deform.	616	gas	UV	[1][2]
		612	Ar	LF	[3]
18b	CC deform.	360	gas	UV	[1][2]
		357	Ar	LF	[3]

$C_6D_5CD_2$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	8a	CC stretch	1593	gas	UV	[1][2]
	19a	CC stretch	1327	gas	UV	[1][2]
			1323	Ar	LF	[3]
	7a	$C-CD_2$ stretch	1204	gas	UV	[1][2]
	1	CC stretch	948	gas	UV	[1][2]
			945	Ar	LF	[3]
	9a	CD deform.	895	gas	UV	[1][2]
	18a	CD deform.	848	gas	UV	[2]
	12a	CC stretch	791	gas	UV	[1][2]
	6a	CC deform.	498	gas	UV	[1][2]
			495	Ar	LF	[3]
a_2	10a	CD deform.	750	gas	UV	[2]
	16a	CC deform.	305	gas	UV	[2]
b_1	16b	CC deform.	376	gas	UV	[2]
b_2	8b	CC stretch	1495	gas	UV	[1][2]
			1490	Ar	LF	[3]
	15	CD deform.	848	gas	UV	[1][2]
	6b	CC deform.	589	gas	UV	[1][2]
			588	Ar	LF	[3]
	18b	CC deform.	305	gas	UV	[1][2]
			303	Ar	LF	[3]

References

[1] L. Grajcar and S. Leach, J. Chim. Phys. 61, 1523 (1964).

[2] L. Watmann-Grajcar, J. Chim. Phys. 66, 1023 (1969).

[3] J. H. Miller and L. Andrews, J. Mol. Spect. 90, 20 (1981).

C_8H_8

(o-Xylylene)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			3105w	Ar	IR	[1]
			3070w	Ar	IR	[1]
			3045w	Ar	IR,Ram	[1]
			2950w	Ar	IR	[1]
			1741w	Ar	IR	[1]
			1576w	Ar	IR,Ram	[1]
			1552m	Ar	IR,Ram	[1]
			1542w	Ar	IR	[1]

o-Xylylene---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1529m	Ar	Ram	[1]
			1490w	Ar	IR	[1]
			1471w	Ar	IR	[1]
			1465w	Ar	IR	[1]
			1427w	Ar	IR	[1]
			1333w	Ar	IR	[1]
			1303w	Ar	IR	[1]
			1293m	Ar	Ram	[1]
			1158w	Ar	IR	[1]
			1000w	Ar	IR	[1]
			953w	Ar	IR	[1]
			870s	Ar	IR,Ram	[1]
			866w	Ar	IR,Ram	[1]
			779w	Ar	IR,Ram	[1]
			776s	Ar	IR	[1]
			742m	Ar	IR	[1]
			737m	Ar	IR	[1]
			675m	Ar	IR	[1]
			638m	Ar	IR	[1]
			442m	Ar	IR	[1]

References

[1] K. L. Tseng and J. Michl, J. Am. Chem. Soc. 99, 4840 (1977).

6.16. Substituted Acetylene and Polyacetylene Cations

$HC{\equiv}CCl^+$ $^2\Pi_{3/2}$ $D_{\infty h}$ Structure: UV [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CH stretch	3146[a]	gas	EF	[2]
	2	C≡C stretch	1984	gas	EF	[2]
	3	CCl stretch	836	gas	EF	[2]
Π	4	HCC deform.	595[a]	gas	EF	[2]
	5	CCCl deform.	235[a]	gas	EF	[2]

$DC{\equiv}CCl^+$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	1	CD stretch	2475[a]	gas	EF	[2]
	2	C≡C stretch	1882	gas	EF	[2]
	3	CCl stretch	816	gas	EF	[2]
Π	4	DCC deform.	476	gas	EF	[2]

[a] Tentative assignment.

References

[1] M. Allan, E. Kloster-Jensen, and J. P. Maier, J. Chem. Soc., Faraday Trans. 2 73, 1406 (1977).

[2] D. Klapstein, R. Kuhn, and J. P. Maier, Chem. Phys. 86, 285 (1984).

$HC{\equiv}CBr^+$ $^2\Pi_{3/2}$ $C_{\infty v}$ Structure: UV [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	3	CBr stretch	674[a]	gas	EF	[2]
Π	5	CCBr deform.	290[a]	gas	EF	[2]

$DC{\equiv}CBr^+$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Π	5	CCBr deform.	273[a]	gas	EF	[2]

[a] $\pm$ 3 cm^{-1}.

References

[1] M. Allan, E. Kloster-Jensen, and J. P. Maier, J. Chem. Soc., Faraday Trans. 2 73, 1406 (1977).

[2] D. Klapstein, R. Kuhn, and J. P. Maier, in press.

$ClC{\equiv}CCl^+$ $^2\Pi_{3/2,u}$ $D_{\infty h}$ Structure: UV [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2107	gas	EF	[2]
	2	C-Cl stretch	504	gas	EF	[2]
Π_g	4	Deformation	318[a]	gas	EF	[2]
Π_u	5	Deformation	198[ab]	gas	EF	[2]

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

[b] Tentative.

References

[1] M. Allan, E. Kloster-Jensen, and J. P. Maier, J. Chem. Soc., Faraday Trans. 2 73, 1417 (1977).

[2] D. Klapstein, J. P. Maier, and W. Zambach, Chem. Phys. 77, 463 (1983).

$BrC{\equiv}CBr^+$ $^2\Pi_{3/2,u}$ $D_{\infty h}$ Structure: UV [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2067	gas	EF	[2]
	2	C-Br stretch	321	gas	EF	[2]
Π_g	4	Deformation	298[a]	gas	EF	[2]
Π_u	5	Deformation	136[a]	gas	EF	[2]

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

References

[1] M. Allan, E. Kloster-Jensen, and J. P. Maier, J. Chem. Soc., Faraday Trans. 2 73, 1417 (1977).

[2] D. Klapstein, J. P. Maier, and W. Zambach, Chem. Phys. 77, 463 (1983).

$IC{\equiv}CI^+$ $^2\Pi_{3/2,u}$ $D_{\infty h}$ Structure: UV [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	1990[a]	gas	EF	[2]
	2	C-I stretch	242	gas	EF	[2]
Π_g	4	Deformation	221[b]	gas	EF	[2]
Π_u	5	Deformation	101[b]	gas	EF	[2]

[a] Value for $^2\Pi_{1/2,u}$ state.

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

References

[1] M. Allan, E. Kloster-Jensen, and J. P. Maier, J. Chem. Soc., Faraday Trans. 2 73, 1417 (1977).

[2] D. Klapstein, J. P. Maier, and W. Zambach, Chem. Phys. 77, 463 (1983).

$NCC{\equiv}CCN^+$ $^2\Pi_u$ $D_{\infty h}$ Structure: UV [1][2]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡N stretch	2210[a]	gas	EF	[1][2]
	2	C≡C stretch	1930[a]	gas	EF	[1][2]
	3	C-C stretch	570[a]	gas	EF	[1][2]

[a] ± 10 cm^{-1}.

References

[1] J. P. Maier, O. Marthaler, and F. Thommen, Chem. Phys. Lett. 60, 193 (1979).

[2] J. P. Maier, L. Misev, and F. Thommen, J. Phys. Chem. 86, 514 (1982).

$H(C{\equiv}C)_2Cl^+$ $^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	C≡C stretch	2190[a]	gas	EF	[1][2]
	3	C≡C stretch	1910[a]	gas	EF	[1][2]
	4	C-C stretch	1180[a]	gas	EF	[1][2]
	5	C-Cl stretch	540[a]	gas	EF	[1][2]
Π	8	Skel. deform.	305[ab]	gas	EF	[2]

[a] ± 10 cm^{-1}.

[b] ½($2\nu_8$).

References

[1] J. P. Maier, O. Marthaler, and E. Kloster-Jensen, J. Electron Spectrosc. Relat. Phenom. 18, 251 (1980).

[2] J. P. Maier, O. Marthaler, L. Misev, and F. Thommen, J. Chem. Soc., Faraday Disc. 71, 181 (1981).

$H(C{\equiv}C)_2Br^+$ $^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	C≡C stretch	2145[a]	gas	EF	[1]
	3	C≡C stretch	1910[a]	gas	EF	[1]
	4	C-C stretch	1110[a]	gas	EF	[1]
	5	C-Br stretch	450[a]	gas	EF	[1]

[a] ± 10 cm^{-1}.

References

[1] J. P. Maier, O. Marthaler, and E. Kloster-Jensen, J. Electron Spectrosc. Relat. Phenom. 18, 251 (1980).

$H(C{\equiv}C)_2CN^+$ $^2\Pi$ $C_{\infty v}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ^+	2	C≡N, C≡C str.	2190[a]	gas	EF	[1]
	3	C≡N, C≡C str.	2070[a]	gas	EF	[1]
	5	C-C stretch	1220[a]	gas	EF	[1]
	6	C-C stretch	630[a]	gas	EF	[1]

[a] ± 10 cm^{-1}.

References

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

$F(C{\equiv}C)_2F^+$ $^2\Pi_g$ $D_{\infty h}$ Structure: PE [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C stretch	2320[a]	gas	EF	[2]
	2	C-F stretch	1550[a]	gas	EF	[2]
	3	C-C stretch	520[a]	gas	EF	[2]
Π_g	7	Deformation	300[ab]	gas	EF	[2]

[a] ± 10 cm^{-1}.

[b] ½($2\nu_7$).

References

[1] G. Bieri, E. Heilbronner, J.-P. Stadelmann, J. Vogt, and W. von Niessen, J. Am. Chem. Soc. 99, 6832 (1977).

[2] M. Allan, J. P. Maier, O. Marthaler, and J.-P. Stadelmann, J. Chem. Phys. 70, 5271 (1979).

$Cl(C{\equiv}C)_2Cl^+$ $^2\Pi_{3/2,g}$ $D_{\infty h}$ Structure: UV [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C s-stretch	2214	gas	EF	[1][2]
	2	C-C stretch	1316	gas	EF	[1][2]
	3	C-Cl s-stretch	393	gas	EF	[1][2]
Σ_u^+	5	C-Cl a-stretch	657	gas	EF	[2]

References

[1] M. Allan, E. Kloster-Jensen, J. P. Maier, and O. Marthaler, J. Electron Spectrosc. 14, 359 (1978).

[2] D. Klapstein, J. P. Maier, and L. Misev, J. Chem. Phys. 78, 5393 (1983).

$Br(C{\equiv}C)_2Br^+$ $^2\Pi_{3/2,g}$ $D_{\infty h}$ Structure: UV [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡C s-stretch	2186	gas	EF	[1][2]
	2	C-C stretch	1225	gas	EF	[1][2]
	3	C-Br s-stretch	252	gas	EF	[1][2]

References

[1] M. Allan, E. Kloster-Jensen, J. P. Maier, and O. Marthaler, J. Electron Spectrosc. 14, 359 (1978).

[2] D. Klapstein, J. P. Maier, and L. Misev, J. Chem. Phys. 78, 5393 (1983).

$I(C{\equiv}C)_2I^+$ $^2\Pi_u$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	3	C-I stretch	190[a]	gas	EF	[1]

[a] ± 10 cm^{-1}.

References

[1] M. Allan, E. Kloster-Jensen, J. P. Maier, and O. Marthaler, J. Electron. Spectrosc. Relat. Phenom. 14, 359 (1978).

$NC(C{\equiv}C)_2CN^+$ $^2\Pi_g$ $D_{\infty h}$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
Σ_g^+	1	C≡N stretch	2180[a]	gas	EF	[1]
	2	C≡C stretch	2100[a]	gas	EF	[1]
	3	C-C stretch	1360[a]	gas	EF	[1]
	4	C-C stretch	460[a]	gas	EF	[1]

[a] ± 10 cm^{-1}.

References

[1] E. Kloster-Jensen, J. P. Maier, O. Marthaler, and M. Mohraz, J. Chem. Phys. 71, 3125 (1979).

$CH_3(C{\equiv}C)_2Cl^+$ ^2E C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C≡C stretch	2240[a]	gas	EF	[1]
	4	CH_3 deform.	1320[a]	gas	EF	[1]
	7	C-Cl stretch	470[a]	gas	EF	[1]

[a] ± 10 cm^{-1}.

References

[1] J. P. Maier, O. Marthaler, and E. Kloster-Jensen, J. Electron Spectrosc. Relat. Phenom. 18, 251 (1980).

$CH_3(C{\equiv}C)_2Br^+$ ^2E C_{3v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	2	C≡C stretch	2210[a]	gas	EF	[1]
	3	C≡C stretch	1980[a]	gas	EF	[1]
	4	CH_3 deform.	1280[a]	gas	EF	[1]
	7	C-Br stretch	380[a]	gas	EF	[1]

[a] ± 10 cm^{-1}.

References

[1] J. P. Maier, O. Marthaler, and E. Kloster-Jensen, J. Electron Spectrosc. Relat. Phenom. 18, 251 (1980).

$CH_3(C{\equiv}C)_2CN^+$ ^2E C_{3v} Structure: UV [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2	C≡C stretch	2207[a]	gas	EF	[2]
	3	C≡C, C≡N str.	2093[a]	gas	EF	[2]
	4	C≡C, C≡N str.	1980[a]	gas	EF	[2]
	5	CH_3 deform.	1340[ab]	gas	EF	[2]
	8	C-C stretch	513[a]	gas	EF	[2]

[a] ± 2 cm^{-1}.

[b] Alternatively, may be assigned to ν_6, a C-C stretching mode.

References

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

[2] D. Klapstein, J. P. Maier, L. Misev, F. Thommen, and W. Zambach, J. Electron Spectrosc. Relat. Phenom. 31, 283 (1983).

$C_2H_5(C{\equiv}C)_2CN^+$ $^2A''$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′	2	C≡N, C≡C str.	2180[a]	gas	EF	[1]
	3	C≡N, C≡C str.	2080[a]	gas	EF	[1]
	5	C-C stretch	1320[a]	gas	EF	[1]
	6	C-C stretch	550[a]	gas	EF	[1]
			460[a]	gas	EF	[1]

[a] ± 10 cm^{-1}.

References

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

$CF_3(C{\equiv}C)_2F^+$ ^2E C_{3v} Structure: PE [1]

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1	C≡C stretch	2280[a]	gas	EF	[2]
	3	C-C a-stretch	1440[a]	gas	EF	[2]
	4	CF stretch	1140[a]	gas	EF	[2]
	5	CF stretch	880[a]	gas	EF	[2]
	6	C-C stretch	710[a]	gas	EF	[2]
	7	CF_3 deform.	340[a]	gas	EF	[2]

[a] ± 10 cm^{-1}.

References

[1] G. Bieri, E. Heilbronner, J.-P. Stadelmann, J. Vogt, and W. von Niessen, J. Am. Chem. Soc. 99, 6832 (1977).

[2] M. Allan, J. P. Maier, O. Marthaler, and J.-P. Stadelmann, J. Chem. Phys. 70, 5271 (1979).

$CF_3(C{\equiv}C)_2CF_3^+$ ^2E_g D_{3d}

(Perfluoro-2,4-Hexadiyne Cation)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	1	C≡C stretch	2239[a]	gas	EF	[1][2]
	2	C-F stretch	1262[a]	gas	EF	[1][2]
	3	C-C stretch	1095[a]	gas	EF	[1][2]
	4	C-C stretch	752[a]	gas	EF	[2]
	5	CF_3 deform.	235[a]	gas	EF	[2]

[a] ± 2 cm^{-1}.

References

[1] M. Allan, J. P. Maier, O. Marthaler, and J.-P. Stadelmann, J. Chem. Phys. 70, 5271 (1979).

[2] D. Klapstein, J. P. Maier, L. Misev, F. Thommen, and W. Zambach, J. Chem. Soc., Faraday Trans. 2 78, 1765 (1982).

6.17. Substituted Benzene Cations

$C_6H_5NH_2^+$ [a] $^2B_1$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	1		837[b]	gas	PI	[1]
	6a	N-ring s-str.	545[c]	gas	PI	[1]
	12	Ring s-stretch	1005[b]	gas	PI	[1]
b_2	15		373[c]	gas	PI	[1]

[a] First overtone of N-atom inversion observed at 904 cm^{-1}, and vibrational spacings of 65, 210, 310, 650, and 947 ± 15 cm^{-1} are tentatively attributed to other fundamentals. Vibrational numbering and assignments parallel those given by Chernoff and Rice (J. Chem. Phys. 70, 2511 (1979)) for aniline.

[b] ± 15 cm^{-1}.

[c] ± 10 cm^{-1}.

References

[1] M. A. Smith, J. W. Hager, and S. C. Wallace, J. Chem. Phys. 80, 3097 (1984).

$1,3\text{-}C_6H_4F_2^+$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4		1560	Ne	LF	[1]
	5		1476	Ne	LF	[1]
	6		1274	Ne	LF	[1]
	7		1092	Ne	LF	[1]
	10		504	Ne	LF	[1]
	11		344	Ne	LF	[1]

References

[1] V. E. Bondybey, J. H. English, and T. A. Miller, Chem. Phys. Lett. 66, 165 (1979).

$1,2,3\text{-}C_6H_3F_3^+$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			877	Ne	LF	[1]
			805	Ne	LF	[1]
			698	Ne	LF	[1]
			601	Ne	LF	[1]
			526	Ne	LF	[1]

$1,2,3\text{-}C_6H_3F_3^+$---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			466	Ne	LF	[1]
			415	Ne	LF	[1]
			389	Ne	LF	[1]
			317	Ne	LF	[1]
			294	Ne	LF	[1]
			197[a]	Ne	LF	[1][2]

$1,2,3\text{-}C_6D_3F_3^+$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			867	Ne	LF	[1]
			781	Ne	LF	[1]
			680	Ne	LF	[1]
			595	Ne	LF	[1]
			464	Ne	LF	[1]
			415	Ne	LF	[1]
			317	Ne	LF	[1]
			292	Ne	LF	[1]
			197[a]	Ne	LF	[1][2]

[a] Identified in [2] as origin of A - X electronic transition.

References

[1] V. E. Bondybey, J. H. English, T. A. Miller, and R. H. Shiley, J. Mol. Spectrosc. 84, 124 (1980).

[2] V. E. Bondybey, J. H. English, and T. A. Miller, J. Mol. Spectrosc. 90, 592 (1981).

$1,2,4\text{-}C_6H_3F_3^+$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a′			1623	gas	UV	[1]
			1623	Ne	LF	[2]
	5		1615	gas	UV,EF	[1][3]
			1616	Ne	LF	[2]
			1608	Ne	LF	[2]
			1595	Ne	LF	[2]
			1407	Ne	LF	[2]
			1119	Ne	LF	[2]
	17		675	gas	EF	[3]

$1,2,4\text{-}C_6H_3F_3^+$---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	18		485	gas	UV,EF	[1][3]
			484	Ne	LF	[2]
	19		405	gas	UV,EF	[1][3]
			403	Ne	LF	[2]
	20		360	gas	UV	[1]
			357	Ne	LF	[2]
	21		293	gas	UV	[1]
			293	Ne	LF	[2]

References

[1] C. Cossart-Magos, D. Cossart, and S. Leach, Mol. Phys. 37, 793 (1979).

[2] V. E. Bondybey, C. R. Vaughn, T. A. Miller, and J. H. English, J. Chem. Phys. 74, 6584 (1981).

[3] R. P. Tuckett, Chem. Phys. 58, 151 (1981).

$1,3,5\text{-}C_6H_3F_3^+$ $^2E''$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1		2911	gas	UV	[1]
	2		1465	gas	UV	[1]
	3		1039.1	gas	UV,EF	[1][4][5]
			1043	Ne	LF	[3]
	4		592.1	gas	UV,LF,EF	[1][3][4][5]
			596	Ne	LF	[3]
e'	9		1665	gas	UV	[1]
			1664	Ne	LF	[3]
	10		1533	gas	UV	[1]
	12		945	Ne	LF	[3]
	13		550.0	gas	UV,LF,EF	[1][3][4][5]
			557	Ne	LF	[3]
	14		334	Ne	LF	[3]

$1,3,5\text{-}C_6D_3F_3^+$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1		2247	gas	UV	[2]
	3		976.1	gas	UV,EF	[2][5]
	4		586.5	gas	UV,EF	[2][5]
			592	Ne	LF	[3]

$1,3,5\text{-}C_6D_3F_3^+$---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	9		1625	gas	UV	[2]
			1612	Ne	LF	[3]
	10		1484	gas	UV	[2]
	11		1053.0	gas	EF	[5]
	12		780	Ne	UV	[3]
	13		532.3	gas	UV,EF	[2][5]
			541	Ne	LF	[3]
	14		334	Ne	LF	[3]

References

[1] C. Cossart-Magos, D. Cossart, and S. Leach, Mol. Phys. 37, 793 (1979).

[2] C. Cossart-Magos, D. Cossart, and S. Leach, Chem. Phys. 41, 345 (1979).

[3] V. E. Bondybey, T. A. Miller, and J. H. English, J. Chem. Phys. 71, 1088 (1979).

[4] R. P. Tuckett, Chem. Phys. 58, 151 (1981).

[5] D. Klapstein, S. Leutwyler, J. P. Maier, C. Cossart-Magos, D. Cossart, and S. Leach, Mol. Phys. 51, 413 (1984).

$C_6H_3F_2OH^+$ C_{2v}

(3,5-Difluorophenol Cation)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	3[a]		992	Ne	LF	[1]
	4		590	Ne	LF	[1]
	9		1608	Ne	LF	[1]
	13		486	Ne	LF	[1]
	14		325	Ne	LF	[1]

[a] As in [1], numbered to show relationship to D_{3h} molecules such as $1,3,5\text{-}C_6H_3F_3^+$.

References

[1] V. E. Bondybey, J. H. English, T. A. Miller, and R. H. Shiley, J. Chem. Phys. 78, 2227 (1983).

$C_6H_3Cl_2F^+$ C_{2v}

(1,3-Dichloro-5-Fluorobenzene Cation)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1747[a]	Ne	LF	[1]
			1680[a]	Ne	LF	[1]
			1306	Ne	LF	[1]
			1289	Ne	LF	[1]
			1107	Ne	LF	[1]
			1101	Ne	LF	[1]
			1062	Ne	LF	[1]
			999	Ne	LF	[1]
			973	Ne	LF	[1]
			961	Ne	LF	[1]
			783	Ne	LF	[1]
			543	Ne	LF	[1]
			529	Ne	LF	[1]
			450	Ne	LF	[1]
			437	Ne	LF	[1]
			422	Ne	LF	[1]
			333	Ne	LF	[1]
			201	Ne	LF	[1]

[a] Polarization not reported. Band with perpendicular polarization displaced 159 cm^{-1} from origin (parallel polarization) was assigned to B - A transition. Only bands with parallel polarization are tabulated.

References

[1] V. E. Bondybey, C. R. Vaughn, T. A. Miller, J. H. English, and R. H. Shiley, J. Chem. Phys. 74, 6584 (1981).

$1,3,5\text{-}C_6H_3Cl_3^+$ $^2E''$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	1		2925	gas	UV	[2]
	2		1189	gas	UV	[2]
			1190	Ne	LF	[1][3]
			1183	Ar	LF	[1]
	3		1068	gas	UV	[2]
			982	Ne	LF	[3]
	4		401	gas	UV	[2]
			442	Ne	LF	[1][3]

$1,3,5\text{-}C_6H_3Cl_3^+$---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
e'	9		1584	gas	UV	[2]
			1588	Ne	LF	[3]
	10		1519	gas	UV	[2]
	11		1074	Ne	LF	[3]
	13		498	gas	UV	[2]
			501	Ne	LF	[1][3]
	14		195	Ne	LF	[1][3]

$1,3,5\text{-}C_6D_3Cl_3^+$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	2		1200	Ne	LF	[3]
	3		940	Ne	LF	[3]
	4		442	Ne	LF	[3]
e'	9		1527	Ne	LF	[3]
	11		853	Ne	LF	[3]
	13		491	Ne	LF	[3]
	14		197	Ne	LF	[3]

References

[1] T. A. Miller, V. E. Bondybey, and J. H. English, J. Chem. Phys. 70, 2919 (1979).

[2] C. Cossart-Magos, D. Cossart, and S. Leach, Chem. Phys. 41, 363 (1979).

[3] V. E. Bondybey, T. A. Miller, and J. H. English, J. Chem. Phys. 71, 1088 (1979).

$sym\text{-}C_6F_3Cl_3^+$ $^2E''$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	3		584	gas	LF	[2]
			585	Ne	LF	[1]
e'	8		1629[a]	Ne	LF	[1]
	9		1428[a]	Ne	LF	[1]
	10		1128[a]	Ne	LF	[1]
	12		409[a]	gas	LF	[2]
			429[a]	Ne	LF	[1]
	13		318[a]	gas	LF	[2]
			324[a]	Ne	LF	[1]
	14		192[a]	Ne	LF	[1]

sym-$C_6F_3Cl_3^+$---Footnote

[a] Transition to v = 1, j = ½ level.

References

[1] V. E. Bondybey, J. Chem. Phys. 71, 3586 (1979).

[2] T. J. Sears, T. A. Miller, and V. E. Bondybey, J. Am. Chem. Soc. 102, 4864 (1980).

sym-$C_6F_3Br_3^+$ $^2E''$ D_{3h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	3		583	Ne	LF	[1]
e'	8		1727	Ne	LF	[1]
	10		1147	Ne	LF	[1]
	12		387	Ne	LF	[1]
	13		292	Ne	LF	[1]

References

[1] V. E. Bondybey, T. J. Sears, T. A. Miller, C. Vaughn, J. H. English, and R. S. Shiley, Chem. Phys. 61, 9 (1981).

sym-$C_6H_2F_3CH_3^+$ C_{2v}

(2,4,6-Trifluorotoluene Cation)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		1648	Ne	LF	[1]
	3		1401	Ne	LF	[1]
	5		1300	Ne	LF	[1]
	9		580	Ne	LF	[1]
	10		427	Ne	LF	[1]
	11		333	Ne	LF	[1]

References

[1] V. E. Bondybey, C. Vaughn, T. A. Miller, J. H. English, and R. H. Shiley, J. Am. Chem. Soc. 103, 6303 (1981).

1,2,3,4-$C_6H_2F_4^+$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		1665	gas	UV,EF	[1][4]
			1665	Ne	LF	[3]
			1228	gas	UV	[1]
	6		1198	Ne	LF	[3]
	7		1083	gas	EF	[4]
			1082	Ne	LF	[3]
	8		678	gas	EF	[4]
			680	Ne	LF	[3]
			593	gas	UV	[1]
	9		441	gas	UV,LF, EF	[1][2] [4]
			443	Ne	LF	[3]
	10		339	gas	EF	[4]
			340	Ne	LF	[3]
	11		271	gas	UV,LF, EF	[1][2] [4]
			273	Ne	LF	[3]

References

[1] C. Cossart-Magos, D. Cossart, and S. Leach, Mol. Phys. 37, 793 (1979).

[2] V. E. Bondybey and T. A. Miller, J. Chem. Phys. 70, 138 (1979).

[3] V. E. Bondybey, J. H. English, and T. A. Miller, J. Mol. Spectrosc. 81, 455 (1980).

[4] R. P. Tuckett, Chem. Phys. 58, 151 (1981).

1,2,3,5-$C_6H_2F_4^+$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		1650	gas	UV,EF	[1][4]
			1647	Ne	LF	[3]
	3		1458	gas	EF	[4]
			1449	Ne	LF	[3]
	5		1318	gas	UV,EF	[1][4]
			1305	Ne	LF	[3]
	8		785	Ne	LF	[3]
	9		584	gas	EF	[4]
			581	Ne	LF	[3]
			586	Ar	LF	[2]
	10		427	gas	UV,EF	[1][4]
			426	Ne	LF	[3]
			429	Ar	LF	[2]

$1,2,3,5\text{-}C_6H_2F_4^+$---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	11		305	gas	UV,EF	[1][4]
			303	Ne	LF	[3]
			307	Ar	LF	[2]

References

[1] C. Cossart-Magos, D. Cossart, and S. Leach, Mol. Phys. 37, 793 (1979).

[2] V. E. Bondybey, T. A. Miller, and J. H. English, J. Am. Chem. Soc. 101, 1248 (1979).

[3] V. E. Bondybey, J. H. English, and T. A. Miller, J. Mol. Spectrosc. 81, 455 (1980).

[4] R. P. Tuckett, Chem. Phys. 58, 151 (1981).

$1,2,4,5\text{-}C_6H_2F_4^+$ D_{2h}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2		1558	gas	EF	[4]
			1558	Ne	LF	[3]
	3		1477	gas	EF	[4]
			1476	Ne	LF	[3]
	4		726	Ne	LF	[3]
	5		482	gas	UV,EF	[1][4]
			485	Ne	LF	[3]
			480	Ar	LF	[2]
	6		287	gas	EF	[4]
			287	Ne	LF	[3]
			289	Ar	LF	[2]

$1,2,4,5\text{-}C_6D_2F_4^+$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_g	2		1542	Ne	LF	[3]
	3		1472	Ne	LF	[3]
	4		706	Ne	LF	[3]
	5		480	Ne	LF	[3]
	6		286	Ne	LF	[3]

References

[1] C. Cossart-Magos, D. Cossart, and S. Leach, Mol. Phys. 37, 793 (1979).

[2] V. E. Bondybey, T. A. Miller, and J. H. English, J. Am. Chem. Soc. 101, 1248 (1979).

[3] V. E. Bondybey, J. H. English, and T. A. Miller, J. Mol. Spectrosc. 81, 455 (1980).

[4] R. P. Tuckett, Chem. Phys. 58, 151 (1981).

$C_6HF_5^+$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		1598	gas	EF	[5]
			1595	Ne	LF	[4]
	3		1546	gas	UV,EF	[1][5]
			1533	Ne	LF	[4]
	5		1356	Ne	LF	[4]
	6		902	Ne	LF	[4]
	8		582	gas	UV,EF	[1][5]
			575	Ne	LF	[4]
	9		457	gas	UV,LF, EF	[1][2] [5]
			460	Ne	LF	[4]
			462	Ar	LF	[3]
	10		423	gas	EF	[5]
			438	Ne	LF	[4]
	11		277	gas	UV,LF, EF	[1][2] [5]
			278	Ne	LF	[4]
			284	Ar	LF	[3]

References

[1] C. Cossart-Magos, D. Cossart, and S. Leach, Mol. Phys. 37, 793 (1979).

[2] V. E. Bondybey and T. A. Miller, J. Chem. Phys. 70, 138 (1979).

[3] V. E. Bondybey, T. A. Miller, and J. H. English, J. Am. Chem. Soc. 101, 1248 (1979).

[4] V. E. Bondybey, J. H. English, and T. A. Miller, J. Mol. Spectrosc. 81, 455 (1980).

[5] R. P. Tuckett, Chem. Phys. 58, 151 (1981).

$C_6F_6^+$ $^2E_{1g}$ D_{6h}

(Hexafluorobenzene Cation)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_{1g}	2		556	gas	UV,LF, EF	[2][4] [5]
			554	Ne	LF	[3]
			557	Ar	LF	[1]
e_{2g}	15		1698	Ne	LF	[3]
	16		1226	Ne	LF	[3]
	17		406	gas	UV,EF	[4][5]
			417	Ne	LF	[3]
			444	Ar	LF	[1]
	18		284	gas	UV,LF, EF	[2][4] [5]
			289	Ne	LF	[3]
			300	Ar	LF	[1]

References

[1] V. E. Bondybey, J. H. English, and T. A. Miller, J. Am. Chem. Soc. 100, 5251 (1978).

[2] C. Cossart-Magos, D. Cossart, and S. Leach, Mol. Phys. 37, 793 (1979).

[3] V. E. Bondybey and T. A. Miller, J. Chem. Phys. 73, 3053 (1980).

[4] T. Sears, T. A. Miller, and V. E. Bondybey, J. Am. Chem. Soc. 103, 326 (1981).

[5] R. P. Tuckett, Chem. Phys. 58, 151 (1981).

$C_6F_5Cl^+$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			590	Ne	LF	[1]
			512	Ne	LF	[1]
			385	Ne	LF	[1]
			252	Ne	LF	[1]
			185[a]	Ne	LF	[1][2]

[a] Identified in [2] as origin of A - X electronic transition.

References

[1] V. E. Bondybey, T. A. Miller, and J. H. English, J. Chim. Phys. 77, 667 (1980).

[2] V. E. Bondybey, C. R. Vaughn, T. A. Miller, J. H. English, and R. H. Shiley, J. Chem. Phys. 74, 6584 (1981).

$C_6F_5OH^+$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	2		1688	Ne	LF	[1]
	3		1656	Ne	LF	[1]
	5		1489	Ne	LF	[1]
	6		1472	Ne	LF	[1]
	7		1350	Ne	LF	[1]
	10		1182	Ne	LF	[1]
	11		1147	Ne	LF	[1]
	16		558	Ne	LF	[1]
	17		431	Ne	LF	[1]
	19		383	Ne	LF	[1]
	21		266	Ne	LF	[1]

References

[1] V. E. Bondybey, J. H. English, T. A. Miller, and C. B. Vaughn, J. Phys. Chem. 85, 1667 (1981).

$C_6F_5CH_3^+$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			277[a]	Ne	LF	[1]

[a] Complicated pattern of unassigned emission peaks results from overlap of B - X and B - A band systems; origin of A - X transition assigned in [2] at 220 cm^{-1}.

References

[1] V. E. Bondybey, T. A. Miller, and J. H. English, J. Chim. Phys. 77, 667 (1980).

[2] V. E. Bondybey, C. R. Vaughn, T. A. Miller, J. H. English, and R. H. Shiley, J. Chem. Phys. 74, 6584 (1981).

$C_6F_5CF_3^+$ C_{2v}

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1617	Ne	LF	[1]
			586	Ne	LF	[1]
			492	Ne	LF	[1]
			292	Ne	LF	[1]
			258	Ne	LF	[1]

References

[1] V. E. Bondybey, T. A. Miller, and J. H. English, J. Chim. Phys. 77, 667 (1980).

6.18. Non-Hydrocarbons with More Than Eight Atoms

$B_3N_3H_3F_3^+$ $^2E''$ D_{3h}

(Tri-B-Fluoroborazine Cation)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1'	2	B-F stretch	1260[a]	gas	EF	[1]
	3	Ring breathing	840[a]	gas	EF	[1]
	4	Ring breathing	430[a]	gas	EF	[1]

[a] $\pm$ 10 cm^{-1}.

References

[1] T. B. Jones, J. P. Maier, and O. Marthaler, Inorg. Chem. 18, 2140 (1979).

$C_3F_6^+$

(Perfluoropropene Cation)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		C=C stretch	1543	Ar	IR	[1]
		$=CF_2$ a-stretch	1414	Ar	IR	[1]
		$=CF_2$ s-stretch	1062	Ar	IR	[1]

References

[1] B. J. Kelsall and L. Andrews, J. Phys. Chem. 85, 1288 (1981).

$n\text{-}C_3F_7$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.[a]
a'	1	CF_3 a-stretch	1354m	Ar	IR	[1]
	2	CF_3 s-stretch	1231s	Ar	IR	[1]
	3	CF_2 s-stretch	1222vs	Ar	IR	[1]
	4	CF_2 s-stretch	1116s	Ar	IR	[1]
	5	C_3 s-stretch	1016m	Ar	IR	[1]
	6	C_3 a-stretch	888m	Ar	IR	[1]
	7	CF_3 s-deform.	750m	Ar	IR	[1]
	8	CF_2 s-deform.	703w	Ar	IR	[1]
	9	CF_2 s-deform.	638m	Ar	IR	[1]
	10	CF_3 a-deform.	520w	Ar	IR	[1]
	11	CF_2 wag	395vw	Ar	IR	[1]
	12	CF_2 wag	306w	Ar	IR	[1]
	13	CF_3 rock	220vw	Ar	IR	[1]
	14	C_3 bend	273w	Ar	IR	[1]

$n\text{-}C_3F_7$---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a"	16	CF_2 a-stretch	1285vs	Ar	IR	[1]
	17	CF_3 a-stretch	1260m	Ar	IR	[1]
	18	CF_2· a-stretch	1191s	Ar	IR	[1]
	19	CF_3 a-deform.	608vw	Ar	IR	[1]
	20	CF_2 twist	472vw	Ar	IR	[1]
	21	CF_2 twist	401vw	Ar	IR	[1]
	22	CF_2 rock	265vw	Ar	IR	[1]
	23	CF_3 rock	248vw	Ar	IR	[1]

[a] Revised assignment offered by [2], based on more detailed study of infrared and Raman spectrum of $n\text{-}C_3F_7I$.

References

[1] R. Butler and A. Snelson, J. Fluorine Chem. 16, 33 (1980).

[2] D. A. C. Compton and D. M. Rayner, J. Phys. Chem. 86, 1628 (1982).

$i\text{-}C_3F_7$ C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a'	1	CF_3 s-stretch	1365s 1362s	Ar	IR	[1]
	2	CF_3 s-stretch	1242vs	Ar	IR	[1]
	3	CF_3 a-stretch	1192m	Ar	IR	[1]
	4	CF_3 a-stretch	1157vs 1152s	Ar	IR	[1]
	5	·CF stretch	1137m 1141w	Ar	IR	[1]
	6	C_3 a-stretch	986vs	Ar	IR	[1]
	7	CF_3 s-deform.	775w	Ar	IR	[1]
	8	CF_3 s-deform.	731w	Ar	IR	[1]
	9	CCF deform.	703m	Ar	IR	[1]
	10	CF_3 a-deform.	499vw	Ar	IR	[1]
	11	CF_3 a-deform.	489vw	Ar	IR	[1]
	12	CF_3 rock	347vw	Ar	IR	[1]
	13	C_3 s-stretch	321vw	Ar	IR	[1]
	14	CF_3 rock	293vw	Ar	IR	[1]
a"	16	CF_3 a-stretch	1249vs	Ar	IR	[1]
	17	CF_3 a-stretch	1206vs	Ar	IR	[1]
	18	CF_3 a-deform.	684w	Ar	IR	[1]
	19	CF_3 a-deform.	543w	Ar	IR	[1]
	20	CF_3 rock	456w	Ar	IR	[1]

$i\text{-}C_3F_7$---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	21	CF_3 rock	255vw	Ar	IR	[1]
	22	CCF deform.	207vw	Ar	IR	[1]

References

[1] R. Butler and A. Snelson, J. Fluorine Chem. 16, 33 (1980).

C_6H_6F C_s

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1428s	Ar	IR	[1]
			1287ms	Ar	IR	[1]
			1094wm	Ar	IR	[1]
			1000ms	Ar	IR	[1]
			924vs	Ar	IR	[1]
			912wm	Ar	IR	[1]
			883s	Ar	IR	[1]
			823wm	Ar	IR	[1]
			693vs	Ar	IR	[1]
			599vs	Ar	IR	[1]

C_6D_6F

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1247s	Ar	IR	[1]
			1013vs	Ar	IR	[1]
			919s	Ar	IR	[1]
			904wm	Ar	IR	[1]
			863s	Ar	IR	[1]
			841m	Ar	IR	[1]
			783m	Ar	IR	[1]
			672m	Ar	IR	[1]
			613s	Ar	IR	[1]
			455vs	Ar	IR	[1]

References

[1] M. E. Jacox, J. Phys. Chem. 86, 670 (1982).

$(CH_3)_2Si$

(Dimethylsilylene)

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CH_3 a-deform.	1438m	Ar	IR	[2][4]
	CH_3 s-deform.	1220s	Ar	IR	[1][4]
	CH_3 s-deform.	1210m	Ar,N_2	IR	[4]
	In-plane CH_3 rock	850s	Ar,N_2	IR	[3][4]
	In-plane CH_3 rock	806vs	Ar,N_2	IR	[4]
	Si-C stretch	735m	Ar,N_2	IR	[4]
	Si-C stretch	690m	Ar,N_2	IR	[4]

[a] Observed by [4] in both Ar and N_2; frequencies in these two matrices were not distinguished.

References

[1] T. J. Drahnak, J. Michl, and R. West, J. Am. Chem. Soc. 101, 5427 (1979).

[2] T. J. Drahnak, J. Michl, and R. West, J. Am. Chem. Soc. 103, 1845 (1981).

[3] H. P. Reisenauer, G. Mihm, and G. Maier, Angew. Chem. 94, 864 (1982); Angew. Chem. Int. Ed. Engl. 21, 854 (1982).

[4] C. A. Arrington, K. A. Klingensmith, R. West, and J. Michl, J. Am. Chem. Soc. 106, 525 (1984).

$CH_3SiH{=}CH_2$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	SiH stretch	2188s	Ar[a]	IR	[1]-[3]
	CH_3 a-deform.	1412m	Ar[a]	IR	[3]
	CH_3 a-deform.	1397m	Ar[a]	IR	[3]
	CH_2 "scissors"	1300m	Ar[a]	IR	[1][3]
	CH_3 s-deform.	1254s	Ar[a]	IR	[1]-[3]
	Si=C stretch	988s	Ar[a]	IR	[1]-[3]
	In-plane def.	880s	Ar[a]	IR	[1]-[3]
	CH_2 OPLA wag	830s	Ar[a]	IR	[3]
	In-plane CH_3 rock	812vs	Ar[a]	IR	[1]-[3]
	Si-C stretch	732m	Ar[a]	IR	[3]
	CH_3 OPLA rock	714m	Ar[a]	IR	[1]-[3]
	In-plane def.	688w	Ar[a]	IR	[3]
	CH_2 torsion	615m	Ar[a]	IR	[1][3]

$CH_3SiH{=}CH_2$---Footnote

[a] Observed by [3] in both Ar and N_2; frequencies in these two matrices were not distinguished.

References

[1] T. J. Drahnak, J. Michl, and R. West, J. Am. Chem. Soc. 103, 1845 (1981).

[2] H. P. Reisenauer, G. Mihm, and G. Maier, Angew. Chem. 94, 864 (1982); Angew. Chem. Int. Ed. Engl. 21, 854 (1982).

[3] C. A. Arrington, K. A. Klingensmith, R. West, and J. Michl, J. Am. Chem. Soc. 106, 525 (1984).

$(CH_3)_2Si{-}CH_2^+$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	H_2C-Si stretch	760[a]	gas	PE	[1]

[a] $\pm$ 30 cm^{-1}.

References

[1] J. M. Dyke, G. D. Josland, R. A. Lewis, and A. Morris, J. Phys. Chem. 86, 2913 (1982).

$(CH_3)_2Si{=}CH_2$ [a] Structure: ED [3]

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1		1251 1260w	Ar	IR	[1][4] [5]
		1004m	Ar	IR	[1][2] [4][5]
	HCSi deform.	818w	Ar	IR	[1][4] [5]
	Si-C stretch	643m	Ar	IR	[1][2] [4][5]
b_1	HCSi deform.	825m	Ar	IR	[1][2] [4][5]

[a] Peaks at 696, 932, and 992 cm^{-1} have also been attributed to $(CH_3)_2Si{=}CH_2$ in an argon matrix in [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.

References

[1] A. K. Mal'tsev, V. N. Khabashesku, and O. M. Nefedov, Dokl. Akad. Nauk SSSR 233, 421 (1977); Dokl. Phys. Chem. 233, 332 (1977).

[2] A. K. Mal'tsev, V. N. Khabashesku, and O. M. Nefedov, Izv. Akad. Nauk SSSR, Ser. Khim., 2152 (1979); Bull. Acad. Sci. USSR, Div. Chem. Sci. 28, 1980 (1979).

[3] P. G. Mahaffy, R. Gutowsky, and L. K. Montgomery, J. Am. Chem. Soc. 102, 2854 (1980).

[4] O. M. Nefedov, A. K. Mal'tsev, V. N. Khabashesku, and V. A. Korolev, J. Organomet. Chem. 201, 123 (1980).

[5] L. E. Gusel'nikov, V. V. Volkova, V. G. Avakyan, and N. S. Nametkin, J. Organomet. Chem. 201, 137 (1980).

$(CH_3)_2Si=C(CH_3)H$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			3020m	Ar	IR	[1][2]
			2980m	Ar	IR	[1][2]
			2965m	Ar	IR	[1][2]
			2940s	Ar	IR	[1][2]
			2900s	Ar	IR	[1][2]
			2870s	Ar	IR	[1][2]
			1450m	Ar	IR	[1][2]
			1410s	Ar	IR	[1][2]
			1370ms	Ar	IR	[1][2]
			1315m	Ar	IR	[1][2]
			1255vs	Ar	IR	[1][2]
			1120m	Ar	IR	[1][2]
			978s	Ar	IR	[1][2]
			883vs	Ar	IR	[1][2]
			808s	Ar	IR	[1][2]
		=CH deform.	795vs	Ar	IR	[1]-[3]
			712m	Ar	IR	[1][2]
			708sh	Ar	IR	[1][2]
		=CH deform.	645s	Ar	IR	[1]-[3]
			608ms	Ar	IR	[1]-[3]
			358m	Ar	IR	[1][2]

References

[1] O. L. Chapman, C.-C. Chang, J. Kolc, M. E. Jung, J. A. Lowe, T. J. Barton, and M. L. Tumey, J. Am. Chem. Soc. 98, 7844 (1976).

[2] M. R. Chedekel, M. Skoglund, R. L. Kreeger, and H. Shechter, J. Am. Chem. Soc. 98, 7846 (1976).

[3] A. K. Mal'tsev, V. A. Korolev, V. N. Khabashesku, and O. M. Nefedov, Dokl. Akad. Nauk SSSR 251, 1166 (1980); Dokl. Phys. Chem. 251, 295 (1980).

C_5SiH_6

(Silabenzene)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SiH stretch	2217	Ar	IR	[1]
			1526	Ar	IR	[1]
			1500	Ar	IR	[1]
			1353	Ar	IR	[1]
			1259	Ar	IR	[1]
			886	Ar	IR	[1]
			598	Ar	IR	[1]
			566	Ar	IR	[1]
			418	Ar	IR	[1]

References

[1] G. Maier, G. Mihm, and H. P. Reisenauer, Angew. Chem. 92, 58 (1980); Angew. Chem. Int. Ed. Engl. 19, 52 (1980).

C_5SiH_6

(Dewar Silabenzene[a])

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		SiH stretch	2142	Ar	IR	[1]
			1890	Ar	IR	[1]
			1263	Ar	IR	[1]
			1084	Ar	IR	[1]
			818	Ar	IR	[1]
			761	Ar	IR	[1]
			728	Ar	IR	[1]
			689	Ar	IR	[1]
			591	Ar	IR	[1]
			559	Ar	IR	[1]

Dewar Silabenzene---Footnote

[a] Formed by 320- or 254-nm irradiation of silabenzene isolated in solid argon; tentative identification.

References

[1] G. Maier, G. Mihm, and H. P. Reisenauer, Angew. Chem. 92, 58 (1980); Angew. Chem. Int. Ed. Engl. 19, 52 (1980).

C_6SiH_8

(1-Methylsilabenzene)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1530	Ar	IR	[1]
			1500	Ar	IR	[1]
			1410	Ar	IR	[1]
			1360	Ar	IR	[1]
			1268	Ar	IR	[1]
			980	Ar	IR	[1]
			965	Ar	IR	[1]
			900	Ar	IR	[1]
			890	Ar	IR	[1]
			883	Ar	IR	[1]
			842	Ar	IR	[1]
			770	Ar	IR	[1]
			697	Ar	IR	[1]
			655	Ar	IR	[1]
			563	Ar	IR	[1]

References

[1] C. L. Kreil, O. L. Chapman, G. T. Burns, and T. J. Barton, J. Am. Chem. Soc. 102, 841 (1980).

$(CH_3)_2Sn$ C_{2v}

(Dimethylstannylene)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH a-stretch	2990wm	Ar	IR	[1]
		CH s-stretch	2924wm	Ar	IR	[1]
		CH_3 deform.	1198w	Ar	IR	[1]
		CH_3 rock	774s	Ar	IR	[1]
		CH_3 rock	739vs	Ar	IR	[1]
		SnC stretch	518sh	Ar	IR	[1]
		SnC stretch	504vs	Ar	IR	[1]

$(CD_3)_2Sn$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD_3 a-stretch	2240	Ar	IR	[1]
		CD_3 s-stretch	2123	Ar	IR	[1]
		CD_3 deform.	1032	Ar	IR	[1]
		CD_3 deform.	932	Ar	IR	[1]
		CD_3 rock	596	Ar	IR	[1]
		CD_3 rock	565	Ar	IR	[1]
		SnC stretch	476	Ar	IR	[1]
		SnC stretch	462	Ar	IR	[1]

References

[1] P. Bleckmann, H. Maly, R. Minkwitz, W. P. Neumann, B. Watta, and G. Olbrich, Tetrahed. Lett. 23, 4655 (1982).

$C_5H_3F_2N^+$

(2,6-Difluoropyridine Cation)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a_1	4		1524	Ne	LF	[1]
	5		1499	Ne	LF	[1]
	6		1372	Ne	LF	[1]
	7		1039	Ne	LF	[1]
	8		967	Ne	LF	[1]
	9		728	Ne	LF	[1]
	10		535	Ne	LF	[1]
	11		365	Ne	LF	[1]

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[1] V. E. Bondybey, J. H. English, and R. H. Shiley, J. Chem. Phys. 77, 4826 (1982).

C_6H_5N

(1-Aza-1,2,4,6-Cycloheptatetraene)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			3025m	Ar	IR	[1]
			1895vs	Ar	IR	[1]
			1348s	Ar	IR	[1]
			1111ms	Ar	IR	[1]
			1105ms	Ar	IR	[1]
			980s	Ar	IR	[1]

1-Aza-1,2,4,6-Cycloheptatetraene---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			940m	Ar	IR	[1]
			748vs	Ar	IR	[1]
			683s	Ar	IR	[1]
			658s	Ar	IR	[1]
			650m	Ar	IR	[1]
			580ms	Ar	IR	[1]
			510ms	Ar	IR	[1]
			370m	Ar	IR	[1]

References

[1] O. L. Chapman and J.-P. Le Roux, J. Am. Chem. Soc. 100, 282 (1978).

C_6H_5N

(3-Pyridylmethylene)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
			1595s	Ar	IR	[1]
			1520s	Ar	IR	[1]
			1379ms	Ar	IR	[1]
			1325m	Ar	IR	[1]
			1233m	Ar	IR	[1]
			1221s	Ar	IR	[1]
			1110m	Ar	IR	[1]
			1015m	Ar	IR	[1]
			990ms	Ar	IR	[1]
			983ms	Ar	IR	[1]
			943m	Ar	IR	[1]
			788vs	Ar	IR	[1]
			688vs	Ar	IR	[1]
			628ms	Ar	IR	[1]
			600wm	Ar	IR	[1]
			550m	Ar	IR	[1]
			505ms	Ar	IR	[1]
			441ms	Ar	IR	[1]
			430wm	Ar	IR	[1]

References

[1] O. L. Chapman and R. S. Sheridan, J. Am. Chem. Soc. 101, 3690 (1979).

Primary $C_2H_4O_3$

(1,2,3-Trioxolane)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CH_2 deform.	1214m	Xe	IR	[2]
		CO stretch + CH_2 deform.	983s	Xe	IR	[2]
			982	CO_2	IR	[1][2]
		CO stretch	927s	Xe	IR	[2]
			926	CO_2	IR	[1][2]
		O_3 s-stretch	846wm	Xe	IR	[2]
		COO bend + CO stretch	727vs	Xe	IR	[2]
			726	CO_2	IR	[1][2]
		O_3 a-stretch	647vs	Xe	IR	[2]
			648	CO_2	IR	[1][2]
		O_3 bend	409m	Xe	IR	[2]
			406	CO_2	IR	[1][2]

Primary $C_2D_4O_3$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		CD_2 deform.	1089wm	Xe	IR	[2]
		CO stretch	892s	Xe	IR	[2]
		O_3 a-stretch	636vs	Xe	IR	[2]
		O_3 bend	387m	Xe	IR	[2]

References

[1] B. Nelander and L. Nord, Tetrahedron Lett. 2821 (1977).

[2] C. K. Kohlmiller and L. Andrews, J. Am. Chem. Soc. 103, 2578 (1981).

Secondary $C_2H_4O_3$ C_2 Structure: MW [1][2][4]

(1,2,4-Trioxolane)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	CH stretch	2973m	Ar	IR	[3][7]
	2	CH stretch	2894vs	Ar	IR	[3][7]
	4	CH_2 wag	1387m	Ar	IR	[3][7]
	5	CH_2 twist	1196m	Ar	IR	[3][7]
	6	CH_2 rock	1129s	Ar	IR	[3][6] [7]
			1130	Xe	IR	[6]

Secondary $C_2H_4O_3$---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	7	C-O_e stretch	955wm	gas	IR	[5]
			952vs	Ar	IR	[3][6][7]
			945	Xe	IR	[6]
	8	C-O_p stretch	926w	Ar	IR	[3][7]
	9	O-O stretch	810w	gas	IR	[5]
			808s	Ar	IR	[3][6][7]
			802	Xe	IR	[6]
	10	Skeletal	737vw	Ar	IR	[3][7]
	11	Ring pucker	352vw	Ar	IR	[3]
b	12	CH stretch	2967s	Ar	IR	[3][7]
	13	CH stretch	2900m	Ar	IR	[3][7]
	14	CH_2 bend	1483vw	Ar	IR	[3]
	15	CH_2 wag	1346m	Ar	IR	[3][7]
	16	CH_2 twist	1202m	Ar	IR	[3][7]
	17	CH_2 rock	1143vw	Ar	IR	[3]
	18	C-O_e stretch	1081.8s	gas	IR	[5]
			1078vs	Ar	IR	[3][6][7]
			1072	Xe	IR	[6]
	19	C-O_p stretch	1029s	Ar	IR	[3][6][7]
			1021	Xe	IR	[6]
	20	Skeletal	698m	Ar	IR	[3][7]
	21	Ring bend	193m	Ar	IR	[3]

Secondary $C_2D_4O_3$

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
a	1	CD stretch	2249m	Ar	IR	[3][7]
	2	CD stretch	2118w	Ar	IR	[3][7]
	3	CD_2 wag + skel.	1160s	Ar	IR	[3][7]
	4	CD_2 def. + skel.	1135s	Ar	IR	[3][7]
	5	Skeletal	1021s	Ar	IR	[3][7]
	6	Skeletal	972m	Ar	IR	[3][7]
	7	CD_2 rock + skel.	911w	Ar	IR	[3][7]
	8	CD_2 twist	851m	Ar	IR	[3][7]
	9	OO stretch	759s	Ar	IR	[3][7]
	10	Skeletal	672m	Ar	IR	[3][7]
	11	Ring pucker	338vw	Ar	IR	[3]

Secondary $C_2D_4O_3$---Continued

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
b	12	CD stretch	2246w	Ar	IR	[3][7]
	13	CD stretch	2092w	Ar	IR	[3][7]
	14	CD_2 wag	1143s	Ar	IR	[3][7]
	15	CD_2 bend	1059vs	Ar	IR	[3][7]
	16	Skeletal	980w	Ar	IR	[3][7]
	17	CD_2 twist	930m	Ar	IR	[3][7]
	18	CD_2 rock	904m	Ar	IR	[3][7]
	19	CD_2 rock	830w	Ar	IR	[3][7]
	20	Skeletal	707w	Ar	IR	[3][7]

[a] Assignments of [3] adopted, except for C-O and O-O stretching modes of sec-$C_2H_4O_3$, for which assignments of [7], suggested by data for ^{18}O-substituted species, are used.

O_p--peroxy O-atom; O_e--ether O-atom.

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[6] C. K. Kohlmiller and L. Andrews, J. Am. Chem. Soc. 103, 2578 (1981).

[7] M. Hawkins, C. K. Kohlmiller, and L. Andrews, J. Phys. Chem. 86, 3154 (1982).

c-$HCOOCH_2OH$

(c-Hydroxymethyl Formate)

Vib. sym.	No.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		OH stretch	3471m	Ar	IR	[4]
		C=O stretch	1760s	gas	IR	[2][3]
			1746vs	Ar	IR	[1][4]
		COH deform.	~1288br[a]	Ar	IR	[4]
		COH deform.	1278ms[a]	Ar	IR	[4]
		C-O stretch	1167s	gas	IR	[2][3]
			1164s	Ar	IR	[1][4]

c-$HCOOCH_2OH$---Continued

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	C-O(H) stretch	1068sh[a]	Ar	IR	[4]
	Skel. stretch	1047s	gas	IR	[2][3]
		1042vs[a]	Ar	IR	[4]
		1035sh[a]	Ar	IR	[4]
	O=C-O deform.	536m[a]	Ar	IR	[4]
	C-O-C deform.	~325m[a]	Ar	IR	[4]

[a] Specific assignment to cis- or trans- structure uncertain.

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[1] H. Kuhne, S. Vaccani, A. Bauder, and H. H. Gunthard, Chem. Phys. 28, 11 (1978).

[2] F. Su, J. G. Calvert, and J. H. Shaw, J. Phys. Chem. 84, 239 (1980).

[3] H. Niki, P. D. Maker, C. M. Savage, and L. P. Breitenbach, J. Phys. Chem. 85, 1024 (1981).

[4] M. Hawkins, C. K. Kohlmiller, and L. Andrews, J. Phys. Chem. 86, 3154 (1982).

t-$HCOOCH_2OH$

(t-Hydroxymethyl Formate)

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	C=O stretch	1786vs	Ar	IR	[1][4]
	COH deform.	~1288br[a]	Ar	IR	[4]
	COH deform.	1278ms[a]	Ar	IR	[4]
	C-O stretch	1139m	Ar	IR	[4]
	C-O(H) stretch	1068sh[a]	Ar	IR	[4]
	Skel. stretch	1047s	gas	IR	[2][3]
		1042vs[a]	Ar	IR	[4]
		1035sh[a]	Ar	IR	[4]
	O=C-O deform.	536m[a]	Ar	IR	[4]
	C-O-C deform.	~325m[a]	Ar	IR	[4]

[a] Specific assignment to cis- or trans- structure uncertain.

References

[1] H. Kuhne, S. Vaccani, A. Bauder, and H. H. Gunthard, Chem. Phys. 28, 11 (1978).

[2] F. Su, J. G. Calvert, and J. H. Shaw, J. Phys. Chem. 84, 239 (1980).

[3] H. Niki, P. D. Maker, C. M. Savage, and L. P. Breitenbach, J. Phys. Chem. 85, 1024 (1981).

[4] M. Hawkins, C. K. Kohlmiller, and L. Andrews, J. Phys. Chem. 86, 3154 (1982).

$C_4H_9O_2$

(t-Butylperoxy)

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		693.7[a]	gas	IR	[1]
		760[b]	gas	IR	[1]

[a] $\pm$ 0.5 cm^{-1}.

[b] $\pm$ 2 cm^{-1}.

References

[1] D. A. Parkes and R. J. Donovan, Chem. Phys. Lett. 36, 211 (1975).

$C_5H_4O_2$

(Cyclopentadienone O-Oxide)

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	OO stretch	1395s 1385vs	Ar	IR	[1][2]
		1184m 1179w	Ar	IR	[1][2]
		1142m	Ar	IR	[1][2]
		1023w	Ar	IR	[1][2]
		983w	Ar	IR	[1][2]
		938vw	Ar	IR	[1][2]
	Ring CH deform.	895vs	Ar	IR	[1][2]
	Ring CH deform.	741s	Ar	IR	[1][2]

References

[1] G. A. Bell and I. R. Dunkin, J. Chem. Soc., Chem. Commun. 1213 (1983).

[2] O. L. Chapman and T. C. Hess, J. Am. Chem. Soc. 106, 1842 (1984).

$(CF_3)_2C_2O$

(Bis(trifluoromethyl)oxirene)

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		1325m	Ar	IR	[1]
		1275s	Ar	IR	[1]
		1160m	Ar	IR	[1]
		875w	Ar	IR	[1]
		730w	Ar	IR	[1]
		660m	Ar	IR	[1]
		560w	Ar	IR	[1]

References

[1] M. Torres, J. L. Bourdelande, A. Clement, and O. P. Strausz, J. Am. Chem. Soc. 105, 1698 (1983).

CF_3CCOCF_3 [a]

(Perfluoroacetylmethylmethylene)

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	C=O stretch	1763m	Ar	IR	[1]
		1751w	Ar	IR	[1]
		1748w	Ar	IR	[1]
		1235m	Ar	IR	[1]
		1226s	Ar	IR	[1]
		1209s	Ar	IR	[1]
		1199s	Ar	IR	[1]
		1167m	Ar	IR	[1]
		1014w	Ar	IR	[1]
		1011w	Ar	IR	[1]
		905w	Ar	IR	[1]
		860m	Ar	IR	[1]
		720w	Ar	IR	[1]
		692m	Ar	IR	[1]
		545w	Ar	IR	[1]
		410w	Ar	IR	[1]

[a] Mixture of two geometric conformers.

References

[1] M. Torres, J. L. Bourdelande, A. Clement, and O. P. Strausz, J. Am. Chem. Soc. 105, 1698 (1983).

$(CF_3)(C_2F_5)C_2O$

(Perfluoromethylethyloxirene)

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		1260	Ar	IR	[1]
		1225	Ar	IR	[1]
		1030	Ar	IR	[1]
		840	Ar	IR	[1]
		750	Ar	IR	[1]
		685	Ar	IR	[1]
		655	Ar	IR	[1]

References

[1] M. Torres, J. L. Bourdelande, A. Clement, and O. P. Strausz, J. Am. Chem. Soc. 105, 1698 (1983).

$(CH_3)_2SiO$

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	Si=O stretch	1204	Ar	IR	[1]

References

[1] C. A. Arrington, R. West, and J. Michl, J. Am. Chem. Soc. 105, 6176 (1983).

$(CH_3)_2CCS$

(Dimethylthiirene)

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
	CH stretch	2970w	Ar	IR	[1][2]
	CH stretch	2921m	Ar	IR	[1][2]
	CH stretch	2865w	Ar	IR	[1][2]
		1923w	Ar	IR	[1][2]
		1440m	Ar	IR	[1][2]
		1427m	Ar	IR	[1][2]
		1041s	Ar	IR	[1][2]
		586w	Ar	IR	[1][2]
		471w	Ar	IR	[1][2]

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[1] A. Krantz and J. Laureni, J. Am. Chem. Soc. 99, 4842 (1977).

[2] A. Krantz and J. Laureni, J. Am. Chem. Soc. 103, 486 (1981).

$C_6H_4S_2$ C_{2v}

(Dithio-p-Benzoquinone)

Vib. No. sym.	Approximate type of mode	cm^{-1}	Med.	Type meas.	Refs.
		1549	Ar	IR	[1]
		1521	Ar	IR	[1]
		1418	Ar	IR	[1]
		1164	Ar	IR	[1]
		844	Ar	IR	[1]
		478	Ar	IR	[1]

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