Submillimeter, Millimeter, and Microwave Spectral Line Catalog

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ABSTRACT

This report describes a computer-accessible catalog of submillimeter, millimeter, and microwave spectral lines in the frequency range between 0 and 10,000 GHz (i.e., wavelengths longer than 30 μm). The catalog can be used as a planning guide or as an aid in the identification and analysis of observed spectral lines. The information listed for each spectral line includes the frequency and its estimated error, the intensity, the lower state energy, and the quantum number assignment. This edition of the catalog has information on 298 atomic and molecular species and includes a total of 1,448,153 lines.

The catalog has been constructed by using theoretical least squares fits of published spectral lines to accepted molecular models. The associated predictions and their estimated errors are based upon the resultant fitted parameters and their covariances. Future versions of this catalog will add more atoms and molecules and update the present listings as new data appear.

The catalog is available on-line via anonymous ftp at spec.jpl.nasa.gov and on the world wide web at `http://spec.jpl.nasa.gov`.

FOREWORD

Revision 2 of the Submillimeter Spectral Line Catalog incorporated a number of changes: (1) a quantum number format, (2) addition of a complete set of partition functions for each species, (3) a computer-accessible directory of species, (4) a table of relative abundances of the isotopes under terrestrial conditions, (5) a new format for the individual species descriptions, (6) eighteen new species, and (7) thirty revised species. The present version is changed only by the addition of new and revised species. The changes are as follows:

NEW SPECIES, REV. 4 (93)

Tag	Name	Tag	Name	Tag	Name
7001	Li-6-H	8001	LiH	8002	Li-6-D
9001	LiD	13003	CH+	19004	H3O+
25002	NaH	27004	C-13-N	28008	HCNH+
28009	CO+	29006	CO-17	29007	HOC+
30010	HOC-13+	30011	NO+	30012	DOC+
31003	HDCO	31004	HO-18-C+	31005	HNO
32006	D2CO	32007	DNO	37002	C3H
37003	c-C3H	38003	C3D	38004	CCC13H
38005	C13CCH	38006	c-C3D	40003	SiC
40004	SiC-v1	40005	KH	41007	SiC-13
41008	CaH	41009	CH3NC	42004	CaD
42005	K-41-H	44010	HCP	44011	AlOH
45009	DCP	45010	HOCO+	45011	AlOD
45012	O-17-CO	46008	CH3OCH3	46009	AlF
46010	NS	46011	DOCO+	46012	HOC-13-O+
46013	O-18-CO	48009	NS-34	49003	C4H
49004	MgCCH	50008	C3N	50009	MgCN
50010	MgNC	51004	HCCNC	51005	HCCNC-v7
51006	HCCNC-v6	51007	HCCNC-v5	51008	HNCCC
52012	DNCCC	53007	C2H3NC	54007	HCCCHO
56007	CCS	56008	C2H3CHO	57001	C-13CS
57002	CC-13S	58001	CCS-34	58002	NaCl
60003	CH3OCHO-A	60004	CH3OCHO-E	60005	NaCl-37
61003	C5H	62005	AlCl	62006	C5D
64003	AlCl-37	66002	OS-34-O	66003	CaNC
69002	C3H7CN	73001	HC6	74001	KCl
74002	C2H5OOCH	75002	H2NCH2COOH-I	75003	H2NCH2COOH-II
76008	KCl-37	76009	C4Si	89001	Sr-88-H
90001	Sr-88-D	92001	C5S	94001	C5-34-S
96001	HOBr-79	98002	HOBr-81	99002	HC7N
112001	Se-80-O2	123001	HC9N	147001	HC11N

REVISED SPECIES, REV. 4 (24)

Tag	Name	Tag	Name	Tag	Name
26001	CN, v = 0, 1	27002	HNC	28001	CO
28007	DNC	29001	C-13-O	30001	CO-18
33001	HO2	34001	O-18-O	34002	H2S
34004	H2O2	38002	c-C3H2	39001	c-HC-13-CCH
39002	c-HCC-13-CH	39005	c-C3HD	41001	CH3CN
46004	C2H5OH	49001	O3-sym-O-17	49002	O3-asym-O-17
52007	SiCC	53001	C2H3CN	55001	C2H5CN
80001	HBr-79	82001	HBr-81	98001	H2SO4

For reference, the changes in Rev. 3 are:

NEW SPECIES, REV. 3 (55)

Tag	Name	Tag	Name	Tag	Name
4001	H2D+	19003	H2O-17	20002	HF
20003	H2O-18	21001	HDO-18	21002	DF
27003	HCN-v2	32005	O2 snglt dlta	33002	O-17-O
37001	DCl	38002	C3H2	39001	C-13-3H2a
39002	C-13-3H2s	39003	C3HD	39004	DCl-37
40002	NaOH	42003	NH2CN	43002	HNCO
43003	AlO	44006	DNCO	44007	HN-15-CO
44008	HNC-13-O	44009	N2O-v2	45005	HCS+
45006	HNCO-18	45007	NN-15-O	45008	N-15-NO
46007	N2O-18	48008	O3-v1,3+v2	50007	CH3Cl-35
51002	ClO-v1	52007	SiCC	52008	CCCO
52009	CH3Cl-37	52010	CH2F2	52011	CH2F2-v4
53003	C-13-CCO	53004	CC-13-CO	53005	CCC-13-O
53006	Cl-37-O-v1	54006	CCCO-18	63002	HNO3-v7
63003	HNO3-v9	63004	HNO3-v6	63005	HNO3-v8
63006	HNO3-v5	66001	COF2	67001	OCl-35-O
68001	CCCS	69001	OCl-37-O	70001	CCCS-34
79001	HOONO2	98001	H2SO4	102001	ClOOCl
104001	Cl-37-OOCl				

REVISED SPECIES, REV. 3 (28)

Tag	Name	Tag	Name	Tag	Name
3001	HD	12001	C-atom	13001	C-13-atom
14002	N-atom-D-state	17001	OH	18003	H2O
19002	HDO	20001	D2O	28001	CO
32001	O2	32002	O2-v1	33001	HO2
34003	PH3	34004	H2O2	36001	HCl
38001	HCl-37	46006	NO2	48004	O3
48005	O3-v2	48006	O3-v1,3	48007	O3-2v2
51002	ClO	52006	HOCl	53002	Cl-37-O
54005	HOCl-37	63001	HNO3	64001	S2
64002	SO2				

For reference, the changes in Rev. 2 are:

NEW SPECIES, REV. 2 (18)

Tag	Name	Tag	Name	Tag	Name
13002	CH	17004	NH3-v2	20001	D2O
25001	CCH	26001	CN	26002	CN-v1
29004	HCO	29005	NNH+	30009	NND+
33001	HO2	46006	NO2	48007	O3-2v2
49001	O3-sym-O-17	49002	O3-asym-O-17	50005	O3-s-O18-v2
50006	O3-a-O18-v2	97002	Cl-35-NO3	99001	Cl-37-NO3

REVISED SPECIES, REV. 2 (30)

Tag	Name	Tag	Name	Tag	Name
16001	O-atom	17001	OH	17002	NH3
18001	OD	18003	H2O	18005	H2O-v2
19001	HO-18	19002	HDO	27001	HCN
29002	HCO+	30002	HC-13-O+	30003	DCO+
31001	HCO-18+	32001	O2	32002	O2-v1
34001	O-18-O	41005	CH3CCD	44001	CS
44002	SiO	45001	C-13-S	46001	CS-34
48004	O3	48005	O3-v2	48006	O3-v1,3
50003	O3-sym-O-18	50004	O3-asym-O-18	52006	HOCl
54005	HOCl-37	63001	HNO3	64002	SO2

For reference, the new and revised species listed in the first revision of this catalog are:

NEW SPECIES, REV. 1 (9)

Tag	Name	Tag	Name	Tag	Name
18004	NH2D	18005	H2O-v2	34004	H2O2
44005	CH3CHO-E	48005	O3-v2	48006	O3-v1,3
52006	HOCl	54005	HOCl-37	63001	HNO3

REVISED SPECIES, REV. 1 (24)

Tag	Name	Tag	Name	Tag	Name
17002	NH3	18002	N-15-H3	18003	H2O
29003	CH2NH	30007	CH2ND	32001	O2
32002	O2-v1	32003	CH3OH	34002	O-18-O
34002	H2S	34003	PH3	45003	NH2CHO
51002	ClO	53002	Cl-37-O	55001	C2H5CN
56001	CH3CH2C-13-N	56002	CH3C-13-H2CN	56003	C-13-H3CH2CN
56005	CH2DCH2CN-s	56006	CH2DCH2CN-a	60001	OCS
61001	OC-13-S	62001	OC-34-S	62002	O-18-CS

Contents

1 INTRODUCTION

This report describes a computer-accessible catalog of submillimeter, millimeter, and microwave spectral lines in the frequency range between 0 and 10,000 GHz (i.e., wavelengths longer than 30 μm). The catalog is intended to be used as a guide in the planning of spectral line observations and as a reference that can facilitate identification and analysis of observed spectral lines. The selection of lines for the catalog is based on the project needs of astronomers and atmospheric scientists.

The catalog is constructed using theoretical least squares fits and predictions based on spectral lines, mostly obtained from the literature. In subsequent versions of the catalog, more molecules will be added and existing molecular listings will be updated as new data appear.

The catalog is available on-line via anonymous ftp at spec.jpl.nasa.gov and on the world wide web at http://spec.jpl.nasa.gov.

The format of the data is given in Section 2. Section 3 gives conversions between different measures of spectral line intensity. General comments on the precision of the spectral line positions and intensities are given in Section 4, while species-specific comments are reserved for Section 6. Section 5 gives the format of quantum numbers as they appear in the catalog.

Documentation for each molecular or atomic species is listed in Section 6 in order of the "species tag." This tag is a six-digit number in which the three most significant digits represent the mass number of the molecule or atom and the last three digits are an accession number for the given mass. Usually there is a separate tag for each vibration-electronic state of a particular molecule.

2 DATA FORMAT

2.1 Line Files

The catalog line files are composed of 80-character lines, with one line entry per spectral line. The format of each line is:

FREQ, ERR, LGINT, DR, ELO, GUP, TAG, QNFMT, QN′, QN″
(F13.4, F8.4, F8.4, I2, F10.4, I3, I7, I4, 6I2, 6I2)

FREQ:	Frequency of the line in MHz.
ERR:	Estimated or experimental error of FREQ in MHz.
LGINT:	Base 10 logarithm of the integrated intensity in units of nm^2·MHz at 300 K. (See Section 3 for conversions to other units.)
DR:	Degrees of freedom in the rotational partition function (0 for atoms, 2 for linear molecules, and 3 for nonlinear molecules).
ELO:	Lower state energy in cm^{-1} relative to the lowest energy spin–rotation level in ground vibronic state.
GUP:	Upper state degeneracy.
TAG:	Species tag or molecular identifier. A negative value flags that the line frequency has been measured in the laboratory. The absolute value of TAG is then the species tag and ERR is the reported experimental error. The three most significant digits of the species tag are coded as the mass number of the species, as explained above.
QNFMT:	Identifies the format of the quantum numbers given in the field QN. These quantum number formats are given in Section 5 and are different from those in the first two editions of the catalog.
QN$'$:	Quantum numbers for the upper state coded according to QNFMT.
QN$''$:	Quantum numbers for the lower state.

2.2 Directory File

The catalog contains a special directory file called catdir.cat Each element of this directory is an 80-character record with the following format:

TAG,	NAME,	NLINE,	QLOG,	VERSION
(I6,X,	A13,	I6,	7F7.4,	I2)

TAG:	The species tag or molecular identifier.
NAME:	An ASCII name for the species.
NLINE:	The number of lines in the catalog.
QLOG:	A seven-element vector containing the base 10 logarithm of the partition function for temperatures of 300 K, 225 K, 150 K, 75 K, 37.5 K, 18.75 K, and 9.375 K, respectively.
VERSION:	The version of the calculation for this species in the catalog.

2.3 Documentation files

The documentation files are stored natively as ASCII LaTex files for each species. Postscript, LaTex, and PDF versions of this publication are also available on line. The documentation files provide the intensity and frequency cut-offs, partition functions at representative temperatures, assumed dipole moments, literature citations for the experimental lines, and a brief description of the nature of the Hamiltonian model used in the calculation. The documentation file also includes a suggested isotopic correction based on cosmic abundances. This correction includes the appropriate statistics for equivalent nuclei. Note the catalog intensities do not include this isotopic correction.

In this edition of the catalog, several of the species have spectra that are extended to 10,000 GHz, so the documentation includes a maximum frequency cutoff. For almost all species, a strength cutoff was also employed:

$$10^{\mathrm{LGINT}} \ > \ 10^{\mathrm{LOGSTR0}} \ + \ (\nu/300GHz)^2 \cdot 10^{\mathrm{LOGSTR1}}$$

A blank entry for LOGSTR1 means that the second term was not included. We have found that LOGSTR1 is often a useful cut-off parameter to account for the decreased sensitivity of instrumentation with increasing frequency or as a means to capture lines with comparable transition dipoles. The partition functions listed (Q) in the catalog include rotation and spin statistics but usually do not include vibrational or electronic corrections. (Exceptions such as H_2O and O_3 are noted.) Calculation of Q is based on a sum over states. At higher temperatures, the sum-over-states calculation is replaced by a classical calculation when the latter is larger due to a limited number of states in the catalog. The spin statistics included in the partition function are sometimes divided by a common factor, but the partition functions are always consistent with the statistics used for intensities in the catalog. This common factor is not always documented, but the choice should be clear from the GUP field in the line file.

3 INTENSITY UNITS AND CONVERSIONS

The units of intensity given in the catalog, $\mathrm{nm}^2\cdot\mathrm{MHz}$, are based on the integral of the absorption cross-section over the spectral line shape. The value of the intensity is calculated for 300 K and is directly comparable with the common infrared intensity unit of $\mathrm{cm}^{-1}/(\mathrm{molecule/cm}^2)$. The latter is obtainable by dividing the catalog intensity by $2.99792458 \times 10^{18}$.

The line intensity in the catalog, I_{ba} (300 K), is obtained from

$$\begin{aligned} I_{ba}(T) &= (8\pi^3/3\mathrm{hc})\nu_{ba}\ {}^xS_{ba}\ \mu_x^2[e^{-E''/kT} - e^{-E'/kT}]/Q_{rs} \qquad (1) \\ &= 4.16231 \times 10^{-5}\nu_{ba}\ {}^xS_{ba}\ \mu_x^2[e^{-E''/kT} - e^{-E'/kT}]/Q_{rs} \qquad (2) \end{aligned}$$

where ν_{ba} is the line frequency, ${}^xS_{ba}$ is the line strength, μ_x is the dipole moment along the molecular axis x, E$''$ and E$'$ are the lower and upper state energies, respectively, and Q_{rs} is the rotation-spin partition function (using the same zero of energy as E$'$ and E$''$). In Eq.(2), I_{ba} has units of $\mathrm{nm}^2\cdot\mathrm{MHz}$, ν_{ba} has units of MHz, and μ_x has units of Debye. In many molecules, there are several dipole moment projections and there even may be mixing between dipoles. In such cases, ${}^xS_{ba}\ \mu_x^2$ is replaced with the sum of the squares of the transition dipoles for each M component in the line. For magnetic dipole transitions, Eq.(2) can be used with the conversion that a Bohr magneton is equivalent to 0.009274 Debye. Note that with this definition the intensities are defined with respect to the total concentration of the vibration-electronic state of the species. No vibrational partition function is included, except where explicitly stated in the documentation. Care is taken to assure that ${}^{x}\mathrm{S}_{ba}$ and Q_{rs} are determined with the same state degeneracies. For the catalog, Eq. (2) is evaluated for T = T $_\circ$ = 300 K.

Values of I_{ba} at other temperatures can also be obtained from Eq.(1) once the temperature dependence of Q_{rs} is known. For linear molecules, Q_{rs} is proportional to T in the limit where the energy spacings are small compared with kT. For nonlinear molecules, Q_{rs} is proportional to $\mathrm{T}^{3/2}$ in the same limit. Explicitly, $I_{ba}(\mathrm{T})$ is

$$\begin{aligned} I_{ba}(T) &= I_{ba}(T_\circ)[Q_{rs}(T_\circ)/Q_{rs}(T)]\frac{e^{-E''/kT} - e^{-E'/kT}}{e^{-E''/kT_\circ} - e^{-E'/kT_\circ}} && (3) \\ &\cong I_{ba}(T_\circ) \cdot (T_\circ/T)^{n+1} e^{-(1/T - 1/T_\circ)E''/k} && (4) \end{aligned}$$

where n = 1 for a linear molecule and 3/2 for a nonlinear molecule. Eq.(4) requires that $E' - E''$ is small compared with kT and $kT_\circ$.

Absorption coefficients of collision-broadened lines can be obtained from I_{ba} with the relation

$$\alpha_{\max} = \frac{I_{ba}(T)}{\Delta\nu}(T_\circ/T) \times 102.458 \text{ cm}^{-1} \tag{5}$$

in which $\Delta\nu$ is the half-width at half-height in MHz at 1 torr partial pressure of the absorber at temperature T, I_{ba} is in units of $\mathrm{nm}^2\cdot\mathrm{MHz}$, and $\alpha_{\max}$ is in units of cm^{-1}. The power transmission through a uniform medium of length L at the peak of the line is $\exp(-\alpha_{\max}L)$. The attenuation is $\alpha_{\max}L \times 4.3429$ in dB. The corresponding value of $\alpha_{\max}$ in the thermal Doppler limit is

$$\alpha_{\max} = \frac{I_{ba}(T)p}{\Delta\nu_d}(T_\circ/T) \times 151.194 \text{ cm}^{-1} \tag{6}$$

in which p is the partial pressure of the absorber in torr, and $\Delta\nu_d$ is the Doppler half-width at half-height in units of MHz. The Doppler width is given by

$$\Delta\nu_d = 1.17221 \times 10^{-6} \times \nu_{ba}\sqrt{(T/T_\circ)(28/m)} \tag{7}$$

in which m is the mass of the absorber (in atomic mass units). The explicit inverse temperature dependence in Eqs.(5) - (6) is due to the conversion of density to pressure units. There is additional implicit temperature dependence in $I_{ba}(T)$ and in the widths. In Eqs.(7) - (10), ν_{ba} is the line frequency in MHz.

The absorption cross-section of an interstellar absorber integrated over a 1 km/s-velocity interval is

$$\sigma_{ba} = \frac{I_{ba}}{\nu_{ba}} \times 2.99792 \times 10^{-9} \text{ cm}^2. \tag{8}$$

The power transmission through a uniform medium of length L and number density ρ is $\exp(-\sigma_{ba}\rho L)$. The inverse of σ_{ba} is the column density per unit optical depth in the same 1 km/s-velocity interval.

The average spontaneous emission rate from the upper states into the lower states is

$$\begin{aligned} A_{ba} &= I_{ba}(T)\ \nu_{ba}^2[Q_{rs}/g^{'}][e^{-E^{''}/kT} - e^{-E^{'}/kT}]^{-1} \times 2.7964 \times 10^{-16}\ \mathrm{sec}^{-1} && (9) \\ &\cong I_{ba}(T_\circ)\ \nu_{ba}[Q_{rs}(T_\circ)/g^{'}]e^{E'/kT_\circ} \times 1.748 \times 10^{-9}\ \mathrm{sec}^{-1} && (10) \end{aligned}$$

in which g$^{'}$ is the degeneracy of the upper state. The value of g$^{'}$ is listed as part of the spectral line information in the catalog. Values of Q$_{rs}$ are listed in the documentation and on the directory file. Eq.(10) requires that $h\nu_{ba}$ is small compared with kT and $kT_\circ$.

It should be noted that the information to make all the intensity conversions given above is available from the directory file and from the line files, with the exception of the collisional broadening coefficients. As a matter of policy, we have not included collisional linewidths in the catalog because of the large variety of different collision partners relevant for the laboratory, the Earth's atmosphere, and the atmospheres of the other planets.

When $\nu \cong \nu_{ba}$, the absorption coefficient is

$$\alpha(\nu) = n \sum_{a,b} I_{ab} f_{ab}(\nu - \nu_{ab}) \tag{11}$$

where n is the number denity of absorbers and $f_{ab}(\delta)$ is an area-normalized line shape. Further away from line center

$$\alpha(\nu) = n\nu \tanh(\nu/2kT) \sum_{a,b} \bar{I}_{ab} \left[f_{ab}(\nu - \nu_{ab}) + f_{ab}(\nu + \nu_{ab})\right] \tag{12}$$

where $\bar{I}_{ab}$ is defined by

$$I_{ab} = \nu_{ab} \tanh(\nu_{ab}/2kT) \bar{I}_{ab} \tag{13}$$

Note that in Eq. (11) and (12), the sum over a and b is restricted to $\nu_{ab} > 0$.

4 GENERAL COMMENTS ON PRECISION

The expected errors of the frequency as listed in the catalog are usually based on a propagation of errors estimated from a least squares fit of the observed frequencies to a model Hamiltonian, using the following equation:

$$\varepsilon_n^2 = \sum_{kj} \frac{\partial \nu_n}{\partial p_k} \frac{\partial \nu_n}{\partial p_j}\ \ V_{kj} \tag{14}$$

in which ε_n is the estimated error of frequency ν_n and V_{kj} is an element of the least square variance-covariance matrix for the parameters p_k. This variance-covariance matrix is determined from the observed lines by

$$(V^{-1})_{kj} = \sum_m \frac{\partial \nu_m}{\partial p_k} \frac{\partial \nu_m}{\partial p_j} \ \varepsilon_m^{-2} \tag{15}$$

in which the summation over m is over the experimental lines using experimental uncertainies, ε_m. The diagonal elements of V are the squares of the parameter uncertainties and the off-diagonal elements of V are products of the parameter uncertainties and correlation coefficients.

The experimental uncertainties generally given in the literature vary from 1.6-σ estimates to 3-σ estimates and are usually "guesstimates." Unfortunately, many authors do not even report their experimental uncertainties. Therefore, the expected errors in predicted lines obtained from fits based on such data will usually reflect this ambiguity in laboratory uncertainties through Eq. (10) and (11). In some cases, the quality of the least squares fit of the parameters to the experimental lines can be a guide to the statistical nature of the experimental uncertainties. Whenever possible, the expected errors in this catalog will reflect an expected 95% confidence interval based on the model used to fit the data. However, the errors can be different from this design goal by factors of three just due to the quality of the input error estimates. Lines with an expected error greater than 1 GHz have been dropped from the catalog.

The expected errors can only be computed relative to the model used. There are at least two ways the model can be "wrong" for the predicted frequencies.

First, higher order centrifugal distortion terms may no longer be negligible for the predicted frequencies. This effect will generally be important for lines of higher J or K than the laboratory-determined data set. In a sense, the predictions are then a form of extrapolation rather than interpolation and are therefore more suspect. A second factor leading to discrepancies in the predicted frequencies comes from "resonances." These resonances come from a near overlap of energy states that are coupled by elements of the Hamiltonian matrix. Poor predictability comes when these elements are neglected in the model or are treated inadequately by some form of perturbation theory. Such a neglect of coupling elements is always necessary at some level in any practical calculation. A major contributing problem is that often the existing data set is not sensitive to the parameters that are needed to characterize the resonances.

Precision in the intensity estimates is generally less critical than precision in the frequency. Contributing to intensity uncertainty are errors in the dipole moment, errors in the line strength ${}^xS_{ba}$, and errors in the rotation-spin partition function (the vibration-electronic partition defined on the basis of concentrations of the given vibration-electronic state). Dipole moment errors come directly from the experimental determination and indirectly from the J dependence of the dipole moment due to centrifugal mixing of the vibrational states. Line strength errors can come from deficiencies in the model Hamiltonian and are particularly severe when resonances have been inadequately accounted for. Partition function errors are relatively benign but can become significant if the classical formulae are used at low temperatures for small molecules. With the exception of unanticipated resonances and poorly determined dipole moments, worst-case errors in the intensity will generally be at the 1% level or lower.

Many molecular models are found in the literature. In principle, a very general model should be able to treat every possible case. In practice, this is hardly ever done. A specific model is most frequently used for every case, mainly because every author starts with a different viewpoint of the problem. In our case, we have tried to develop a program that will treat a wide variety of problems with a minimum of adaptation. This saves a great deal of time in the initial setup, and provides a uniform output format for the final results. Most importantly, the basic treatment is the same for every molecule, regardless of the model used, so that a high degree of consistency can be maintained, facilitating comparisons between different molecules. The particular model needed to analyze a specific problem is treated as a subroutine. For certain problems, this subroutine can be quite simple, but for others, it is more complex.

Simple singlet sigma diatomic, linear, and symmetric rotor molecules are treated together. Asymmetric rotors with and without various complicating interactions are treated exactly, without any perturbation expansions. This is done by employing the Hamiltonian operators to generate the matrix elements. All possible operators can be used, so any conceivable interaction can be included initially.

Comments on specific models are given for the individual species.

5 FORMAT OF QUANTUM NUMBERS

For the later editions of this catalog, we have attempted to use a quantum number format convention that allows the quantum numbers to be accessed easily by computer (see Table 1). First, the upper and lower quantum number sets have been separated into distinct fields. Second, the quantum format designations have been defined to have more accessible information encoded in them. The quantum number format designation, QNFMT, is a 4-digit quantity in the catalog. We divide QNFMT into a series of digits so that

$$\mathrm{QNFMT} = Q \cdot 100 + H \cdot 10 + NQN$$

in which Q determines the type of molecule (see Table 1), H determines the coding of half-integer quantum numbers, and NQN is the number of quantum numbers for each state. Q is defined so that MOD(Q,5) is the number of primary quantum numbers. If NQN is greater than the number of primary quantum numbers, the degeneracy is derived from the last quantum number. Otherwise, the degeneracy is derived from the first quantum number. H is a 3-bit binary code for the existence of half-integer quantum numbers for the *last three* quantum numbers. The least significant bit refers to quantum number NQN and is 1 if the last quantum number is half-integer. In the catalog, all half-integer quantum numbers are rounded **up** to the next integer.

The parity given may not always be experimentally determined, but the parity convention is guaranteed to produce parities of the same sign for interacting states and to produce a change in parity across dipole allowed transitions. It should be noted that for symmetric top transitions with no K splitting, the parity designation is frequently dropped. Unless otherwise stated below, the parity of prolate symmetric tops follows the parity of K_{+1} for the corresponding asymmetric top level, while for oblate tops, the parity follows K_{-1}. For example, the level $5_{3,2}$ for an asymmetric rotor has $K = 3$ for a prolate symmetric top quantum field, and $K = -2$ for an oblate top. Hund's case (b) quanta are similar to symmetric top quanta except that K is replaced with Λ. Hunds's case (a) quanta also have parity encoded in the Λ field. The correlation between parity and e,f designations should follow the recommendations of J. M. Brown *et al.*, 1975, J. Mol. Spect. **55**, 500. For reference, this convention is

TABLE 1. QUANTUM NUMBER FORMATS

Type	**Q**	**DR**	**Quantum Order**
Atom	0	0	(J),(F),$\cdots$
Linear — Σ	1	2	N,(J),(F_1),(F_2)(F)
Linear — Case b	2	2	N, Λ,(F_1),(F_2),(F)
Linear — Case a (2S+1 odd)	3	2	J,Ω, Λ,(F_1),(F_2),(F)
Linear — Case a (2S+1 even)	8	2	J+$\frac{1}{2}$,$\Omega + \frac{1}{2}$, Λ,(F_1), (F_2),(F)
Symmetric rotor	2	3	N,K,(J),(F_1),(F_2),(F)
Symmetric rotor with vibration	13	3	N,K,v,(J),(F_1),(F)
Asymmetric rotor	3	3	N,K_{-1},K_{+1},(J),(F_1),(F)
Asymmetric rotor with vibration	14	3	N,K_{-1},K_{+1},v,(J),(F)

Conventions:

1. Half-integer quantum numbers are rounded up.
2. The sign of Λ and K refers to the parity under inversion of spatial coordinates, *not* the sign of the operator.
3. Quantum numbers in parentheses are optional.

For odd-spin multiplicity:

$$\begin{array}{llcrll} \text{if} & p(-1)^{J+1/2} & = & -1, & \text{then} & e \\ \text{if} & p(-1)^{J+1/2} & = & 1, & \text{then} & f \end{array}$$

For even-spin multiplicity:

$$\begin{array}{llcrll} \text{if} & p(-1)^{J} & = & 1, & \text{then} & f \\ \text{if} & p(-1)^{J} & = & -1, & \text{then} & e \end{array}$$

where p is ±1 according to the parity. Care must be used because this convention is not universally followed in the literature.

6 DOCUMENTATION BY SPECIES

In this edition of the catalog, several of the species have spectra that are extended to 10,000 GHz, so the documentation below includes a maximum frequency cutoff. For almost all species, a strength cutoff was also employed:

$$10^{\mathrm{LGINT}} > 10^{\mathrm{LOGSTR0}} + (\nu/300GHz)^2 \cdot 10^{\mathrm{LOGSTR1}}$$

A blank entry for LOGSTR1 means that the second term was not included. The partition functions listed (Q) include rotation and spin statistics but usually do not include vibrational corrections. (Exceptions such as H_2O and O_3 are noted.) Calculation of Q is based on a sum over states. At higher temperatures, the sum-over-states calculation is replaced by a classical calculation when the latter is larger due to a limited number of states in the catalog. The spin statistics included are only a partial set but are consistent with the intensities in the catalog.

6.1 Isotope Corrections

For convenience, we have included an isotope correction for the rarer isotopes that includes effects of redundant substitution. The atomic abundances used are listed in Table 2. It should be stressed that the intensities in the catalog do not contain an isotope correction.

TABLE 2. ASSUMED RELATIVE ISOTOPIC ABUNDANCES FOR CATALOG DESCRIPTION

Isotope	Log (abundance)	Isotope	Log (abundance)
^{1}H	0.000	^{2}H	-3.824
^{6}Li	-1.131	^{7}Li	-0.033
^{12}C	0.000	^{13}C	-1.955
^{14}N	0.000	^{15}N	-2.432
^{16}O	0.000	^{17}O	-3.432
^{18}O	-2.690	^{28}Si	-0.035
^{29}Si	-1.327	^{30}Si	-1.506
^{32}S	-0.022	^{33}S	-2.125
^{34}S	-1.376	^{35}Cl	-0.122
^{37}Cl	-0.611	^{79}Br	-0.296
^{81}Br	-0.306		

6.2 List of Species in This Catalog

Table 3 lists all the species provided in this catalog, by tag and name.

TABLE 3. LIST OF SPECIES

Tag	Name	Tag	Name	Tag	Name
1001	H-atom	2001	D-atom	3001	HD
4001	H2D+	7001	Li-6-H	8001	LiH
8002	Li-6-D	9001	LiD	12001	C-atom
13001	C-13-atom	13002	CH	13003	CH+
14001	N-atom	14002	N-atom-D-st	15001	NH
16001	O-atom	17001	OH	17002	NH3
17003	CH3D	17004	NH3-v2	17005	OH-v1,2
18001	OD	18002	N-15-H3	18003	H2O
18004	NH2D	18005	H2O-v2	19001	HO-18
19002	HDO	19003	H2O-17	19004	H3O+
20001	D2O	20002	HF	20003	H2O-18
21001	HDO-18	21002	DF	25001	CCH
25002	NaH	26001	CN, v = 0, 1	27001	HCN
27002	HNC	27003	HCN-v2	27004	C-13-N
28001	CO	28002	HC-13-N	28003	HCN-15
28004	DCN	28005	HNC-13	28006	HN-15-C
28007	DNC	28008	HCNH+	28009	CO+
29001	C-13-O	29002	HCO+ v=0,1,2	29003	CH2NH
29004	HCO	29005	NNH+	29006	CO-17
29007	HOC+	30001	CO-18	30002	HC-13-O+
30003	DCO+	30004	H2CO	30005	C-13-H2NH
30006	CH2N-15-H	30007	CH2ND	30008	NO
30009	NND+	30010	HOC-13+	30011	NO+
30012	DOC+	31001	HCO-18+	31002	H2C-13-O
31003	HDCO	31004	HO-18-C+	31005	HNO
32001	O2	32002	O2-v1	32003	CH3OH
32004	H2CO-18	32005	O2-snglt-dlta	32006	D2CO
32007	DNO	33001	HO2	33002	O-17-O
33003	SH v=0,1	34001	O-18-O	34002	H2S
34003	PH3	34004	H2O2	34005	SD
35001	HDS	36001	HCl	37001	DCl

TABLE 3. (continued)

Tag	Name	Tag	Name	Tag	Name
37002	C3H	37003	c-C3H	38001	HCl-37
38002	c-C3H2	38003	C3D	38004	c-CCC-13-H
38005	c-C-13-CCH	38006	c-C3D	39001	c-HC-13-CCH
39002	c-HCC-13-CH	39003	c-C3HD	39004	DCl-37
40001	CH3CCH	40002	NaOH	40003	SiC
40004	SiC-v1	40005	KH	40006	C2O
40007	MgO	41001	CH3CN v8=0,1	41002	CH3CC-13-H
41003	CH3C-13-CH	41004	C-13-H3CCH	41005	CH3CCD
41006	CH2DCCH	41007	SiC-13	41008	CaH
41009	CH3NC	42001	CH3CN-15	42002	CH2CO
42003	NH2CN	42004	CaD	42005	K-41-H
42006	C-13-H3CN	42007	CH3C-13-N	42008	CH2DCN
42009	H2CSi	42010	SiN	43001	CHDCO
43002	HNCO	43003	AlO	43004	CP
44001	CS	44002	SiO	44003	CH3CHO-a
44004	N2O	44005	CH3CHO-e	44006	DNCO
44007	HN-15-CO	44008	HNC-13-O	44009	N2O-v2
44010	HCP	44011	AlOH	44012	N2O-2v2
45001	C-13-S	45002	Si-29-O	45003	NH2CHO
45005	HCS+	45006	HNCO-18	45007	NN-15-O
45008	N-15-NO	45009	DCP	45010	HOCO+
45011	AlOD	45012	O-17-CO	45013	PN v=0-4
46001	CS-34	46002	Si-30-O	46003	H2CS
46004	C2H5OH	46005	HCOOH	46006	NO2
46007	N2O-18	46008	CH3OCH3	46009	AlF
46010	NS	46011	DOCO+	46012	HOC-13-O+
46013	O-18-CO	47001	H2C-13-S	47002	HC-13-OOH
47003	DCOOH	47004	HCOOD	47005	PO+ v=0-4
47006	PO	48001	SO	48002	SO-v1
48003	H2CS-34	48004	O3	48005	O3-v2
48006	O3-v1,3	48007	O3-2v2	48008	O3-v1,3+v2
48009	NS-34	48010	SO+	49001	O3-sym-O-17
49002	O3-asym-O-17	49003	C4H	49004	MgCCH
50001	S-34-O	50002	SO-18	50003	O3-sym-O-18
50004	O3-asym-O-18	50005	O3-s-O18-v2	50006	O3-a-O18-v2

TABLE 3. (continued)

Tag	Name	Tag	Name	Tag	Name
50007	CH3Cl-35	50008	C3N	50009	MgCN
50010	MgNC	51001	HCCCN	51002	ClO
51003	ClO-v1	51004	HCCNC	51005	HCCNC-v7
51006	HCCNC-v6	51007	HCCNC-v5	51008	HNCCC
52001	HCCC-13-N	52002	HCC-13-CN	52003	HC-13-CCN
52004	HCCCN-15	52005	DCCCN	52006	HOCl
52007	SiCC	52008	CCCO	52009	CH3Cl-37
52010	CH2F2	52011	CH2F2-v4	52012	DNCCC
52013	CNCN	53001	C2H3CN	53002	Cl-37-O
53003	C-13-CCO	53004	CC-13-CO	53005	CCC-13-O
53006	Cl-37-O-v1	53007	C2H3NC	53008	HNCCN+
54001	CH2CHC-13-N	54002	CH2C-13-HCN	54003	C-13-H2CHCN
54004	CH2CDCN	54005	HOCl-37	54006	CCCO-18
54007	HCCCHO	55001	C2H5CN	56001	CH3CH2C-13-N
56002	CH3C-13-H2CN	56003	C-13-H3CH2CN	56004	C2H5CN-15
56005	CH2DCH2CN-s	56006	CH2DCH2CN-a	56007	CCS
56008	C2H3CHO	56009	MgS	57001	C-13CS
57002	CC-13S	58001	CCS-34	58002	NaCl
60001	OCS	60002	SiS	60003	CH3OCHO-A
60004	CH3OCHO-E	60005	NaCl-37	61001	OC-13-S
61002	Si-29-S	61003	C5H	62001	OC-34-S
62002	O-18-CS	62003	Si-30-S	62004	SiS-34
62005	AlCl	62006	C5D	63001	HNO3
63002	HNO3-v7	63003	HNO3-v9	63004	HNO3-v6
63005	HNO3-v8	63006	HNO3-v5	63007	PS
63008	PO2	64001	S2	64002	SO2
64003	AlCl-37	64004	C4O	64005	SO2-v2
65001	S-33-O2	66001	COF2	66002	S-34-O2
66003	CaNC	66004	SOO-18	67001	OCl-35-O
68001	CCCS	69001	OCl-37-O	69002	C3H7CN 1
70001	CCCS-34	71001	MnO	73001	C6H
74001	KCl	74002	C2H5OOCH	75001	HCCCCCN
75002	H2NCH2COOH I	75003	H2NCH2COOH II	76001	HCCCCC-13-N
76002	HCCCC-13-CN	76003	HCCC-13-CCN	76004	HCC-13-CCCN
76005	HC-13-CCCCN	76006	HCCCCCN-15	76007	DCCCCCN

TABLE 3. (continued)

Tag	Name	Tag	Name	Tag	Name
76008	KCl-37	76009	C4Si	76010	C5O
79001	HOONO2	80001	HBr-79	81001	Cl-35-NO2
82001	HBr-81	88001	C6O	89001	Sr-88-H
90001	Sr-88-D	92001	C5S	94001	C5-34-S
95001	Br-79-O	95002	Br-79-O v=1	96001	HOBr-79
97001	Br-81-O	97002	Cl-35-ONO2	97003	Br-81-O v=1
98001	H2SO4	98002	HOBr-81	99001	Cl-37-ONO2
99002	HC7N	100001	C7O	102001	ClOOCl
104001	Cl-37-OOCl	111001	OBr-79-O	112001	Se-80-O2
112002	C8O	113001	OBr-81-O	123001	HC9N
124001	C9O	147001	HC11N		

Species Tag:	1001	Name:	H-atom
Version:	1		$^{2}\mathrm{S}_{1/2}$ ground state
Date:	Oct. 1979		
Contributor:	H. M. Pickett		

Lines Listed:	1	Q(300.0)=	4.000
Freq. (GHz) $<$	2	Q(225.0)=	4.000
Max. J:	1	Q(150.0)=	4.000
LOGSTR0=	-9.1	Q(75.00)=	4.000
LOGSTR1=		Q(37.50)=	4.000
Isotope Corr.:	0.0	Q(18.75)=	4.000
Egy. (cm^{-1}) $>$	0.0479	Q(9.375)=	4.000
μ_a =		A=	
μ_b =		B=	
μ_c =		C=	

The atomic hydrogen line at 21 cm has been measured to a precision of 0.001 Hz (L. Essen, R. W. Donaldson, M. J. Bangham, and E. G. Hope, 1971, Nature **229**, 110). The average spontaneous emission lifetime of the three F = 1 states is 2.876×10^{-15} sec^{-1}.

Species Tag:	2001	Name:	D-atom
Version:	1		$^2S_{1/2}$ ground state
Date:	Oct. 1979		
Contributor:	H. M. Pickett		
Lines Listed:	1	Q(300.0)=	6.00
Freq. (GHz) <	1	Q(225.0)=	6.00
Max. J:	2	Q(150.0)=	6.00
LOGSTR0=	-10.3	Q(75.00)=	6.00
LOGSTR1=	-4.3	Q(37.50)=	6.00
Isotope Corr.:	-3.824	Q(18.75)=	6.00
Egy. (cm^{-1}) >	0.0	Q(9.375)=	6.00
μ_a =		A=	
μ_b =		B=	
μ_c =		C=	

The atomic deuterium line at 327 MHz has been measured to an accuracy of 0.002 Hz (D. J. Wineland and N. F. Ramsey, 1972, Phys. Rev. A **5**, 821). The average spontaneous emission lifetime for the four F = 3/2 states is 4.695×10^{-17} sec^{-1}.

Species Tag:	3001	Name:	HD
Version:	2		Mono-deuterated
Date:	Oct. 1989		molecular hydrogen
Contributor:	H. M. Pickett		
Lines Listed:	1	Q(300.0)=	5.016
Freq. (GHz) <	2675	Q(225.0)=	3.858
Max. J:	1	Q(150.0)=	2.701
LOGSTR0=	-5.6	Q(75.00)=	1.571
LOGSTR1=	-7.5	Q(37.50)=	1.098
Isotope Corr.:	-3.523	Q(18.75)=	1.003
Egy. (cm^{-1}) >	0.0	Q(9.375)=	1.000
μ_a =	0.000585	A=	
μ_b =		B=	1339100.
μ_c =		C=	

The dipole moment is from M. Trefler and H. P. Gush, 1968, Phys. Rev. Lett. **20**, 703. The frequency has been measured by K. M. Evenson *et al.*, 1988, Astrophys. J. **330**, L135. This measurement has also been confirmed at JPL using laser sideband techniques (unpublished data).

Species Tag:	4001	Name:	H2D+
Version:	1		
Date:	Oct. 1989		
Contributor:	H. M. Pickett		

Lines Listed:	19	Q(300.0)=	73.824
Freq. (GHz) <	5539	Q(225.0)=	49.477
Max. J:	5	Q(150.0)=	27.530
LOGSTR0=	-7.2	Q(75.00)=	9.727
LOGSTR1=	-3.4	Q(37.50)=	3.102
Isotope Corr.:	-3.347	Q(18.75)=	1.215
Egy. (cm^{-1}) >	0.0	Q(9.375)=	1.004
μ_a =	0.6	A=	1299960.
μ_b =		B=	873685.
μ_c =		C=	491480.

The frequency fit included rotational lines measured by M. Bogey *et al.*, 1984, Astron. Astrophys. **137**, 137, and Saito *et al.*, 1985, J. Chem. Phys. **82**, 45. Infrared combination differences from T. Amano and J. K. G. Watson, 1984, J. Chem. Phys. **81**, 2869, were also used.

Species Tag:	7001	Name:	Li-6-H
Version:	1		Lithium hydride,
Date:	July 1995		^{6}Li isotope
Contributor:	M. L. Delitsky		$\nu = 0, 1$
	H. M. Pickett		
Lines Listed:	33	Q(300.0)=	28.137
Freq. (GHz) <	7210	Q(225.0)=	21.127
Max. J:	17	Q(150.0)=	14.174
LOGSTR0=	-20	Q(75.00)=	7.249
LOGSTR1=	-100	Q(37.50)=	3.804
Isotope Corr.:	-1.13	Q(18.75)=	2.101
Egy. (cm^{-1}) >	0	Q(9.375)=	1.299
$\mu_a =$	5.882	A=	
$\mu_b =$		B=	226633.2
$\mu_c =$		C=	

The line frequencies were taken from: Maki, Olson and Thompson, 1990, J. Mol. Spect. **144**, 257. Bellini, *et al.*, 1994, Astrophys. J. **424**, 507, and Plummer, Herbst and DeLucia , 1984, J. Chem. Phys. **81**, 4893. Additional lines were measured by F. Matsushima, *et. al.*, 1994, J. Jpn. Appl. Phys. **33**, 315. These were not included in the analysis due to poor agreement with other data. Further work is required to resolve the differences between these two data sets.

The dipole moment is from L. Warton, L. P. Gold and W. Klemperer, 1960, J. Chem. Phys. **33**, 1255. It has been assumed to be the same for all isotopomers.

Species Tag:	8001	Name:	LiH
Version:	1		Lithium hydride,
Date:	July 1995		^{7}Li isotope
Contributor:	M. L. Delitsky		$\nu = 0, 1$
	H. M. Pickett		
Lines Listed:	40	Q(300.0)=	28.717
Freq. (GHz) <	8122	Q(225.0)=	21.559
Max. J:	20	Q(150.0)=	14.461
LOGSTR0=	-20	Q(75.00)=	7.393
LOGSTR1=	-100	Q(37.50)=	3.875
Isotope Corr.:	-0.03	Q(18.75)=	2.136
Egy. (cm^{-1}) >	0.0	Q(9.375)=	1.314
μ_a =	5.882	A=	
μ_b =		B=	222027.4
μ_c =		C=	

The line frequencies were taken from: Bellini, *et al.*, 1994, Astrophys. J., **424**, 507, and Plummer, Herbst and DeLucia, 1984, J. Chem. Phys., **81**, 4893. Maki, Olson and Thompson, 1990, J. Mol. Spect. **144**, 257. We also note line frequencies in: Matsushima, et al., 1994, Jpn. J. Appl. Phys. **33**, 315. However, these lines were not included in the fit due to poor agreement with the measurements of Bellini. We include it here for reference. Further work is required to resolve the differences between these two data sets.

The dipole moment is from L. Warton, L. P. Gold and W. Klemperer, 1960, J. Chem. Phys. **33**, 1255.

Species Tag:	8002	Name:	Li-6-D
Version:	1		Lithium deuteride,
Date:	Aug 1995		^{6}Li, ^{2}H isotopes
Contributor:	M. L. Delitsky		$\nu = 0, 1$
	H. M. Pickett		
Lines Listed:	40	Q(300.0)=	48.988
Freq. (GHz) <	4939	Q(225.0)=	36.572
Max. J:	20	Q(150.0)=	24.425
LOGSTR0=	-20	Q(75.00)=	12.363
LOGSTR1=	-100	Q(37.50)=	6.352
Isotope Corr.:	-4.95	Q(18.75)=	3.359
Egy. (cm^{-1}) >	0.0	Q(9.375)=	1.885
μ_a =	5.882	A=	
μ_b =		B=	130170.89
μ_c =		C=	

The transition frequencies were taken from: Maki, Olson and Thompson, 1990, J. Mol. Spect. **144**, 257. Plummer, Herbst and DeLucia, 1984, J. Chem. Phys. **81**, 4893. E. F. Pearson and W. Gordy, 1969, Phys. Rev. **177**, 59.

The dipole moment is assumed to be the same as the parent species which was reported by L. Warton, L. P. Gold and W. Klemperer, 1960, J. Chem. Phys. **33**, 1255.

Species Tag:	9001	Name:	LiD
Version:	1		Lithium deuteride,
Date:	Aug 1995		^{7}Li, ^{2}H isotopes
Contributor:	M. L. Delitsky		$\nu = 0, 1$
	H. M. Pickett		
Lines Listed:	40	Q(300.0)=	50.812
Freq. (GHz) <	4772	Q(225.0)=	37.915
Max. J:	20	Q(150.0)=	25.314
LOGSTR0=	-20	Q(75.00)=	12.807
LOGSTR1=	-100	Q(37.50)=	6.573
Isotope Corr.:	-3.85	Q(18.75)=	3.469
Egy. (cm^{-1}) >	0.0	Q(9.375)=	1.938
μ_a =	5.882	A=	
μ_b =		B=	125538.0
μ_c =		C=	

The transition frequencies were taken from: Maki, Olson and Thompson, 1990, J. Mol. Spect. **144**, 257. Plummer, Herbst and De Lucia , 1984, J.Chem. Phys., **81**, 4893. E. F. Pearson and W. Gordy, 1969, Phys. Rev. **177**, 59.

The observed line in Plummer, *et al.* for $J = 1 \leftarrow 0$ $\nu = 0$ was a typographical error (Herbst, personal communication, 8/95). The correct 251043.53 MHz line frequency of Pearson and Gordy was used in our calculation.

The dipole moment is from L. Warton, L. P. Gold and W. Klemperer, 1960, J. Chem. Phys. **33**, 1255. It has been assumed to be the same for all isotopomers.

Species Tag:	12001	Name:	C-atom
Version:	2		^{3}P ground state
Date:	Jan. 1991		
Contributor:	H. M. Pickett		
Lines Listed:	2	Q(300.0)=	7.832
Freq. (GHz) <	810	Q(225.0)=	7.489
Max. J:	2	Q(150.0)=	6.860
LOGSTR0=	-4.5	Q(75.00)=	5.364
LOGSTR1=	-4.9	Q(37.50)=	3.543
Isotope Corr.:	0	Q(18.75)=	2.030
Egy. (cm^{-1}) >	0.0	Q(9.375)=	1.248
μ_a =		A=	
μ_b =		B=	
μ_c =		C=	

The lines of atomic carbon have been measured by Laser Magnetic Resonance (A. L. Cooksy, R. J. Saykally, J. M. Brown, and K. M. Evenson, 1980, Astrophys. J. **309**, 828). Intensities were calculated using the free electron g factor.

Species Tag:	13001	Name:	C-13-atom
Version:	2		^{13}C isotope
Date:	Jan. 1991		
Contributor:	H. M. Pickett		
Lines Listed:	7	Q(300.0)=	15.668
Freq. (GHz) <	810	Q(225.0)=	14.976
Max. J:	3	Q(150.0)=	13.721
LOGSTR0=	-15.4	Q(75.00)=	10.728
LOGSTR1=	-6.0	Q(37.50)=	7.086
Isotope Corr.:	-1.955	Q(18.75)=	4.060
Egy. (cm^{-1}) >	0.0	Q(9.375)=	2.496
μ_a =		A=	
μ_b =		B=	
μ_c =		C=	

The far-infrared lines of ^{13}C carbon have been measured by Laser Magnetic Resonance (A. L. Cooksy, R. J. Saykally, J. M. Brown, and K. M. Evenson, 1980, Astrophys. J. **309**, 828). The hyperfine intervals of G. Wolber, H. Figger, R. A. Haberstroh, and S. Peneselin, 1969, Phys. Lett. **A29**, 461, and the far-infrared lines were used for the line frequencies. Intensities were calculated using the free electron g factor.

Species Tag:	13002	Name:	CH
Version:	1		Methylidyne
Date:	Feb. 1984		X $^2\Pi$ states
Contributor:	H. M. Pickett		

Lines Listed:	324	Q(300.0)=	120.837
Freq. (GHz) <	9926	Q(225.0)=	91.369
Max. J:	12	Q(150.0)=	62.001
LOGSTR0=	-9.5	Q(75.00)=	32.923
LOGSTR1=	-6.9	Q(37.50)=	18.845
Isotope Corr.:	0.	Q(18.75)=	12.201
Egy. (cm^{-1}) >	0.0	Q(9.375)=	8.960
μ_a =	1.46	A=	
μ_b =		B=	425472.8
μ_c =		C=	

The laboratory spectra of C. R. Brazier and J. M. Brown, 1983, J. Chem. Phys. **78**, 1608–1610, and M. Bogey, C. Demuynck, and J. L. Destombes, 1983, Chem. Phys. Lett. **100**, 105-109, were combined with the data of O. E. H. Rydbeck *et al.*, 1974, Astron. Astrophys. **34**, 479, and the predictions of the rotational lines given by J. M. Brown and K. M. Evenson, 1983, Astrophys. J. **268**, L51, in a fit to a Hund's case (b) Hamiltonian with eight fine structure parameters, the B and D parameters, and seven hyperfine parameters. Calculated values are given for the rotational transition. The dipole moment was taken from D. J. Phelps and F. W. Dalby, 1966, Phys. Rev. Lett. **16**, 3.

Species Tag:	13003	Name:	CH+
Version:	1		Methylidynium
Date:	Feb. 1996		X $^1\Sigma$
Contributor:	H. M. Pickett M. L. Delitsky		
Lines Listed:	9	Q(300.0)=	15.3503
Freq. (GHz) <	7400	Q(225.0)=	11.5904
Max. J:	9	Q(150.0)=	7.8376
LOGSTR0=	-9.0	Q(75.00)=	4.0969
LOGSTR1=		Q(37.50)=	2.2449
Isotope Corr.:	0.	Q(18.75)=	1.3621
Egy. (cm^{-1}) >	0.0	Q(9.375)=	1.0418
μ_a =	1.	A=	
μ_b =		B=	417616.89
μ_c =		C=	

There are no reported pure rotational lines reported for CH$^+$. However, the electronic spectra reported by A. Carrington and D. A. Ramsay, 1982, Phys. Scripta. **25**, 272, provides adequate rotation and centrifugal distortion constants for a prediction of the rotational spectrum. The dipole used is arbitrary.

Species Tag:	14001	Name:	N-atom
Version:	1		$^4\mathrm{S}_{3/2}$ ground state
Date:	Oct. 1979		
Contributor:	H. M. Pickett		
Lines Listed:	2	Q(300.0)=	12.001
Freq. (GHz) $<$	1	Q(225.0)=	12.001
Max. J:	3	Q(150.0)=	12.001
LOGSTR0=	-12.8	Q(75.00)=	12.001
LOGSTR1=	-4.2	Q(37.50)=	12.001
Isotope Corr.:	0.	Q(18.75)=	12.001
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	12.001
μ_a =		A=	
μ_b =		B=	
μ_c =		C=	

The hyperfine transitions of atomic nitrogen at 14.6 and 26.1 MHz were obtained from J. M. Hirsch, G. H. Zimmerman, III, D. J. Larson, and N. F. Ramsey, 1977, Phys. Rev. **A16**, 484. Intensities were calculated using the experimental g_J value.

Species Tag:	14002	Name:	N-atom D-state
Version:	3		
Date:	Dec. 1989		
Contributor:	H. M. Pickett		
Lines Listed:	6	Q(300.0)=	29.512
Freq. (GHz) $<$	262	Q(225.0)=	29.349
Max. J:	3	Q(150.0)=	29.034
LOGSTR0=	-48.2	Q(75.00)=	28.151
LOGSTR1=	-48.1	Q(37.50)=	26.583
Isotope Corr.:	0.0	Q(18.75)=	24.138
Egy. (cm^{-1}) $>$	19223.0	Q(9.375)=	21.120
μ_a =		A=	
μ_b =		B=	
μ_c =		C=	

The ^{2}D$_{5/2}$ state is 19,223 cm^{-1} above the ground ^{4}S$_{3/2}$ state (C. E. Moore, 1949, Atomic Energy Levels I, National Bureau of Standards). The ^{2}D$_{3/2}$ - ^{2}D$_{5/2}$ inverted fine structure transition at 261 GHz has been measured by M. Bogey *et al.*, 1989, Astrophys. J. **339**, L49. The average spontaneous emission rate from the ^{2}D states to the ^{4}S states is 1.06×10^{-6} sec^{-1}. In contrast, the spontaneous emission rate from ^{2}D$_{3/2}$ F = 5/2 to ^{2}D$_{5/2}$ F = 7/2 is 3.15×10^{-9} sec^{-1}.

Species Tag:	15001	Name:	NH
Version:	1		Imidogen or Imin
Date:	Aug. 1997		X $^3\Sigma^-$
Contributor:	H. S. P. Müller		
Lines Listed:	91	Q(300.0)=	236.347
Freq. (GHz) <	9943	Q(225.0)=	178.699
Max. J:	91	Q(150.0)=	121.163
LOGSTR0=	-10.0	Q(75.00)=	63.845
LOGSTR1=	-10.0	Q(37.50)=	35.574
Isotope Corr.:	0.0	Q(18.75)=	22.446
Egy. (cm^{-1}) >	0.0	Q(9.375)=	18.353
μ_a =	1.389	A=	
μ_b =		B=	489959.2
μ_c =		C=	

The measurements of the $N = 1 - 0$ transition were reported by (1) Th. Klaus, S. Takano, and G. Winnewisser, 1997, Astron. Astrophys. **184**, L1. Infrared measurements by (2) P. F. Bernath and T. Amano, 1982, J. Mol. Spectr. **95**, 359 were used to determine D. Additional distortion terms have been fixed to values from (3) C. R. Brazier, R. S. Ram, and P. F. Bernath, 1986, J. Mol. Spectr. **120**, 381. The dipole moment was taken from (4) E. A. Scarl and F. W. Dalby, 1974, Can. J. Phys. **52**, 1429. Some magnetic dipole transitions have also been predicted.

Species Tag: 16001
Version: 2
Date: Mar. 1984
Contributor: H. M. Pickett

Lines Listed: 2
Freq. (GHz) < 3000
Max. J: 1
LOGSTR0= -3.5
LOGSTR1= -5.2
Isotope Corr.: 0.0
Egy. (cm^{-1}) > 0.0
μ_a =
μ_b =
μ_c =

Name: O-atom
^{3}P ground state

Q(300.0)= 6.741
Q(225.0)= 6.324
Q(150.0)= 5.770
Q(75.00)= 5.156
Q(37.50)= 5.007
Q(18.75)= 5.000
Q(9.375)= 5.000
A=
B=
C=

The 68 cm^{-1} J = 1-2 and the 158.3 cm^{-1} J = 0-1 lines of oxygen have been measured by Laser Magnetic Resonance (R. J. Saykally and K. M. Evenson, 1979, J. Chem Phys. **71**, 1564). Intensities were calculated using the free electron g factor.

Species Tag:	17001	Name:	OH
Version:	4		Hydroxyl radical
Date:	Dec. 2000		X $^2\Pi$ states
Contributor:	H. M. Pickett		

Lines Listed:	1160	Q(300.0)=	81.494
Freq. (GHz) $<$	4000	Q(225.0)=	60.296
Max. J:	50	Q(150.0)=	40.144
LOGSTR0=	-30.0	Q(75.00)=	22.754
LOGSTR1=	-35.0	Q(37.50)=	17.034
Isotope Corr.:	0.0	Q(18.75)=	16.004
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	15.929
$\mu_a =$	1.65520	A=	
$\mu_b =$		B=	556174.
$\mu_c =$		C=	

The microwave data have been reported in R. A. Beaudet and R. L. Poynter, 1978, J. Phys. Chem. Ref. Data **7**, 311. Far-infrared data are from: G. A. Blake, J. Farhoomand, and H. M. Pickett, 1986, J. Mol. Spect. **115**, 226. J. Farhoomand, G. A. Blake, and H. M. Pickett, 1985, Astrophys. J. **291**, L19. J. M. Brown *et al.*, 1986, Astrophys. J. **307**, 410.

The mid-infrared lines of B. Lemoine, M. Bogey, and J. L. Destombes, 1985, Chem. Phys. Lett. **117**, 532, were also used in the fit. The calculation involved fitting the spectra to effective parameters for the two $^2\Pi$ states using a Hund's case (b) basis, but the quanta have been converted to Hund's case (a).

The dipole moment is from K. I. Peterson, G. T. Fraser, and W. A. Klemperer, 1984, Can. J. Phys. **62**, 1502.

Species Tag:	17002	Name:	NH3
Version:	3		Ammonia
Date:	Jan. 1984		
Contributor:	R. L. Poynter		

Lines Listed:	446	Q(300.0)=	579.029
Freq. (GHz) <	9497	Q(225.0)=	378.443
Max. J:	19	Q(150.0)=	207.109
LOGSTR0=	-15.2	Q(75.00)=	74.559
LOGSTR1=	-11.0	Q(37.50)=	27.606
Isotope Corr.:	0.	Q(18.75)=	11.251
Egy. (cm^{-1}) >	0.4	Q(9.375)=	5.398
μ_a =	0	A=	B
μ_b =	0	B=	298117.06
μ_c =	1.476	C=	186726.36

The computational method and most of the microwave data are given in R. L. Poynter and R. K. Kakar, 1975, Astrophys. J. Suppl. **29**, 87. Additional microwave transitions have been reported by B. V. Shinha and P. D. P. Smith, 1980, J. Mol. Spect. **80**, 231. The rotational transitions and energy levels were taken from R. Poynter and J. S. Margolis, 1983, Mol. Phys. **48**, 401. The analysis was based on a very extensive set of accurate ν_2 measurements reported by R. Poynter and J. S. Margolis, 1984, Mol. Phys. **51**, 393, and upon a series of ‘forbidden’ transitions in the ν_4 band, reported by E. A. Cohen, W. H. Weber, R. L. Poynter, and J. S. Margolis, 1983, Mol. Phys. **50**, 727. The work of Cohen *et al.* allowed the C, D_K, H_K, and L_K constants to be determined, thus fixing the energy level scale. The J = 1 → 0, K = 0 rotational transition was taken from P. Helminger, F. C. De Lucia, and W. Gordy, 1971, J. Mol. Spect. **39**, 94. Because of the important applications of these rotational lines, the upper frequency limit has been extended to 335 cm^{-1} (9.5 THz). Hyperfine splittings have not been included.

Species Tag:	17003	Name:	CH3D
Version:	1		Mono-deutero
Date:	Feb. 1980		methane
Contributor:	R. L. Poynter		
Lines Listed:	80	Q(300.0)=	402.161
Freq. (GHz) <	2999	Q(225.0)=	315.138
Max. J:	13	Q(150.0)=	142.692
LOGSTR0=	-7.6	Q(75.00)=	51.086
LOGSTR1=	-8.5	Q(37.50)=	18.467
Isotope Corr.:	-3.824	Q(18.75)=	7.029
Egy. (cm^{-1}) >	0.0	Q(9.375)=	2.980
μ_a =	0.0056	A=	157412.
μ_b =		B=	116325.
μ_c =		C=	B

The J = 0 → 1 line has been measured by H. M. Pickett, E. A. Cohen, and T. G. Phillips, 1980, Astrophys. J. Lett. Ed. **226**, L43. Predicted lines are based on the constants given by C. Chakerian and G. Guelachvili, 1980, J. Mol. Spect. **84**, 447. The dipole moment has been measured by I. Ozier, W. Ho, and G. Birnbaum, 1969, J. Chem. Phys. **51**, 4873, and by S. C. Wofsy, J. S. Muenter, and W. Klemperer, 1970, J. Chem. Phys. **53**, 4005.

Species Tag:	17004	Name:	NH3-v2
Version:	1		NH_3 ammonia,
Date:	Mar. 1984		ν_2 vibrational state
Contributor:	R. L. Poynter		

Lines Listed:	442	Q(300.0)=	579.029
Freq. (GHz) <	11589	Q(225.0)=	378.443
Max. J:	17	Q(150.0)=	207.109
LOGSTR0=	-11.9	Q(75.00)=	74.559
LOGSTR1=	-11.6	Q(37.50)=	27.606
Isotope Corr.:		Q(18.75)=	11.251
Egy. (cm^{-1}) >	948.6	Q(9.375)=	5.398
μ_a =		A=	B
μ_b =		B=	299196.11
μ_c =	1.253	C=	183595.39

The lines for this species were derived by combination differences from the ν_2 lines reported by R. L. Poynter and J. S. Margolis, 1984, Mol. Phys. **81**, 393. Some measurements have been reported by: F. Y. Chu and S. M. Freund, 1973, J. Mol. Spect. **48**, 183. S. Urban *et al.*, 1980, J. Mol. Spect. **79**, 455. E. N. Karyakin *et al.*, 1977, J. Mol. Spect. **66**, 177. S. Urban *et al.*, 1981, J. Mol. Spect. **88**, 274.

The transition dipole moment was reported by B. J. Orr and T. Oka, 1977, J. Mol. Spect. **66**, 302.

Species Tag:	17005	Name:	OH
Version:	1		Hydroxyl radical
Date:	Dec. 2000		X $^2\Pi$ states
Contributor:	H. M. Pickett		v = 1,2

Lines Listed:	1765	Q(300.0)=	81.494
Freq. (GHz) <	3000	Q(225.0)=	60.296
Max. J:	50	Q(150.0)=	40.144
LOGSTR0=	-30.0	Q(75.00)=	22.754
LOGSTR1=	-35.0	Q(37.50)=	17.034
Isotope Corr.:	0.0	Q(18.75)=	16.004
Egy. (cm^{-1}) >	3568.5	Q(9.375)=	15.929
μ_a =	1.66257, 1.6648	A=	
μ_b =		B=	534348.
μ_c =		C=	

The microwave data have been reported by T. Thissen, H. Spiecker, and P. Andresen, 1999, J. Mol. Spect. **200**, 277 and J. A Coxon, K. V. L. N. Sastry, J. A. Austin, and D. H. Levy, 1979, Can. J. Phys., **57**, 619. Infrared data for v = 1 are from T. Amano, 1984, J. Mol. Spect. **103**, 436. For v = 2, term values up to N = 7 from J. A. Coxon, 1980, Can. J. Phys. **58**, 993 were used as synthetic data with an uncertainty of 150 MHz. For both vibrational states, H was fixed to the values given in Coxon, 1980.

The calculation involved fitting the spectra along with v=0 data (see species 17001) to effective parameters for the $^2\Pi$ states using a Hund's case (b) basis, but the quanta have been converted to Hund's case (a).

The dipole moments are from K. I. Peterson, G. T. Fraser, and W. A. Klemperer, 1984, Can. J. Phys. **62**, 1502.

Species Tag:	18001	Name:	OD
Version:	1		Hydroxyl radical,
Date:	May 1983		X $^2\Pi$ states
Contributor:	H. M. Pickett		deuterium isotope
Lines Listed:	912	Q(300.0)=	212.422
Freq. (GHz) <	9926	Q(225.0)=	153.391
Max. J:	17	Q(150.0)=	97.477
LOGSTR0=	-10.3	Q(75.00)=	48.967
LOGSTR1=	-10.3	Q(37.50)=	30.896
Isotope Corr.:	-3.824	Q(18.75)=	25.021
Egy. (cm^{-1}) >	0.0	Q(9.375)=	24.010
μ_a =	1.653	A=	
μ_b =		B=	296312.
μ_c =		C=	

The microwave data have been reported in R. A. Beaudet and R. L. Poynter, 1978, J. Phys. Chem. Ref. Data **7**, 311. Additional data have been reported in J. M. Brown and J. E. Schubert, 1982, J. Mol. Spect. **95**, 194. Predictions of the rotational lines were included in the fit. The calculation involved fitting the spectra to effective parameters for the two $^2\Pi$ states.

Species Tag:	18002	Name:	N-15-H3
Version:	2		Ammonia,
Date:	Jan. 1981		^{15}N isotope
Contributor:	R. L. Poynter		

Lines Listed:	235	Q(300.0)=	575.837
Freq. (GHz) <	2992	Q(225.0)=	451.232
Max. J:	20	Q(150.0)=	206.205
LOGSTR0=	-16.4	Q(75.00)=	74.714
LOGSTR1=	-11.8	Q(37.50)=	27.669
Isotope Corr.:	-2.432	Q(18.75)=	11.277
Egy. (cm^{-1}) >	0.4	Q(9.375)=	5.415
μ_a =		A=	B
μ_b =		B=	297390.8
μ_c =	1.476	C=	186711.

The same computational method was used here as for $^{14}NH_3$. These lines are based upon the precision molecular beam measurements by S. G. Kukolich, 1967, Phys. Rev. **156**, 83, and 1968, Phys. Rev. **172**, 59, and upon the most recent microwave measurements of H. Sasada, 1980, J. Mol. Spect. **83**, 15. The energy levels were computed from the recent far-infrared measurements of M. Carlotti, A. Trombetti, B. Velino, and J. Vrbanchich, 1980, J. Mol. Spect. **83**, 401. The C rotational constant was assumed to be the same as for $^{14}NH_3$. The dipole moment was assumed to be the same as for $^{14}NH_3$.

Species Tag:	18003	Name:	H2O
Version:	5		Water
Date:	Nov. 1999		
Contributor:	J. C. Pearson H. M. Pickett		
Lines Listed:	3086	Q(300.0)=	178.115
Freq. (GHz) $<$	29800	Q(225.0)=	116.011
Max. J:	23	Q(150.0)=	63.680
LOGSTR0=	-26.7	Q(75.00)=	23.169
LOGSTR1=	-26.7	Q(37.50)=	8.580
Isotope Corr.:	0.0	Q(18.75)=	3.033
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	1.257
μ_a =		A=	835840.3
μ_b =	1.84718	B=	435351.7
μ_c =		C=	278138.7

The data set used in this fit includes all the micorowave measurements reviewed in J. C. Pearson, T. Anderson, E. Herbst, F. C. De Lucia and P. Helminger, 1991, Astrophys J. **379**, L41, additional measurements were used from J. C. Pearson, 1995, Ph.D. Thesis Duke University, S. Belov, 1996, Private Communication, F. Matsushima, H. Odashima, T. Iwasaki, S. Tsunekawa, K. Takagi, 1995, J. Mol. Struct. **352-353**, 371, and P. Chen, J. C. Pearson, S. Matsuura, G. A. Blake and H. M. Pickett, 1999, Astrophys. J., In Press. FTIR rotational data was taken from J. Kauppinen, T. Karkkainen and E. Kyro, 1978, J. Mol. Spectrosc. **71**, 15, J. W. C. Johns, 1985, J. Opt. Soc. Am. **B2**, 1340, R. Paso and V. M. Hornman, 1995, J. Opt. Soc. Am. **B12**, 1813 and R. A. Toth, 1999, Private Communication, FTIR band transitions were taken from R. A. Toth, 1999, Private Communication and Energy Levels taken from R. A. Toth, 1998, J. Mol. Spectrosc. **190**, 379 and O. L. Polyansky, N. Zobov, S. Viti, J. Tennyson, P. Bernath and L. Wallace, 1997, J. Mol. Spectrosc. **186**, 422. All the data was forced into the fit and a reduced RMS of 1.9 was obtained for a combined fit of the ground and ν_2 data. This represents the ground state version only. It should be noted that there is minimal data at the highest J values. The quoted errors are expected to be about $1/2\sigma$. The fitting method is described in P. Chen *et al.*.

The intensities were calculated using the method in C. Camy-Peyret *et al.*, 1985, J. Mol. Spectrosc. **113**, 208. A value of 1.84718 Debye was used along with corrections for the planarity conditions. This agrees will with observed IR intensities up to $\Delta K_a = 3$ transitions. Higher order planarity terms are needed for agreement with $\Delta K_a = 5, 7, 9...$ transitions. The partition function includes the ν_2 state. Classical corrections for higher temperatures are given in P. Chen *et al.*.

Species Tag:	18004	Name:	NH2D
Version:	1		Mono-deutero
Date:	Jan. 1981		ammonia
Contributor:	H. M. Pickett		
Lines Listed:	5036	Q(300.0)=	3790.531
Freq. (GHz) <	3000	Q(225.0)=	2408.795
Max. J:	14	Q(150.0)=	1293.302
LOGSTR0=	-10.0	Q(75.00)=	434.310
LOGSTR1=	-12.0	Q(37.50)=	136.993
Isotope Corr.:	-3.347	Q(18.75)=	40.439
Egy. (cm^{-1}) >	0.0	Q(9.375)=	13.240
μ_a =	-0.18	A=	290125.
μ_b =		B=	192194.
μ_c =	1.463	C=	140795.

The experimental lines were measured by F. C. DeLucia and P. Helminger, 1975, J. Mol. Spect. **54**, 200, and by E. A. Cohen and H. M. Pickett, 1982, J. Mol. Spect. **93**, 83. The dipole moments and quadrupole splitting were also determined by Cohen and Pickett. The Hamiltonian included terms up to the 8th power in angular momentum, as well as a $P_aP_c + P_cP_a$ interaction term. The relative sign of the dipoles is determinable and is important for intensities because of mixing by the interaction term.

Species Tag:	18005	Name:	H2O-v2
Version:	3		Water,
Date:	Nov. 1999		(010) bending state
Contributor:	J. C. Pearson H. M. Pickett		
Lines Listed:	2847	Q(300.0)=	178.115
Freq. (GHz) <	29800	Q(225.0)=	116.011
Max. J:	23	Q(150.0)=	63.680
LOGSTR0=	-31.2	Q(75.00)=	23.169
LOGSTR1=	-31.2	Q(37.50)=	8.580
Isotope Corr.:	0.	Q(18.75)=	3.033
Egy. (cm^{-1}) >	1594.8	Q(9.375)=	1.257
μ_a =		A=	993052
μ_b =	1.81552	B=	440318.
μ_c =		C=	273710.

The data set used in this fit includes all the micorowave measurements reviewed in J. C. Pearson, T. Anderson, E. Herbst, F. C. De Lucia and P. Helminger, 1991, Astrophys. J. **379**, L41, additional measurements were used from J. C. Pearson, 1995, Ph.D. Thesis Duke University, S. Belov, 1996, Private Communication, F. Matsushima, H. Odashima, T. Iwasaki, S. Tsunekawa, K. Takagi, 1995, J. Mol. Struct. **352-353**, 371, and P. Chen, J. C. Pearson, S. Matsuura, G. A. Blake and H. M. Pickett, 1999, Astrophys. J., In Press. FTIR rotational data was taken from J. Kauppinen, T. Karkkainen and E. Kyro, 1978, J. Mol. Spectrosc. **71**, 15, J. W. C. Johns, 1985, J. Opt. Soc. Am. **B2**, 1340, R. Paso and V. M. Hornman, 1995, J. Opt. Soc. Am. **B12**, 1813 and R. A. Toth, 1999, Private Communication, FTIR band transitions were taken from R. A. Toth, 1999, Private Communication and Energy Levels taken from R. A. Toth, 1998, J. Mol. Spectrosc. **190**, 379 and O. L. Polyansky, N. Zobov, S. Viti, J. Tennyson, P. Bernath and L. Wallace, 1997, J. Mol. Spectrosc. **186**, 422. All the data was forced into the fit and a reduced RMS of 1.9 was obtained for a combined fit of the ground and ν_2 data. This represents the ν_2 state version only. It should be noted that there is minimal data at the highest J values. The quoted errors are expected to be about $1/2\sigma$ The fitting method is described in P. Chen *et al.*.

The intensities were calculated using the method in C. Camy-Peyret *et al.*, 1985, J. Mol. Spectrosc. **113**, 208. A value of 1.81552 Debye was used along with corrections for the planarity conditions. This agrees will with observed IR intensities up to $\Delta K_a = 3$ transitions. Higher order planarity terms are needed for agreement with $\Delta K_a = 5, 7, 9...$ transitions. The partition function includes the ν_2 state. Classical corrections for higher temperatures are given in P. Chen *et al.*.

Species Tag:	19001	Name:	HO-18
Version:	2		Hydroxyl radical,
Date:	May 1983		X $^{\Pi}$ states
Contributor:	H. M. Pickett		^{18}O isotope

Lines Listed:	295	Q(300.0)=	81.941
Freq. (GHz) $<$	9839	Q(225.0)=	60.618
Max. J:	14	Q(150.0)=	40.327
LOGSTR0=	-9.9	Q(75.00)=	22.824
LOGSTR1=	-9.6	Q(37.50)=	17.053
Isotope Corr.:	-2.690	Q(18.75)=	16.007
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	15.929
μ_a =	1.667	A=	
μ_b =		B=	552470.
μ_c =		C=	

The microwave data have been reported in R. A. Beaudet and R. L. Poynter, 1978, J. Phys. Chem. Ref. Data **7**, 311. The fit involved constraining the constants by isotope relations to the mean of those for OH and OD, since only Λ doubling data are available. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	19002	Name:	HDO
Version:	3		Water,
Date:	Oct. 1989		singly deuterated
Contributor:	H. M. Pickett		

Lines Listed:	1401	Q(300.0)=	146.859
Freq. (GHz) <	9995	Q(225.0)=	95.565
Max. J:	17	Q(150.0)=	52.300
LOGSTR0=	-12.8	Q(75.00)=	18.850
LOGSTR1=	-11.3	Q(37.50)=	6.952
Isotope Corr.:	-3.523	Q(18.75)=	2.711
Egy. (cm^{-1}) >	0.0	Q(9.375)=	1.334
μ_a =	0.657	A=	701931.5
μ_b =	1.732	B=	272912.6
μ_c =	0.	C=	192055.2

The far-infrared lines used in this fit are from J. W. C. Johns, 1985, J. Opt. Soc. Am. B Opt. Phys. **2**, 1340. Microwave lines are from J. K. Messer *et al.*, 1984, J. Mol. Spect. **105**, 139.

Species Tag:	19003	Name:	H2O-17
Version:	1		Water,
Date:	Jan. 1988		^{17}O isotope
Contributor:	E. A. Cohen R. L. Poynter		
Lines Listed:	404	Q(300.0)=	178.813
Freq. (GHz) <	9975	Q(225.0)=	116.520
Max. J:	12	Q(150.0)=	63.959
LOGSTR0=	-6.8	Q(75.00)=	23.270
LOGSTR1=	-8.0	Q(37.50)=	8.616
Isotope Corr.:	-3.432	Q(18.75)=	3.044
Egy. (cm^{-1}) >	0.0	Q(9.375)=	1.259
$\mu_a =$		A=	830283.294
$\mu_b =$	1.8546	B=	435350.957
$\mu_c =$		C=	277511.176

The microwave and millimeter line measurements were taken from F. C. De Lucia and P. Helminger, 1975, J. Mol. Spect. **56**, 138, and G. Steenbeckeliers and J. Bellet, 1971, Compt. Rend. Acad. Sci. **273B**, 471. Combination-differences from new high-resolution infrared measurements of R. A. Toth, private communication, were used in a combined fit with the microwave data. The data set has been truncated at $J = 12$. The dipole moment was assumed to be the same as for the parent molecular species. Splittings due to the ^{17}O nucleus are not included in this calculation.

Species Tag:	19004	Name:	H_3O^+
Version:	1		Hydronium ion,
Date:	Jan. 1996		$\nu_2 = 0, 1$
Contributor:	H. M. Pickett		
	M. L. Delitsky		
Lines Listed:	420	Q(300.0)=	523.7663
Freq. (GHz) <	9999	Q(225.0)=	329.2979
Max. J:	16	Q(150.0)=	175.2980
LOGSTR0=	-10.0	Q(75.00)=	62.9188
LOGSTR1=	-10.0	Q(37.50)=	26.7436
Isotope Corr.:	0.0	Q(18.75)=	15.8847
Egy. (cm^{-1}) >	0.0	Q(9.375)=	11.5358
μ_a =		A=	337388.49
μ_b =		B=	A
μ_c =	1.44	C=	181374.00

The two inversion states of the ground state and the $\nu_2 = 1$ state are included in this calculation. The vibrational designation 0, 1, 2, and 3 are the 0^+, 0^-, 1^+, and 1^- states of ν_2, respectively. The values of C and D_K cannot be determined and are fixed to those of M. Gruebele, M. Polak, and R. J. Sakally, 1987, J. Chem. Phys. **87**, 3347. The experimental measurements were reported by D. J. Liu and T. Oka, 1985, Phys. Rev. Lett. **54**, 1787; D. J. Liu, N. N. Haese, and T. Oka, 1985, J. Chem. Phys. **82**, 5368; M. Bogey, C. Demuynck, M. Denis, and J. L. Destombes, 1985, Astron. Astrophys. **148**, L11; G. M. Plummer, E. Herbst, and F. C. DeLucia, 1985, J. Chem. Phys. **83**, 1428.

The dipole moment was calculated by P. Botschwina, P. Rosmus, and E. A. Reinsch, 1984, Chem. Phys. Lett. **102**, 299. The dipoles used are $\mu_{01} = 1.44$D, $\mu_{12} = 0.673$D, $\mu_{03} = 0.302$D, and $\mu_{23} = 1.10$D.

Species Tag:	20001	Name:	D2O
Version:	2		Water,
Date:	Dec. 1989		doubly deuterated
Contributor:	H. M. Pickett R. L. Poynter		
Lines Listed:	1137	Q(300.0)=	1044.720
Freq. (GHz) <	9998	Q(225.0)=	679.517
Max. J:	18	Q(150.0)=	371.193
LOGSTR0=	-9.3	Q(75.00)=	133.107
LOGSTR1=	-11.5	Q(37.50)=	48.562
Isotope Corr.:	-7.648	Q(18.75)=	18.557
Egy. (cm^{-1}) >	0.0	Q(9.375)=	8.644
μ_a =		A=	462278.8
μ_b =	1.8545	B=	218038.4
μ_c =		C=	145258.0

The far-infrared data used in this fit are from J. W. C. Johns, 1985, J. Opt. Soc. Am. B Opt. Phys. **2**, 1340.

The dipole moment is from T. R. Dyke and J. S. Muenter, 1973, J. Chem. Phys. **59**, 3125.

The microwave and submillimeter lines are from: J. Bellet and G. Steenbeckeliers, 1970, Compt. Rend. Acad. Sci. **271B**, 1208. W. S. Benedict *et al.*, 1970, J. Chem. Phys. **53**, 2565. H. Bluyssen, 1978, Thesis, Nijmegen. G. Eriandsson and J. Cox, 1956, J. Chem. Phys. **25**, 778. C. K. Jen, D. R. Bianco, and J. T. Massey, 1953, J. Chem. Phys. **21**, 520. J. K. Messer, F. C. De Lucia, and P. Helminger, 1984, J. Mol. Spect. **105**, 139. G. Steenbeckeliers and J. Bellet, 1970, Compt. Rend. Acad. Sci. **270B**,1039. G. Steenbeckeliers and J. Bellet, 1970, J. Mol. Spect. **45**,10. D. A. Stephenson and R. G. Strauch, 1970, J. Mol. Spect. **35**, 494. J. Verhoeven, H. Bluyssen, and A. Dymanus, 1968, Phys. Letters **26A**, 424.

Species Tag:	20002	Name:	HF
Version:	1		Hydrogen fluoride
Date:	June 1989		
Contributor:	H. M. Pickett		

Lines Listed:	8	Q(300.0)=	10.503
Freq. (GHz) <	9733	Q(225.0)=	7.960
Max. J:	8	Q(150.0)=	5.424
LOGSTR0=	0.5	Q(75.00)=	2.899
LOGSTR1=	-2.5	Q(37.50)=	1.664
Isotope Corr.:	0.0	Q(18.75)=	1.128
Egy. (cm^{-1}) >	0.0	Q(9.375)=	1.006
$\mu_a =$	1.826526	A=	
$\mu_b =$		B=	616365.
$\mu_c =$		C=	

The experimental measurements were reported by I. G. Nolt *et al.*, 1987, J. Mol. Spect. **125**, 274. The dipole moment was measured by J. S. Muenter and W. Klemperer, 1970, J. Chem. Phys. **52**, 6033.

Species Tag:	20003	Name:	H2O-18
Version:	1		Water,
Date:	Dec. 1988		^{18}O isotope
Contributor:	R. L. Poynter		

Lines Listed:	726	Q(300.0)=	179.639
Freq. (GHz) <	9996	Q(225.0)=	117.004
Max. J:	16	Q(150.0)=	64.210
LOGSTR0=	-9.4	Q(75.00)=	23.361
LOGSTR1=	-8.0	Q(37.50)=	8.648
Isotope Corr.:	-2.690	Q(18.75)=	3.054
Egy. (cm^{-1}) >	0.0	Q(9.375)=	1.260
μ_a =		A=	825367.80
μ_b =	1.8546	B=	435354.05
μ_c =		C=	276951.05

The microwave and submillimeter line measurements have been taken from F. C. De Lucia *et al.*, 1972, Phys. Rev. A **6**, 1324. Far-infrared line measurements have been taken from J. W. C. Johns, 1985, J. Opt. Soc. Am. B Opt. Phys. **2**, 1340. Infrared line measurements have been taken from G. Guelachvili, 1983, J. Opt. Soc. Am. **73**, 137, and from R. A. Toth, private communication. The dipole moment was assumed to be the same as for the parent molecular species.

Species Tag:	21001	Name:	HDO-18
Version:	1		Water,
Date:	Jan. 1991		singly deuterated ^{18}O
Contributor:	E. A. Cohen		isotope

Lines Listed:	952	Q(300.0)=	148.730
Freq. (GHz) <	9981	Q(225.0)=	96.783
Max. J:	13	Q(150.0)=	52.954
LOGSTR0=	-8.9	Q(75.00)=	19.081
LOGSTR1=	-8.8	Q(37.50)=	7.034
Isotope Corr.:	-6.2130	Q(18.75)=	2.740
Egy. (cm^{-1}) >	0.0	Q(9.375)=	1.341
μ_a =	0.6715	A=	692844.04
μ_b =	1.7261	B=	271457.501
μ_c =		C=	190812.982

We have used G. Steenbeckeliers' microwave data as compiled by F. J. Lovas, 1978, J. Phys. Chem. Ref. Data **7**, 1445. These data have been combined with energy levels derived by R. A. Toth, private communication, from new high-resolution infrared spectra to produce the fit upon which the calculation is based. The dipole moment components were estimated from those of HDO.

Species Tag:	21002	Name:	DF
Version:	1		Deuterium fluoride
Date:	Jan. 1991		
Contributor:	E. A. Cohen		

Lines Listed:	20	Q(300.0)=	19.575
Freq. (GHz) <	12474	Q(225.0)=	14.760
Max. J:	20	Q(150.0)=	9.949
LOGSTR0=	-9	Q(75.00)=	5.150
LOGSTR1=	-9	Q(37.50)=	2.764
Isotope Corr.:	-3.824	Q(18.75)=	1.601
Egy. (cm^{-1}) >	0.0	Q(9.375)=	1.107
μ_a =	1.818805	A=	
μ_b =		B=	325584.862
μ_c =		C=	

The dipole moment was measured by J. S. Muenter and W. Klemperer, 1970, J. Chem. Phys. **52**, 6033. The molecular parameters are derived from a fit to far-infrared and infrared data supplied by J. A. Coxon (personal communication) and from the submillimeter measurement of P. Helminger *et al.*, 1970, Phys. Rev. Lett. **25**, 1397. See also J. A. Coxon and P. G. Hajigeorgiou, 1990, J. Mol. Spect. **142**, 254, and J. A. Coxon and J. F. Oglvie, 1989, Can. J. Phys. **34**, 137.

Species Tag:	25001	Name:	CCH
Version:	1		Ethynyl, X $^2\Sigma$
Date:	Mar. 1983		
Contributor:	H. M. Pickett		
Lines Listed:	114	Q(300.0)=	574.249
Freq. (GHz) <	2351	Q(225.0)=	430.923
Max. J:	28	Q(150.0)=	287.674
LOGSTR0=	-5.0	Q(75.00)=	144.477
LOGSTR1=	-4.0	Q(37.50)=	72.912
Isotope Corr.:	0	Q(18.75)=	37.145
Egy. (cm^{-1}) >	0.0	Q(9.375)=	19.284
μ_a =	0.8	A=	
μ_b =		B=	43674.534
μ_c =		C=	

The spectral data and Hamiltonian are from C. A. Gottlieb, E. W. Gottlieb, and P. Thaddeus, 1983, Astrophys. J. **264**, 740–745. The dipole moment is an assumed value.

Species Tag:	25002	Name:	NaH
Version:	1		Sodium hydride,
Date:	Aug 1995		$\nu = 0, 1$
Contributor:	M. L. Delitsky H. M. Pickett		
Lines Listed:	52	Q(300.0)=	43.920
Freq. (GHz) $<$	7073	Q(225.0)=	32.851
Max. J:	27	Q(150.0)=	21.965
LOGSTR0=	-20	Q(75.00)=	11.137
LOGSTR1=	-100	Q(37.50)=	5.741
Isotope Corr.:	0.0	Q(18.75)=	3.056
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	1.739
μ_a =	6.7	A=	
μ_b =		B=	144952.4
μ_c =		C=	

The rotational line frequencies were taken from: Leopold, Zink, Evenson, and Jennings, 1987, J. Mol. Spect. **122**, 150, and Sastry, Herbst and Delucia, 1981, Astrophys. J. **248**, L53.

The IR line frequencies used in the analysis are from: Maki and Olson, 1989, J. Chem. Phys. **90**, 6887, and Magg and Jones, 1988, Chem. Phys. Lett.**146**, 415.

The dipole moment was taken from : E. S. Sachs, J. Hinze and N. H. Switalski, 1975, J. Chem. Phys. **62**, 3367.

Species Tag:	26001	Name:	CN
Version:	2		Cyanide radical, X $^2\Sigma^+$
Date:	Jan. 1996		$v = 0, 1$
Contributor:	H. S. P. Müller		^{12}C isotope

Lines Listed:	511 / 363	Q(300.0)=	664.0906
Freq. (GHz) <	4000	Q(225.0)=	498.4499
Max. J:	35	Q(150.0)=	332.9077
LOGSTR0=	-8.0 / -10.0	Q(75.00)=	167.4335
LOGSTR1=	-8.0 / -10.0	Q(37.50)=	84.7308
Isotope Corr.:	-0.006	Q(18.75)=	43.4081
Egy. (cm^{-1}) >	0.0 / 2042.4	Q(9.375)=	22.7963
μ_a =	1.45	A=	
μ_b =		B=	56693.47 / 56171.10
μ_c =		C=	

The data are from D. D. Skatrud F. C. De Lucia, G. A. Blake, and K. V. L. N. Sastry, 1983, J. Mol. Spect. **99**, 35 and E. Klisch, Th. Klaus, S. P. Belov, G. Winnewisser, and E. Herbst, 1995, Astron. Astrophys., 304, L5.

The data were used in a combined fit of all four observed vibrational states.

The dipole moment was taken from R. Thomson and F. W. Dalby, 1968, Can. J. Phys. **46**, 53. It was assumed to be the same for all vibrational states.

Species Tag:	27001	Name:	HCN
Version:	2		Hydrogen cyanide
Date:	Jan. 1984		
Contributor:	R. L. Poynter		
Lines Listed:	40	Q(300.0)=	424.326
Freq. (GHz) <	2913	Q(225.0)=	318.493
Max. J:	33	Q(150.0)=	212.618
LOGSTR0=	-3.8	Q(75.00)=	106.807
LOGSTR1=	-3.4	Q(37.50)=	53.914
Isotope Corr.:	0.0	Q(18.75)=	27.473
Egy. (cm^{-1}) >	0	Q(9.375)=	14.272
μ_a =	2.984	A=	
μ_b =		B=	44315.975
μ_c =		C=	

The observed transitions are from F. C. De Lucia and W. Gordy, 1969, Phys. Rev. **187**, 58, and from F. C. Van den Heuvel, W. L. Meerts, and A. Dymanus, 1982, Chem. Phys. Lett. **92**, 215. The dipole moment is from G. Tomasevich, 1970, Thesis, Harvard University.

Species Tag:	27002	Name:	HNC
Version:	2		Hydrogen isocyanide
Date:	Feb. 1995		
Contributor:	M. L. Delitsky		
	H. M. Pickett		
Lines Listed:	49	Q(300.0)=	138.311
Freq. (GHz) <	4395.	Q(225.0)=	103.801
Max. J:	49	Q(150.0)=	69.301
LOGSTR0=	-5.0	Q(75.00)=	34.814
LOGSTR1=	-100	Q(37.50)=	17.575
Isotope Corr.:	0	Q(18.75)=	8.960
Egy. (cm^{-1}) >	0.0	Q(9.375)=	4.659
μ_a =	3.05	A=	
μ_b =		B=	45331.99
μ_c =		C=	

The observed lines are from T. Okabayashi and M. Tanimoto, 1993, J. Chem. Phys., **99**, 3268.

The dipole moment is from G. L. Blackman, *et al.*, 1976, Nature, **261**, 395.

Species Tag:	27003	Name:	HCN-v2
Version:	1		Hydrogen cyanide,
Date:	Aug. 1991		$\nu_2 = 1$ state
Contributor:	E. A. Cohen		

Lines Listed:	132	Q(300.0)=	141.442
Freq. (GHz) <	4322	Q(225.0)=	106.164
Max. J:	49	Q(150.0)=	70.873
LOGSTR0=	-8.7	Q(75.00)=	35.602
LOGSTR1=	-8.7	Q(37.50)=	17.971
Isotope Corr.:	0.0	Q(18.75)=	9.158
Egy. (cm^{-1}) >	716.5	Q(9.375)=	4.757
μ_a =	2.942	A=	
μ_b =		B=	44422.616
μ_c =		C=	

The microwave data have been taken from a compilation by A. G. Maki, 1974, J. Phys. Chem. Ref. Data **3,** 221. Combination differences up to $J' = 22$ are included in the fit. These have been derived from the high-resolution FTIR spectrum of the ν_2 band reported by J. Hietanen *et al.*, 1988, J. Mol. Spect. **127**, 272. Hyperfine structure is not given for this state in the catalog. The partition function used in the calculation reflects this.

Species Tag:	27004	Name:	C-13-N
Version:	1		Cyanide radical, X $^2\Sigma^+$
Date:	Jan. 1996		^{13}C isotope
Contributor:	H. S. P. Müller		

Lines Listed:	1218	Q(300.0)=	1385.2788
Freq. (GHz) <	2500	Q(225.0)=	1039.7457
Max. J:	23	Q(150.0)=	694.3442
LOGSTR0=	-8.0	Q(75.00)=	349.0809
LOGSTR1=	-8.0	Q(37.50)=	176.5182
Isotope Corr.:	-1.957	Q(18.75)=	90.2909
Egy. (cm^{-1}) >	0.0	Q(9.375)=	47.2688
μ_a =	1.45	A=	
μ_b =		B=	54343.14
μ_c =		C=	

The data were taken from and have been fit according to M. Bogey, C. Demuynck, and J. L. Destombes, 1984, Can. J. Phys. **62**, 1248.

The dipole moment was assumed to be the same as that of the ^{12}CN isotopomer; its value was taken from R. Thomson and F. W. Dalby, 1968, Can. J. Phys. **46**, 53.

Species Tag:	28001	Name:	CO
Version:	4		Carbon monoxide
Date:	Aug. 1997		
Contributor:	H. S. P. Müller		

Lines Listed:	91	Q(300.0)=	108.865
Freq. (GHz) <	9943	Q(225.0)=	81.718
Max. J:	91	Q(150.0)=	54.581
LOGSTR0=	-36.5	Q(75.00)=	27.455
LOGSTR1=	-36.5	Q(37.50)=	13.897
Isotope Corr.:	0.0	Q(18.75)=	7.122
Egy. (cm^{-1}) >	0.0	Q(9.375)=	3.744
μ_a =	0.11011	A=	
μ_b =		B=	57635.968
μ_c =		C=	

The experimental measurements were reported by (1) G. Winnewisser,S. P. Belov, Th. Klaus, and R. Schieder, 1997, J. Mol. Spect. **184**, . The dipole moment and dipole centrifugal corrections are taken from (2) D. Goorvitch, 1994, Astrophys. J. Suppl. **95**, 535.

Species Tag:	28002	Name:	HC-13-N
Version:	1		Hydrogen cyanide,
Date:	Dec. 1979		^{13}C isotope
Contributor:	R. L. Poynter		
Lines Listed:	45	Q(300.0)=	435.412
Freq. (GHz) <	2923	Q(225.0)=	326.964
Max. J:	34	Q(150.0)=	218.273
LOGSTR0=	-3.9	Q(75.00)=	109.623
LOGSTR1=	-3.4	Q(37.50)=	55.310
Isotope Corr.:	-1.955	Q(18.75)=	28.171
Egy. (cm^{-1}) >	0.0	Q(9.375)=	14.622
μ_a =	2.984	A=	
μ_b =		B=	43170.137
μ_c =		C=	

The measured lines are from E. F. Pearson, R. A. Creswell, M. Winnewisser, and G. Winnewisser, 1976, Z. Naturforsch. **31a**, 1394. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	28003	Name:	HCN-15
Version:	1		Hydrogen cyanide,
Date:	Dec. 1979		^{15}N isotope
Contributor:	R. L. Poynter		
Lines Listed:	35	Q(300.0)=	145.680
Freq. (GHz) <	2998	Q(225.0)=	109.345
Max. J:	35	Q(150.0)=	72.996
LOGSTR0=	-2.5	Q(75.00)=	36.661
LOGSTR1=	-3.5	Q(37.50)=	18.497
Isotope Corr.:	-2.432	Q(18.75)=	9.421
Egy. (cm^{-1}) >	0.0	Q(9.375)=	4.889
μ_a =	2.984	A=	
μ_b =		B=	43027.69
μ_c =		C=	

The measured lines are from E. F. Pearson, R. A. Creswell, M. Winnewisser, and G. Winnewisser, 1976, Z. Naturforsch. **31a**, 1394. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	28004	Name:	DCN
Version:	1		Hydrogen cyanide, deuterium isotope
Date:	Dec. 1979		
Contributor:	R. L. Poynter		
Lines Listed:	54	Q(300.0)=	518.920
Freq. (GHz) <	2954	Q(225.0)=	389.583
Max. J:	41	Q(150.0)=	260.016
LOGSTR0=	-4.1	Q(75.00)=	130.497
LOGSTR1=	-4.1	Q(37.50)=	65.751
Isotope Corr.:	-3.824	Q(18.75)=	33.389
Egy. (cm^{-1}) >	0.0	Q(9.375)=	17.223
μ_a =	2.984	A=	
μ_b =		B=	36207.46
μ_c =		C=	

The observed transitions are from F. C. De Lucia and W. Gordy, 1969, Phys. Rev. **187**, 58. The dipole moment is from G. Tomasevich, 1970, Thesis, Harvard University.

Species Tag:	28005	Name:	HNC-13
Version:	1		Hydrogen isocyanide, ^{13}C isotope
Date:	Dec. 1979		
Contributor:	R. L. Poynter		
Lines Listed:	34	Q(300.0)=	143.880
Freq. (GHz) <	2946	Q(225.0)=	108.044
Max. J:	34	Q(150.0)=	72.127
LOGSTR0=	-2.6	Q(75.00)=	36.224
LOGSTR1=	-3.5	Q(37.50)=	18.281
Isotope Corr.:	-1.955	Q(18.75)=	9.313
Egy. (cm^{-1}) >	0.0	Q(9.375)=	4.835
$\mu_a =$	2.699	A=	
$\mu_b =$		B=	43545.61
$\mu_c =$		C=	

The observed lines are from R. A. Creswell, E. F. Pearson, M. Winnewisser, and G. Winnewisser, 1976, Z. Naturforsch. **31a**, 221, and E. F. Pearson, R. A. Creswell, M. Winnewisser, and G. Winnewisser, 1976, Z. Naturforsch. **31a**, 1394.

Species Tag:	28006	Name:	HN-15-C
Version:	1		Hydrogen isocyanide,
Date:	Dec. 1979		^{15}N isotope
Contributor:	R. L. Poynter		
Lines Listed:	33	Q(300.0)=	141.059
Freq. (GHz) <	2919	Q(225.0)=	105.901
Max. J:	33	Q(150.0)=	70.697
LOGSTR0=	-2.6	Q(75.00)=	35.514
LOGSTR1=	-3.3	Q(37.50)=	17.923
Isotope Corr.:	-2.432	Q(18.75)=	9.135
Egy. (cm^{-1}) >	0.0	Q(9.375)=	4.746
μ_a =	2.699	A=	
μ_b =		B=	44433.04
μ_c =		C=	

The observed lines are from R. A. Creswell, E. F. Pearson, M. Winnewisser, and G. Winnewisser, 1976, Z. Naturforsch. **31a**, 221, and E. F. Pearson, R. A. Creswell, M. Winnewisser, and G. Winnewisser, 1976, Z. Naturforsch. **31a**, 1394.

Species Tag:	28007	Name:	DNC
Version:	2		Hydrogen isocyanide, deuterium isotope
Date:	Feb. 1995		
Contributor:	M. L. Delitsky H. M. Pickett		
Lines Listed:	53	Q(300.0)=	164.271
Freq. (GHz) <	4002	Q(225.0)=	123.268
Max. J:	53	Q(150.0)=	82.278
LOGSTR0=	-5.0	Q(75.00)=	41.301
LOGSTR1=	-100	Q(37.50)=	20.818
Isotope Corr.:	-3.824	Q(18.75)=	10.580
Egy. (cm^{-1}) >	0.0	Q(9.375)=	5.466
μ_a =	3.050	A=	
μ_b =		B=	38152.998
μ_c =		C=	

The observed lines are from T. Okabayashi and M. Tanimoto, 1993, J. Chem. Phys. **99**, 3268.

The dipole moment is from G. L. Blackman *et al.*, 1976, Nature **261**, 395.

Species Tag:	28008	Name:	HCNH+
Version:	1		Amidogen ion, protonated HCN
Date:	Dec. 1995		
Contributor:	M. L. Delitsky		
Lines Listed:	74	Q(300.0)=	169.0989
Freq. (GHz) <	5406	Q(225.0)=	126.8938
Max. J:	74	Q(150.0)=	84.6981
LOGSTR0=	-100.0	Q(75.00)=	42.5123
LOGSTR1=	-100.0	Q(37.50)=	21.4241
Isotope Corr.:	0.0	Q(18.75)=	10.8833
Egy. (cm^{-1}) >	0.0	Q(9.375)=	5.6181
$\mu_a =$	0.3	A=	
$\mu_b =$		B=	37055.7526
$\mu_c =$		C=	

The experimental frequency measurements and dipole moment were taken from M. Bogey, C. Demuynck, and J. L. Destombes, 1985, J. Chem. Phys. **83**, 3703. Other calculations for dipole moments are mentioned in T. J. Lee and H. F. Schaefer, 1984, J. Chem. Phys. **80**, 2977.

Species Tag:	28009	Name:	CO+
Version:	1		Carbon monoxide cation,
Date:	Jan. 1996		X $^2\Sigma^+$
Contributor:	J. C. Pearson		

Lines Listed:	88	Q(300.0)=	212.736
Freq. (GHz) <	3520	Q(225.0)=	159.717
Max. J:	30	Q(150.0)=	106.685
LOGSTR0=	-8.0	Q(75.00)=	53.670
LOGSTR1=	-8.0	Q(37.50)=	27.174
Isotope Corr.:	0.0	Q(18.75)=	13.935
Egy. (cm^{-1}) >	0.0	Q(9.375)=	7.333
μ_a =	1.0	A=	
μ_b =		B=	58983.0.
μ_c =		C=	

The experimental measurements were reported by K. V. Sastry, P. Helminger, E. Herbst and F. C. De Lucia, 1981, Astrophys. J. **250**, L91. The dipole moment has not been measured so unit dipole was used in the calculation.

Species Tag:	29001	Name:	C-13-O
Version:	3		Carbon monoxide,
Date:	Aug. 1997		^{13}C isotope
Contributor:	H. S. P. Müller		

Lines Listed:	60	Q(300.0)=	113.858
Freq. (GHz) <	6468	Q(225.0)=	85.463
Max. J:	60	Q(150.0)=	57.077
LOGSTR0=	-16.5	Q(75.00)=	28.702
LOGSTR1=	-16.5	Q(37.50)=	14.520
Isotope Corr.:	-1.955	Q(18.75)=	7.434
Egy. (cm^{-1}) >	0.0	Q(9.375)=	3.899
μ_a =	0.11046	A=	
μ_b =		B=	55101.011
μ_c =		C=	

The experimental measurements were reported by (1) M. Winnewisser, B. P. Winnewisser, and G. Winnewisser, in 1985, "Molecular Astrophysics, Series C" (G. H. F. Diercksen, W. F. Huebner, and P. W. Langhoff, Eds.), Vol. 157, pp. 375 – 402. Reidel, Dordrecht. The dipole moment and dipole centrifugal corrections are taken from (2) D. Goorvitch, 1994, Astrophys. J. Suppl. **95**, 535. Additional rotational lines up to R(60) from (2) were included in the fit.

Species Tag:	29002	Name:	HCO+
Version:	3		Formyl cation /
Date:	Jan. 1997		Oxomethylium,
Contributor:	J. C. Pearson		X $^1\Sigma^+$
			nu_2=0,1,2,nu_1=1,nu_3=1
Lines Listed:	246	Q(300.0)=	145.8870
Freq. (GHz) <	3561	Q(225.0)=	106.5539
Max. J:	40	Q(150.0)=	70.4886
LOGSTR0=	-10.0	Q(75.00)=	35.3833
LOGSTR1=	-8.0	Q(37.50)=	17.8600
Isotope Corr.:	0.	Q(18.75)=	9.1023
Egy. (cm^{-1}) >	0.0	Q(9.375)=	4.7298
μ_a =	3.30	A=	
μ_b =		B=	44594.4
μ_c =		C=	

The observed microwave lines are from R. C. Woods, T. A. Dixon, R. J. Saykally, and P. G. Szanto, 1975, Phys. Rev. Lett. **35**, 1269; K. V. L. N. Sastry, E. Herbst, and F. C. De Lucia, 1981, J. Chem. Phys. **75**, 4169; and F. C. van den Heuvel and A. Dymanus, 1982, Chem. Phys. Lett. **92**, 21, G. A. Blake, K. B. Laughlin, R. C. Cohen, K. L. Busarow and R. J. Saykally, 1987, Astrophys. J. **316**, L45; E. Hirota and Y. Endo, 1988, J. Mol. Spectrosc. **127**, 527. The observed infrared transitions were taken from P. B. Davies and W. J. Rothwell, 1984, J. Chem. Phys. **81**, 5239; K. Kawaguchi, C. Yamada, S. Saito and E. Hirota, 1985, J. Chem. Phys. **82**, 1750; P. B. Davies, P. A. Hamilton and W. J. Rothwell, 1984, J. Chem. Phys. **81**, 1598; S. C. Foster, A. R. W. McKeller and T. J. Sears, 1984, J. Chem. Phys. **81**, 578; C. S. Gudeman, M. H. Begemann, J. Pfaff and R. J. Saykally, 1983, Phys. Rev. Lett. **50**, 727; T. Amano, 1983, J. Chem. Phys. **79**, 3595; D.-J. Liu, S.-T. Lee and T. Oka, 1988, J. Mol. Spectrosc. **128**, 236.

The vibrational state are as follows: v=0 is the ground, v=1 is nu_2=1 (bend), v=2 is nu_2=2 l=0 (bend), v=3 is nu_3=1 (C-O stretch), and v=4 is nu_1=1 (C-H stretch). Only l=0 components for the nu_2=2 state have been reported. These were fit to an effective Hamiltonian as in E. Hirota and Y. Endo.

The dipole moment was estimated theoretically by Woods *et al.*, above and was assumed for all the states.

Species Tag:	29003	Name:	CH2NH
Version:	2		Methylenimine
Date:	Jan. 1981		
Contributor:	R. L. Poynter		

Lines Listed:	2957	Q(300.0)=	5892.504
Freq. (GHz) <	2998	Q(225.0)=	3800.143
Max. J:	33	Q(150.0)=	2084.970
LOGSTR0=	-8.0	Q(75.00)=	740.457
LOGSTR1=	-6.8	Q(37.50)=	263.390
Isotope Corr.:	0.	Q(18.75)=	94.297
Egy. (cm^{-1}) >	0.0	Q(9.375)=	34.206
μ_a =	1.325	A=	196211.045
μ_b =	1.530	B=	34532.395
μ_c =		C=	29352.232

The data set and computational method are referenced in W. H. Kirchhoff, D. R. Johnson, and F. J. Lovas, 1973, J. Phys. Chem. Ref. Data **2**, 1.

Species Tag:	29004	Name:	HCO
Version:	1		Formyl radical /
Date:	June 1983		Oxomethyl, X $^2A'$
Contributor:	H. M. Pickett G. A. Blake		
Lines Listed:	2454	Q(300.0)=	3024.128
Freq. (GHz) <	2992	Q(225.0)=	1963.360
Max. J:	31	Q(150.0)=	1068.071
LOGSTR0=	-6.7	Q(75.00)=	378.355
LOGSTR1=	-5.0	Q(37.50)=	134.834
Isotope Corr.:	0.	Q(18.75)=	48.989
Egy. (cm^{-1}) >	0.0	Q(9.375)=	20.310
μ_a =	1.3626	A=	7829365.
μ_b =	0.700	B=	44788.
μ_c =	0	C=	41930.4

The data include some lines recently measured at Duke University by G. A. Blake as well as those from S. Saito, 1972, Astrophys. J. **178**, L95; J. A. Austin *et al.*, 1974, J. Chem. Phys. **60**, 207; and H. M. Pickett and T. L. Boyd, 1978, Chem. Phys. Lett. **58**, 446.

Species Tag:	29005	Name:	NNH+
Version:	1		Diazenylium
Date:	Jan. 1984		X $^1\Sigma^+$
Contributor:	R. L. Poynter		

Lines Listed:	34	Q(300.0)=	1210.877
Freq. (GHz) <	2971	Q(225.0)=	909.076
Max. J:	32	Q(150.0)=	607.016
LOGSTR0=	-3.3	Q(75.00)=	304.930
LOGSTR1=	-3.1	Q(37.50)=	153.993
Isotope Corr.:	0.	Q(18.75)=	78.560
Egy. (cm^{-1}) >	0.0	Q(9.375)=	40.888
μ_a =	3.40	A=	
μ_b =		B=	46586.867
μ_c =		C=	

The experimental measurements were reported by: R. J. Saykally, T. A. Dixon, T. G. Anderson, P. G. Szanto, and R. C. Woods, 1976, Astrophys. J. Lett. Ed. **205**, L101. K. V. L. N. Sastry, P. Helminger, E. Herbst, and F. C. De Lucia, 1981, Chem. Phys. Lett. **84**, 286. F. C. Van den Heuvel and A. Dymanus, 1982, Chem. Phys. Lett. **92**, 219.

The dipole moment was estimated theoretically by S. Green, J. A. Montgomery, Jr., and P. Thaddeus, 1974, Astrophys. J. **193**, L89.

Species Tag:	29006	Name:	CO-17
Version:	2		Carbon monoxide,
Date:	Aug. 1997		^{17}O isotope
Contributor:	H. S. P. Müller		

Lines Listed:	50	Q(300.0)=	111.678
Freq. (GHz) <	5532	Q(225.0)=	83.828
Max. J:	50	Q(150.0)=	55.987
LOGSTR0=	-12.5	Q(75.00)=	28.157
LOGSTR1=	-12.5	Q(37.50)=	14.248
Isotope Corr.:	-3.432	Q(18.75)=	7.298
Egy. (cm^{-1}) >	0.0	Q(9.375)=	3.831
μ_a =	0.11034	A=	
μ_b =		B=	56179.990
μ_c =		C=	

The experimental measurements were reported by (1) M. Winnewisser, B. P. Winnewisser, and G. Winnewisser, in 1985, "Molecular Astrophysics, Series C" (G. H. F. Diercksen, W. F. Huebner, and P. W. Langhoff, Eds.), Vol. 157, pp. 375 – 402. Reidel, Dordrecht. No hyperfine splittings due to ^{17}O have been reported in this study. Hyperfine splittings for the J = 1 – 0 transition were reported in (2) F. J. Lovas and E. Tiemann, 1974, J. Phys. Chem. Ref. Data **3**, 609-770. The experimental line positions and uncertainties, the logarithmic line strengths, and the quantum numbers $F' + 1/2$ and $F'' + 1/2$, are
112358.7200 0.1000 -5.6952 2 3
112358.9800 0.0200 -5.3942 4 3
112360.0160 0.0200 -5.5191 3 3
The dipole moment and dipole centrifugal corrections are taken from (3) D. Goorvitch, 1994, Astrophys. J. Suppl. **95**, 535. Additional rotational lines up to R(60) from (3) were included in the fit.

Species Tag:	29007	Name:	HOC+
Version:	1		Hydroxymethylidynium,
Date:	Jan. 1996		X $^1\Sigma^+$
Contributor:	J. C. Pearson		
Lines Listed:	40	Q(300.0)=	140.139
Freq. (GHz) <	3550	Q(225.0)=	105.170
Max. J:	40	Q(150.0)=	70.212
LOGSTR0=	-3.2	Q(75.00)=	35.267
LOGSTR1=	-3.2	Q(37.50)=	17.801
Isotope Corr.:	0.	Q(18.75)=	9.073
Egy. (cm^{-1}) >	0.0	Q(9.375)=	4.715
μ_a =	4.0	A=	
μ_b =		B=	44743.9
μ_c =		C=	

The observed lines are from: C. S. Gudeman and R. C. Woods, 1982, Phys. Rev. Lett. **48**, 1344. G. A. Blake, P. Helminger, E. Herbst and F. C. De Lucia, 1983, Astrophys. J. **264**, L69. The dipole was estimated by Gudeman and Woods.

Species Tag:	30001	Name:	CO-18
Version:	3		Carbon monoxide,
Date:	Aug. 1997		^{18}O isotope
Contributor:	H. S. P. Müller		

Lines Listed:	60	Q(300.0)=	114.292
Freq. (GHz) <	6444	Q(225.0)=	85.788
Max. J:	60	Q(150.0)=	57.294
LOGSTR0=	-16.5	Q(75.00)=	28.810
LOGSTR1=	-16.5	Q(37.50)=	14.574
Isotope Corr.:	-2.690	Q(18.75)=	7.461
Egy. (cm^{-1}) >	0.0	Q(9.375)=	3.912
μ_a =	0.11079	A=	
μ_b =		B=	54891.420
μ_c =		C=	

The experimental measurements were reported by (1) M. Winnewisser, B. P. Winnewisser, and G. Winnewisser, in 1985, "Molecular Astrophysics, Series C" (G. H. F. Diercksen, W. F. Huebner, and P. W. Langhoff, Eds.), Vol. 157, pp. 375 – 402. Reidel, Dordrecht. The dipole moment and dipole centrifugal corrections are taken from (2) D. Goorvitch, 1994, Astrophys. J. Suppl. **95**, 535. Additional rotational lines up to R(60) from (2) were included in the fit.

Species Tag:	30002	Name:	HC-13-O+
Version:	2		Formyl cation
Date:	Dec. 1983		Oxomethylium,
Contributor:	R. L. Poynter		X $^1\Sigma^+$
			^{13}C isotope
Lines Listed:	34	Q(300.0)=	144.444
Freq. (GHz) <	2938	Q(225.0)=	108.468
Max. J:	34	Q(150.0)=	72.410
LOGSTR0=	-2.4	Q(75.00)=	36.366
LOGSTR1=	-3.3	Q(37.50)=	18.353
Isotope Corr.:	-1.955	Q(18.75)=	9.348
Egy. (cm^{-1}) >	0.0	Q(9.375)=	4.852
μ_a =	3.3	A=	
μ_b =		B=	43377.32
μ_c =		C=	

Only two lines of this molecule have been measured by R. C. Woods, R. J. Saykally, T. A. Dixon, P. G. Szanto, and T. Anderson, 1976, 31st Symposium on Molecular Spectroscopy, Columbus, Ohio, and by M. Bogey, C. Demuynck, and J. L. Destombes, 1981, Mol. Phys. **43**, 1043. A least squares analysis cannot be done with such limited data. The catalog entries are therefore just simple calculations from the B and D rotational constants, and no error estimates can be given beyond the two measured lines. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	30003	Name:	DCO+
Version:	2		Formyl cation /
Date:	Dec. 1983		Oxomethylium,
Contributor:	R. L. Poynter		X $^1\Sigma^+$,
			Deuterium isotope
Lines Listed:	41	Q(300.0)=	521.915
Freq. (GHz) <	2939	Q(225.0)=	391.652
Max. J:	41	Q(150.0)=	261.397
LOGSTR0=	-2.7	Q(75.00)=	131.190
LOGSTR1=	-4.0	Q(37.50)=	66.085
Isotope Corr.:	-3.824	Q(18.75)=	33.558
Egy. (cm^{-1}) >	0.0	Q(9.375)=	17.306
μ_a =	3.3	A=	
μ_b =		B=	36019.76
μ_c =		C=	

The observed lines are from: R. C. Woods, R. J. Saykally, T. A. Dixon, P. G. Szanto, and T. Anderson, 1976, 31st Symposium on Molecular Spectroscopy, Columbus, Ohio. M. Bogey, C. Demuynck, and J. L. Destombes, 1981, Mol. Phys. **43**, 1043. K. V. L. N. Sastry, E. Herbst, and F. C. De Lucia, 1981, J. Chem. Phys. **75**, 4169. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	30004	Name:	H2CO
Version:	2		Formaldehyde
Date:	Nov. 1997		
Contributor:	H. S. P. Müller		

Lines Listed:	3506	Q(300.0)=	2883.014
Freq. (GHz) <	9999	Q(225.0)=	1872.622
Max. J:	57	Q(150.0)=	1019.971
LOGSTR0=	-20.0	Q(75.00)=	361.720
LOGSTR1=	-9.0	Q(37.50)=	128.649
Isotope Corr.:	0.	Q(18.75)=	44.681
Egy. (cm^{-1}) >	0.0	Q(9.375)=	13.801
μ_a =	2.331	A=	281970.58
μ_b =		B=	38833.987
μ_c =		C=	34004.244

The experimental data was reported by (1) R. Bocquet *et al.*, 1996, J. Mol. Spect. **177**, 154.

The dipole moment was measured by (2) K. Kondo and T. Oka, 1960, J. Phys. Soc. Jap. **15**, 307.

Species Tag:	30005	Name:	C-13-H2NH
Version:	1		Methylenimine,
Date:	Jan. 1980		^{13}C isotope
Contributor:	R. L. Poynter		
Lines Listed:	439	Q(300.0)=	2012.334
Freq. (GHz) <	2975	Q(225.0)=	1307.074
Max. J:	10	Q(150.0)=	711.541
LOGSTR0=	-7.9	Q(75.00)=	251.536
LOGSTR1=	-6.6	Q(37.50)=	88.941
Isotope Corr.:	0.	Q(18.75)=	31.441
Egy. (cm^{-1}) >	0.0	Q(9.375)=	11.117
μ_a =	1.325	A=	194195.217
μ_b =	1.530	B=	33747.87
μ_c =		C=	28707.05

The computational method is the same as that used on the parent species, CH_2NH. The data are from R. Pearson, Jr., and F. J. Lovas, 1977, J. Chem. Phys. **66**, 4149. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	30006	Name:	CH2N-15-H
Version:	1		Methylenimine,
Date:	Jan. 1980		^{15}N isotope
Contributor:	R. L. Poynter		

Lines Listed:	440	Q(300.0)=	2015.580
Freq. (GHz) <	2994	Q(225.0)=	1309.182
Max. J:	10	Q(150.0)=	712.689
LOGSTR0=	-7.9	Q(75.00)=	251.942
LOGSTR1=	-6.6	Q(37.50)=	89.084
Isotope Corr.:	-2.432	Q(18.75)=	31.492
Egy. (cm^{-1}) >	0.0	Q(9.375)=	11.135
μ_a =	1.325	A=	195738.07
μ_b =	1.530	B=	33736.10
μ_c =		C=	28688.61

The computational method is the same as that used on the parent species, CH_2NH. The data are from R. Pearson, Jr., and F. J. Lovas, 1977, J. Chem. Phys. **66**, 4149. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	30007	Name:	CH2ND
Version:	1		Methylenimine,
Date:	Feb. 1981		deuterium isotope
Contributor:	R. L. Poynter		on nitrogen atom
Lines Listed:	1834	Q(300.0)=	7181.249
Freq. (GHz) <	2989	Q(225.0)=	4664.446
Max. J:	14	Q(150.0)=	2542.728
LOGSTR0=	-8.0	Q(75.00)=	811.708
LOGSTR1=	-6.8	Q(37.50)=	297.852
Isotope Corr.:	-3.824	Q(18.75)=	92.619
Egy. (cm^{-1}) >	0.0	Q(9.375)=	43.381
μ_a =	1.325	A=	157673.877
μ_b =	1.530	B=	32069.366
μ_c =		C=	26563.849

The computational method is the same as that used for CH_2NH. The data are from R. Pearson, Jr., and F. J. Lovas, 1977, J. Chem. Phys. **66**, 4149. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	30008	Name:	NO
Version:	1		Nitric oxide,
Date:	Feb. 1980		X $^2\Pi$ states
Contributor:	H. M. Pickett		

Lines Listed:	1909	Q(300.0)=	1159.578
Freq. (GHz) <	2994	Q(225.0)=	816.958
Max. J:	36	Q(150.0)=	492.266
LOGSTR0=	-19.8	Q(75.00)=	209.701
LOGSTR1=	-21.5	Q(37.50)=	99.472
Isotope Corr.:	0.	Q(18.75)=	52.000
Egy. (cm^{-1}) >	0.0	Q(9.375)=	28.867
μ_a =	0.15872	A=	
μ_b =		B=	50849.06
μ_c =		C=	

The spectrum of NO was fitted to the fine-structure Hamiltonian described by C. Amiot, R. Bacis, and G. Guelachvili, 1978, Can. J. Phys. **56**, 251, along with the hyperfine Hamiltonian described by W. L. Meerts, 1976, Chem. Phys. **14**, 421. The radio frequency lines are from W. L. Meerts and A. Dymanus, 1972, J. Mol. Spect. **44**, 320. The millimeter lines were measured at JPL by H. M. Pickett and E. A. Cohen. The partition function was determined by a sum over states to J = 35.5.

Species Tag:	30009	Name:	NND+
Version:	1		Diazenylium,
Date:	Jan. 1984		Deuterium isotope,
Contributor:	R. L. Poynter		X $^1\Sigma^+$

Lines Listed:	41	Q(300.0)=	487.641
Freq. (GHz) <	2993	Q(225.0)=	365.932
Max. J:	39	Q(150.0)=	244.231
LOGSTR0=	-3.5	Q(75.00)=	122.631
LOGSTR1=	-3.9	Q(37.50)=	61.816
Isotope Corr.:	-3.824	Q(18.75)=	31.420
Egy. (cm^{-1}) >	0.0	Q(9.375)=	16.241
μ_a =	3.40	A=	
μ_b =		B=	38554.719
μ_c =		C=	

The experimental measurements were reported by T. G. Anderson, T. A. Dixon, N. D. Piltch, R. J. Saykally, P. G. Szanto, and R. C. Woods, 1977, Astrophys. J. Lett. Ed. **216**, L85, and by K. V. L. N. Sastry, P. Helminger, E. Herbst, and F. C. De Lucia, 1981, Chem. Phys. Lett. **84**, 826. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	30010	Name:	HOC-13+
Version:	1		Hydroxymethylidynium,
Date:	Jan. 1996		X $^{1}\Sigma^{+}$,
Contributor:	J. C. Pearson		^{13}C isotope

Lines Listed:	40	Q(300.0)=	146.236
Freq. (GHz) <	3400	Q(225.0)=	109.740
Max. J:	40	Q(150.0)=	73.258
LOGSTR0=	-3.2	Q(75.00)=	36.790
LOGSTR1=	-3.2	Q(37.50)=	18.563
Isotope Corr.:	-1.955	Q(18.75)=	9.453
Egy. (cm^{-1}) >	0.0	Q(9.375)=	4.905
μ_a =	4.0	A=	
μ_b =		B=	42876.6
μ_c =		C=	

The observed line is from: C. S. Gudeman and R. C. Woods, 1982, Phys. Rev. Lett. **48**, 1344. The dipole was estimated by Gudeman and Woods.

Since it is impossible to get a meaningful least squares fit of one line, the D constant was taken from the normal species with uncertainty increased according to the ratio of the B constants and the B constant was assigned the ground states uncertainty.

Species Tag:	30011	Name:	NO+
Version:	1		Nitrosyl cation,
Date:	Jan. 1996		X $^1\Sigma^+$
Contributor:	J. C. Pearson		

Lines Listed:	154	Q(300.0)=	315.814
Freq. (GHz) $<$	3675	Q(225.0)=	237.103
Max. J:	30	Q(150.0)=	158.382
LOGSTR0=	-8.0	Q(75.00)=	79.685
LOGSTR1=	-8.0	Q(37.50)=	40.351
Isotope Corr.:	0.0	Q(18.75)=	20.699
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	10.898
μ_a =	0.5	A=	
μ_b =		B=	59597.1
μ_c =		C=	

The experimental measurements were reported by W. C. Bowman, E. Herbst and F. C. De Lucia, 1982, J. Chem. Phys. **77**, 4261. The dipole moment has been calculated to be 0.66(38) Debye by Ch. Jungen and H. Lefebvre-Brion, 1970, J. Mol. Spect. **33**, 520. Another calculation by F. P. Billingsley, 1973, Chem. Phys. Lett. **23**, 160 placed the value at 0.31 Debye. An intermediate value of 0.5 was used in the calculation.

Species Tag:	30012	Name:	DOC+
Version:	1		hydroxymethylidynium,
Date:	Feb. 1996		X $^1\Sigma^+$,
Contributor:	J. C. Pearson		deuterium isotope

Lines Listed:	40	Q(300.0)=	164.1268
Freq. (GHz) <	3032	Q(225.0)=	123.1582
Max. J:	40	Q(150.0)=	82.2006
LOGSTR0=	-2.4	Q(75.00)=	41.2600
LOGSTR1=	-2.4	Q(37.50)=	20.7971
Isotope Corr.:	-3.824	Q(18.75)=	10.5697
Egy. (cm^{-1}) >	0.0	Q(9.375)=	5.4616
μ_a =	4.0	A=	
μ_b =		B=	38193.2
μ_c =		C=	

The observed lines are from: M. Bogey, C. Demuynck and J. L. Destombes, 1986, J. Mol. Spect. **115**, 229.

The dipole was fixed to the parent species value of: C. S. Gudeman and R. C. Woods, 1982, Phys. Rev. Lett. **48**, 1344.

Species Tag:	31001	Name:	HCO-18+
Version:	2		Formyl cation /
Date:	Dec. 1983		Oxomethylium,
Contributor:	R. L. Poynter		X $^1\Sigma^+$,
			^{18}O isotope
Lines Listed:	34	Q(300.0)=	147.163
Freq. (GHz) <	2886	Q(225.0)=	110.459
Max. J:	34	Q(150.0)=	73.739
LOGSTR0=	-2.4	Q(75.00)=	37.034
LOGSTR1=	-3.2	Q(37.50)=	18.690
Isotope Corr.:	-2.690	Q(18.75)=	9.515
Egy. (cm^{-1}) >	0.0	Q(9.375)=	4.936
μ_a =	3.30	A=	
μ_b =		B=	42581.21
μ_c =		C=	

Only two lines of this molecule have been measured, by C. Woods, R. J. Saykally, T. A. Dixon, P. G. Szanto, and T. Anderson, 1976, 31st Symposium on Molecular Spectroscopy, Columbus, Ohio, and by M. Bogey, C. Demuynck, and J. L. Destombes, 1981, Mol. Phys. **43**, 1043. A least squares analysis cannot be done with such limited data. The catalog entries are therefore just simple calculations from the B and D rotational constants, and no error estimates can be given. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	31002	Name:	H2C-13-O
Version:	1		Formaldehyde,
Date:	Jan. 1980		^{13}C isotope
Contributor:	R. L. Poynter		

Lines Listed:	601	Q(300.0)=	2949.850
Freq. (GHz) <	2985	Q(225.0)=	1925.307
Max. J:	30	Q(150.0)=	1047.611
LOGSTR0=	-9.2	Q(75.00)=	370.937
LOGSTR1=	-6.2	Q(37.50)=	131.856
Isotope Corr.:	-1.995	Q(18.75)=	45.783
Egy. (cm^{-1}) >	0.0	Q(9.375)=	14.129
μ_a =	2.331	A=	281930.85
μ_b =		B=	37811.92
μ_c =		C=	33213.19

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. **41**, 333. The measurements were taken from: D. Dangoisse, E. Willemot, and J. Bellet, 1978, J. Mol. Spect. **71**, 414. D. R. Johnson, F. Lovas, and W. H. Kirchhoff, 1972, J. Phys. Chem. Ref. Data **1**, 1011. R. B. Lawrence and M. W. P. Strandberg, 1951, Phys. Rev. **83**, 363. R. Nerf, 1972, Astrophys. J. **174**, 467. T. Oka, H. Hirakawa, and K. Shimoda, 1960, J. Phys. Soc. Jap. **15**, 2265. T. Oka, T. Takagi, and Y. Morino, 1964, J. Mol. Spect. **14**, 27. K. D. Tucker, G. R. Tomasevich, and P. Thaddeus, 1972, Astrophys. J. **174**, 463, and 1971, Astrophys. J. **169**, 429. The dipole moment was assumed to be the same as for the parent H_2CO.

Species Tag:	31003	Name:	HDCO
Version:	1		Formaldehyde,
Date:	Feb. 1995		deuterium isotope
Contributor:	H. M. Pickett		
	M. L. Delitsky		
Lines Listed:	4204	Q(300.0)=	1929.1277
Freq. (GHz) <	9999	Q(225.0)=	1256.9963
Max. J:	90	Q(150.0)=	686.2959
LOGSTR0=	-10	Q(75.00)=	243.6807
LOGSTR1=	-8	Q(37.50)=	86.7182
Isotope Corr.:	-3.523	Q(18.75)=	31.0537
Egy. (cm^{-1}) >	0.0	Q(9.375)=	11.2679
$\mu_a =$	2.324	A=	198111.99
$\mu_b =$	0.182	B=	34910.84
$\mu_c =$		C=	29561.07

The experimental frequencies were taken from D. Dangoisse, E. Willemot, and J. Bellet, 1978, J. Mol. Spect. **71**, 414.

The total dipole moment was assumed to be the same as for the parent H_2CO, but the components are obtained by rotating the axes by an amount which is calculated from the structure.

Species Tag:	31004	Name:	HO-18-C+
Version:	1		Hydroxymethylidynium,
Date:	Jan. 1996		X $^1\Sigma^+$,
Contributor:	J. C. Pearson		^{18}O isotope

Lines Listed:	40	Q(300.0)=	144.788
Freq. (GHz) <	3435	Q(225.0)=	108.654
Max. J:	40	Q(150.0)=	72.534
LOGSTR0=	-3.2	Q(75.00)=	36.428
LOGSTR1=	-3.2	Q(37.50)=	18.382
Isotope Corr.:	-2.69	Q(18.75)=	9.363
Egy. (cm^{-1}) >	0.0	Q(9.375)=	4.860
μ_a =	4.0	A=	
μ_b =		B=	43306.0
μ_c =		C=	

The observed line is from: C. S. Gudeman and R. C. Woods, 1982, Phys. Rev. Lett. **48**, 1344. The dipole was estimated by Gudeman and Woods.

Since it is impossible to get a meaningful least squares fit of one line, the D constant was taken from the normal species with uncertainty increased according to the ratio of the B constants and the B constant was assigned the ground state uncertainty.

Species Tag:	31005	Name:	HNO
Version:	1		Nitrosylhydride,
Date:	Feb. 1996		X $^1\Sigma^+$
Contributor:	J. C. Pearson		

Lines Listed:	10293	Q(300.0)=	2751.7066
Freq. (GHz) <	9952	Q(225.0)=	1790.4519
Max. J:	30	Q(150.0)=	975.4327
LOGSTR0=	-8.0	Q(75.00)=	346.0358
LOGSTR1=	-8.0	Q(37.50)=	123.3276
Isotope Corr.:		Q(18.75)=	44.4254
Egy. (cm^{-1}) >	0.0	Q(9.375)=	17.2300
μ_a =	1.03	A=	553898.9
μ_b =	1.31	B=	42312.9
μ_c =		C=	39165.1

The observed lines are from: S. Satio and K. Takagi, 1972, Astrophys J. **175**, L47. K. Takagi and S. Saito, 1973, J. Mol. Spect. **47**, 99. J. E. T. Corrie, G. W. Kirby, A. E. Laird, L. W. Mackinnon and J. K. Tyler, 1978, Chem. Comm., 275. K. V. L. N. Sastry, P. Helminger, G. M. Plummer, E. Herbst and F. C. De Lucia, 1984, Astrophys. J. Suppl. **55**, 563.

The dipole was measured by Takagi and Saito. The H_K constant was fixed to the IR/microwave/electronic value of J. W. C. Johns, A. R. W. McKeller and E. Weinberger, 1983, Can. J. Phys. **61**, 1106.

The molecule was first observed in interstellar emission by B. L. Ulich, J. M. Hollis and L. E. Snyder, 1977, Astrophys. J. **217**, L105.

Species Tag:	32001	Name:	O2
Version:	3		Molecular oxygen, $^{16}O_2$
Date:	June 1989		X $^3\Sigma_g^-$, v = 0
Contributor:	H. M. Pickett		

Lines Listed:	237	Q(300.0)=	218.675
Freq. (GHz) <	9928	Q(225.0)=	164.135
Max. J:	61	Q(150.0)=	109.597
LOGSTR0=	-31.5	Q(75.00)=	55.195
LOGSTR1=	-18.7	Q(37.50)=	28.035
Isotope Corr.:	0	Q(18.75)=	14.514
Egy. (cm^{-1}) >	0.0	Q(9.375)=	7.870
μ_a =	magnetic	A=	
μ_b =		B=	43099.795
μ_c =		C=	

Additional partition function values are:
Q(275) = 200.426
Q(250) = 182.231
Q(200) = 145.919

The measurements and calculational method are from T. Amano and E. Hirota, 1974, J. Mol. Spect. **53**, 346. The Raman lines of O_2 (M. Loete and H. Berger, 1977, J. Mol. Spect. **68**, 317) were used with the millimeter wavelength measurements and the submillimeter line of W. Steinbach and W. Gordy (1973, Phys. Rev. **A8**, 1953) in a combined fit of the v = 0 and v = 1 transitions. New measurements in the far-infrared by L. R. Zink and M. Mizushima, 1987, J. Mol. Spect. **125**, 154, are included. The intensities of the magnetic dipole transitions have been calculated using the g values obtained from magnetic resonance by K. D. Bowers, R. A. Kamper, and C. D. Lustig, 1959, Proc. Roy. Soc. London **A251**, 565. The zero-frequency absorption is included but the frequency is set to a synthetic frequency of $|g|J$ for the given level. The intensity of these zero-frequency absorptions is based on the synthetic frequency, using the equations for integrated intensity given in Section 3.

Species Tag:	32002	Name:	O2-v1
Version:	4		Molecular oxygen, $^{16}\mathrm{O}_2$
Date:	Dec. 1983		X $^3\Sigma_g^-$, v = 1
Contributor:	H. M. Pickett		

Lines Listed:	237	Q(300.0)=	218.675
Freq. (GHz) <	9817	Q(225.0)=	164.135
Max. J:	61	Q(150.0)=	109.597
LOGSTR0=	-34.7	Q(75.00)=	55.195
LOGSTR1=	-21.8	Q(37.50)=	28.035
Isotope Corr.:	0	Q(18.75)=	14.514
Egy. (cm^{-1}) >	1556.4	Q(9.375)=	7.870
μ_a =	magnetic	A=	
μ_b =		B=	42626.96
μ_c =		C=	

The calculations are described for the ground state (Species 32001). The vibrational excited state, v = 1, is 1556.38 ± 0.01 cm^{-1} above the ground state (M. Leote and H. Berger, 1977, J. Mol. Spect. **68**, 317). Intensities were calculated using the ground state g values.

Species Tag:	32003	Name:	CH3OH
Version:	2		Methyl alcohol,
Date:	Nov. 1980		lowest A, E_1, and E_2
Contributor:	H. M. Pickett		vibrational states
Lines Listed:	709	Q(300.0)=	6413.573
Freq. (GHz) <	1470	Q(225.0)=	4165.815
Max. J:	12	Q(150.0)=	2267.776
LOGSTR0=	-9.9	Q(75.00)=	801.678
LOGSTR1=	-5.2	Q(37.50)=	283.465
Isotope Corr.:	0	Q(18.75)=	100.207
Egy. (cm^{-1}) >	0.0	Q(9.375)=	35.432
μ_a =	0.885	A=	127484.
μ_b =	1.440	B=	24679.98
μ_c =		C=	23769.70

The lines below 200 GHz are reported by R. M. Lees, F. J. Lovas, W. H. Kirchhoff, and D. R. Johnson, 1973, J. Phys. Chem. Ref. Data **2**, 205. Additional lines are referenced in F. J. Lovas, L. E. Snyder, and D. R. Johnson, 1979, Astrophys. J. Suppl. **41**, 451. The lines above 200 GHz were measured at JPL. Frequencies were predicted using energy polynomials in J (J + 1) for each value of K. The **v** quantum numbers in the catalog are:

v	**Species**	**Asymmetric Rotor Correspondence**
1	A	Upper K state for K even, lower for K odd
2	A-	Upper K state for K odd, lower for K even
3	E_1	No direct correspondence
4	E_2	No direct correspondence

Species Tag:	32004	Name:	H2CO-18
Version:	1		Formaldehyde,
Date:	Feb. 1980		^{18}O isotope
Contributor:	R. L. Poynter		

Lines Listed:	449	Q(300.0)=	3017.171
Freq. (GHz) <	1424	Q(225.0)=	1959.747
Max. J:	20	Q(150.0)=	1066.842
LOGSTR0=	-8.8	Q(75.00)=	379.228
LOGSTR1=	-9.3	Q(37.50)=	134.865
Isotope Corr.:	0	Q(18.75)=	46.806
Egy. (cm^{-1}) >	0.0	Q(9.375)=	14.441
μ_a =	-2.331	A=	281993.0
μ_b =		B=	36903.6
μ_c =		C=	32514.7

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. **41**, 333. The measurements were taken from:

D. Dangoisse, E. Willemot, and J. Bellet, 1978, J. Mol. Spect. **71**, 414.

D. R. Johnson, F. Lovas, and W. H. Kirchhoff, 1972, J. Phys. Chem. Ref. Data **1**, 1011.

R. B. Lawrence and M. W. P. Strandberg, 1951, Phys. Rev. **83**, 363.

T. Oka, H. Hirakawa, and K. Shimoda, 1960, J. Phys. Soc. Jap. **15**, 2265.

T. Oka, T. Takagi, and Y. Morino, 1964, J. Mol. Spect. **14**, 27.

R. D. Tucker, G. R. Tomasevich, and P. Thaddeus, 1972, Astrophys. J. **174**, 463, 1971, and Astrophys. J. **169**, 429.

The dipole moment was assumed to be the same as for the parent species.

Species Tag:	32005	Name:	O2-snglt-dlta
Version:	1		Oxygen molecule,
Date:	Sept. 1985		metastable $a\,^1\Delta_g$ state
Contributor:	E. A. Cohen		
Lines Listed:	67	Q(300.0)=	149.555
Freq. (GHz) <	5665	Q(225.0)=	112.746
Max. J:	69	Q(150.0)=	75.928
LOGSTR0=	-15.3	Q(75.00)=	39.165
LOGSTR1=	-17.8	Q(37.50)=	20.831
Isotope Corr.:	0.0	Q(18.75)=	11.754
Egy. (cm^{-1}) >	0.0	Q(9.375)=	7.389
μ_a =		A=	
μ_b =	magnetic	B=	42505.7440
μ_c =		C=	

The data and parameters are reported in K. W. Hillig *et al.*, 1985, J. Mol. Spectrosc. **109**, 205. The partition function is calculated as if the metastable $a\,^1\Delta_g$ state is a separate molecule. The state is essentially unpopulated in thermal equilibrium.

Species Tag:	32006	Name:	D_2CO
Version:	1		Formaldehyde,
Date:	Feb. 1995		di-deuterium isotope
Contributor:	H. M. Pickett		
	M. L. Delitsky		
Lines Listed:	3682	Q(300.0)=	11433.3263
Freq. (GHz) <	9999	Q(225.0)=	7425.5670
Max. J:	60	Q(150.0)=	4043.4608
LOGSTR0=	-10	Q(75.00)=	1432.7604
LOGSTR1=	-8	Q(37.50)=	509.2633
Isotope Corr.:	-7.648	Q(18.75)=	182.2097
Egy. (cm^{-1}) >	0.0	Q(9.375)=	67.3395
μ_a =	2.331	A=	141653.54
μ_b =		B=	32283.55
μ_c =		C=	26185.31

The experimental frequencies were taken from D. Dangoisse, E. Willemot, and J. Bellet, 1978, J. Mol. Spect. **71**, 414.

The dipole moment was assumed to be the same as for the parent H_2CO.

Species Tag:	32007	Name:	DNO
Version:	1		Nitrosylhydride,
Date:	Feb. 1996		X $^1\Sigma^+$,
Contributor:	J. C. Pearson		deuterium isotope

Lines Listed:	14739	Q(300.0)=	4060.4046
Freq. (GHz) $<$	9500	Q(225.0)=	2646.0465
Max. J:	30	Q(150.0)=	1441.7924
LOGSTR0=	-8.0	Q(75.00)=	511.1894
LOGSTR1=	-8.0	Q(37.50)=	181.9931
Isotope Corr.:	-3.824	Q(18.75)=	65.2955
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	23.8962
μ_a =	1.18	A=	315497.2
μ_b =	1.22	B=	38735.0
μ_c =		C=	34350.7

The observed lines are from: K. Takagi and S. Saito, 1972, J. Mol. Spect. **44**, 81. K.V.L.N. Sastry, P. Helminger, G. M. Plummer, E. Herbst and F. C. De Lucia, 1984, Astrophys. J. Suppl. **55**, 563.

The dipole was measured by Takagi and Saito. The H_K constant was fixed to the IR/microwave/electronic value of J. W. C. Johns, A. R. W. McKeller and E. Weinberger, 1983, Can. J. Phys. **61**, 1106.

Species Tag:	33001	Name:	HO2
Version:	3		Hydroperoxyl radical
Date:	Mar. 1996		X $^2A''$
Contributor:	H. S. P. Müller		

Lines Listed:	21954	Q(300.0)=	4375.7031
Freq. (GHz) <	9999	Q(225.0)=	2841.7306
Max. J:	41	Q(150.0)=	1547.2823
LOGSTR0=	-7.5	Q(75.00)=	548.4641
LOGSTR1=	-8.5	Q(37.50)=	195.1806
Isotope Corr.:	0	Q(18.75)=	70.2146
Egy. (cm^{-1}) >	0.0	Q(9.375)=	27.5930
μ_a =	1.412	A=	610273.
μ_b =	1.541	B=	33514.
μ_c =		C=	31672.

The data were obtained from A. Charo and F. C. De Lucia, 1982, J. Mol. Spect. **94**, 426; Y. Beers and C. J. Howard, 1975, J. Chem. Phys. **63**, 4121; S. Saito, 1977, J. Mol. Spect. **65**, 229; K. V. Chance, K. Park, K. M. Evenson, L. R. Zink, and F. Stroh, 1995, J. Mol. Spect. **172**, 407; and FIR lines from A. von Bargen, M. Birk, and G. Wagner, DLR, to be published. The spectrum was computed using a full diagonalization of the spin-rotation Hamiltonian.

Species Tag:	33002	Name:	O-17-O
Version:	1		Oxygen molecule $^{17}O^{16}O$
Date:	June 1989		
Contributor:	E. A. Cohen		

Lines Listed:	10787	Q(300.0)=	2692.775
Freq. (GHz) <	9992	Q(225.0)=	2018.831
Max. J:	62	Q(150.0)=	1345.860
LOGSTR0=	-32.0	Q(75.00)=	672.977
LOGSTR1=	-35.0	Q(37.50)=	337.054
Isotope Corr.:	-3.1310	Q(18.75)=	169.707
Egy. (cm^{-1}) >	0.0	Q(9.375)=	87.036
μ_a =	magnetic	A=	
μ_b =		B=	41830.97
μ_c =		C=	

The data were reported by G. Cazzoli *et al.*, 1981, Nuovo Ciminto **62**, 243.

Species Tag:	33003	Name:	SH
Version:	1		nu=0,1
Date:	Jan. 1997		$^2\Pi_i$ State
Contributor:	J. C. Pearson		
Lines Listed:	646	Q(300.0)=	113.4337
Freq. (GHz) <	9999	Q(225.0)=	81.9754
Max. J:	21	Q(150.0)=	54.3911
LOGSTR0=	-14.0	Q(75.00)=	30.9151
LOGSTR1=	-12.0	Q(37.50)=	20.5682
Isotope Corr.:	-0.022	Q(18.75)=	16.7001
Egy. (cm^{-1}) >	0.0	Q(9.375)=	16.0151
μ_a =	0.7580	A=	
μ_b =		B=	283587.6
μ_c =		C=	

The data were taken from: E. Klisch, Th. Klaus, S. P. Belov, A. Dolgner, R. Schieder, G. Winnewisser and E. Herbst, 1996, Astrophys. J. **473**, 1118, I. Morino and K. Kawaguchi, 1995, J. Mol. Spectrosc. **170**, 172, W. L. Meerts and A. Dymanus, 1974, Astrophys. J. **187**, L45, W. L. Meerts and A. Dymanus, 1975, Can J. Phys. **53**, 2123, P. F. Bernath, T. Amano and M. Wong, 1983, J. Mol. Spectrosc. **98**, 20, J. R. Winkel, Jr. and S. P. Davis, 1984, Can J. Phys. **62**, 1420, and R. S. Ram, P. F. Bernath, R. Engleman, Jr. and J. W. Brault, 1995, J. Mol. Spectrosc. **172**, 34. The ground state A value was fixed to the electronic value of S. H. Ashworth and J. M. Brown, 1992, J. Mol. Spectrosc. **153**, 41.

The dipole moment is from W. L. Meerts and A. Dymanus, 1975, Can J. Phys. **53**, 2123. The ground state dipole was assumed for the nu=1 state.

Species Tag:	34001	Name:	O-18-O
Version:	3		Molecular oxygen,
Date:	Feb. 1996		single substituted
Contributor:	E. A. Cohen		^{18}O isotope

Lines Listed:	400	Q(300.0)=	461.087
Freq. (GHz) $<$	5961	Q(225.0)=	345.728
Max. J:	57	Q(150.0)=	230.431
LOGSTR0=	-31.3	Q(75.00)=	115.215
LOGSTR1=	-15.0	Q(37.50)=	57.680
Isotope Corr.:	-2.389	Q(18.75)=	29.017
Egy. (cm^{-1}) $>$	-0.6	Q(9.375)=	14.863
μ_a =	magnetic	A=	
μ_b =		B=	40708.
μ_c =		C=	

The measurements are from T. Amano and E. Hirota, 1974, J. Mol. Spect. **53**, 346. W. Steinbach and W. Gordy, 1975, Phys. Rev. **A11**, 729, and R. L. Crownover, F. C. De Lucia and E. Herbst, 1990, Astrophys.J. **349,** L29. The calculation included the high resolution spectrum of the $a^1\Delta - X^3\Sigma$ band, J. Brault, unpublished, and two microwave transitions from the $a^1\Delta$ state from E. A. Cohen, M. Okunishi, and J. J. Oh, J. Mol. Struct. **352/353,** 283. Intensities of magnetic dipole transitions have been calculated using the g values obtained from magnetic resonance by K. D. Bowers, R. A. Kamper, and C. D. Lustig, 1959, Proc. Roy. Soc. London **A251**, 565. The zero-frequency absorption is included but the frequency is set to a synthetic frequency of |g| J for the given level.

Species Tag:	34002	Name:	H2-32-S
Version:	3		Hydrogen sulfide
Date:	Jan. 1996		^{32}S isotope
Contributor:	H. S. P. Müller		

Lines Listed:	1525	Q(300.0)=	514.4470
Freq. (GHz) $<$	9999	Q(225.0)=	334.5222
Max. J:	21	Q(150.0)=	182.7622
LOGSTR0=	-8.9	Q(75.00)=	65.5265
LOGSTR1=	-9.9	Q(37.50)=	23.8654
Isotope Corr.:	-0.022	Q(18.75)=	8.6996
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	2.9106
μ_a =		A=	310583.57
μ_b =	0.974	B=	270367.68
μ_c =		C=	141820.03

The experimental measurements were analyzed using the methods described in S. P. Belov *et al.*, 1995, J. Mol. Spect. **173**, 380. The Hamiltonian contains distortion constants up to tenth order. The measurements were taken from S. P. Belov *et al.*, which includes measurements from P. Helminger, R. L. Cook, and F. C. De Lucia, 1972, J. Chem. Phys. **56**, 481, and P. Helminger, F. C. De Lucia, and W. H. Kirchhoff, 1973, J. Phys. Chem. Ref. Data **2**, 213. Also included in the fit are FIR lines from K. M. T. Yamada and S. Klee, 1994, J. Mol. Spect. **166**, 395. Wherever a line has been measured more than once, the one with the smaller uncertainty is listed. The highest J and K_a included in the fit are 16 and 13 respectively. The uncertainties of transitions beyond these values are only qualitative and should be taken with care. The dipole moment was reported by C. Huiszoon and A. Dymanus, 1965, Physica **31**, 1049.

Species Tag:	34003	Name:	PH3
Version:	3		Phosphine
Date:	Jan. 1991		
Contributor:	R. L. Poynter H. M. Pickett		
Lines Listed:	728	Q(300.0)=	803.896
Freq. (GHz) <	5635	Q(225.0)=	527.351
Max. J:	27	Q(150.0)=	288.802
LOGSTR0=	-17.0	Q(75.00)=	103.086
LOGSTR1=	-10.0	Q(37.50)=	37.196
Isotope Corr.:	0.0	Q(18.75)=	13.916
Egy. (cm^{-1}) >	0.0	Q(9.375)=	5.796
μ_a =	0.000072*	A=	B
μ_b =		B=	133480.22
μ_c =	0.574	C=	117488.39

*centrifugally induced

The measured lines are taken from: D. Helms and W. Gordy, 1971, J. Mol. Spect. **66**, 206. F. Y. Chu and T. Oka, 1974, J. Chem. Phys. **60**, 4612. P. B. Davies, R. M. Newman, S. C. Wofsy, and W. Klemperer, 1971, J. Chem. Phys. **55**, 3564. A. F. Krupnov, A. A. Melnikov, and V. A. Skvortsov, 1979, Opt. Spectrosc. (USSR) **46** (5), 570. H. M. Pickett, R. L. Poynter, and E. A. Cohen, 1981, J. Quant. Spectrosc. Radiat. Transfer **26**, 197. S. P. Belov *et al.*, 1981, J. Mol. Spect. **90**, 579.

The dipole moment measured by P. B. Davies *et al.*, above, is 0.57395 ± 0.0003D. The sign of the K = 3, 6, 9 levels represents the parity under inversion.

Species Tag:	34004	Name:	H2O2
Version:	4		Hydrogen peroxide,
Date:	Sept. 1995		H_2O_2,
Contributor:	J. C. Pearson		first 5 torsional states

Lines Listed:	38357	Q(300.0)=	9785.505
Freq. (GHz) $<$	9999	Q(225.0)=	5760.578
Max. J:	60	Q(150.0)=	2814.265
LOGSTR0=	-10.0	Q(75.00)=	895.518
LOGSTR1=	-10.0	Q(37.50)=	288.930
Isotope Corr.:	0.0	Q(18.75)=	88.856
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	26.680
$\mu_a =$		A=	301878.
$\mu_b =$		B=	26211.9
$\mu_c =$	1.5724	C=	25099.14

The spectral lines and method of calculation are from D. T. Petkie, T. M. Goyette, J. J. Holton, F. C. De Lucia and P. Helminger, 1995, J. Mol. Spect. **171**, 145-159. This paper included the previous lines of P. Helminger, W. C. Bowman and F. C. De Lucia, 1981, J. Mol. Spect. **85**, 120. E. A. Cohen and H. M. Pickett, 1981, J. Mol. Spect. **87**, 582. Also used in the analysis were energy levels from C. Cammy-Peyret, J.-M. Flaud, J. W. C. Johns and M. Noel, 1992, J. Mol. Spect. **155**, 84-104. Dipoles are from A. Perrin, J.-M. Flaud, C. Camy-Peyret, R. Schermaul, M. Winnewisser, J.-Y. Mandin, V. Danna, M. Badaoui, and J. Koput, Line Intensities in the Far-Infrared Spectrum of H_2O_2, in preparation.

The dipole moment is c-type in all cases. The value given is for the ground state transitions only. The vibrational quantum number designation is as follows:

v(catalog)	n	τ_{even}	τ_{odd}
0	0	1	2
1	1	1	2
2	2	1	2
3	0	4	3
4	1	4	3

τ_{even} is the value of τ when K_a is even, and τ_{odd} is the value of τ when K_a is odd. The analysis must be separated into τ = odd and τ = even parts due to torsional staggering.

Species Tag:	34005	Name:	SD
Version:	1		nu=0,1
Date:	Jan. 1997		$^2\Pi_i$ State
Contributor:	J. C. Pearson		Deuterium isotope

Lines Listed:	1125	Q(300.0)=	313.6878
Freq. (GHz) <	9999	Q(225.0)=	223.5794
Max. J:	33	Q(150.0)=	114.5516
LOGSTR0=	-14.0	Q(75.00)=	76.5070
LOGSTR1=	-12.0	Q(37.50)=	44.8539
Isotope Corr.:	-0.022	Q(18.75)=	30.2154
Egy. (cm^{-1}) >	0.0	Q(9.375)=	24.8860
μ_a =	0.7571	A=	
μ_b =		B=	146885.3
μ_c =		C=	

The data were taken from: E. Klisch, Th. Klaus, S. P. Belov, A. Dolgner, R. Schieder, G. Winnewisser and E. Herbst, 1996, Astrophys. J. **473**, 1118, W. L. Meerts and A. Dymanus, 1975, Can. J. Phys. **53**, 2123. The ground state A value was fixed to the electronic value of D. Zeitz, W. Bohle, J Werner, A. Hinz and W. Urban, 1985, Mol. Phys. **54**, 953.

The dipole moment is from W. L. Meerts and A. Dymanus, 1975, Can. J. Phys. **53**, 2123.

Species Tag:	35001	Name:	HDS
Version:	1		Hydrogen sulfide,
Date:	Jan. 1980		deuterium isotope
Contributor:	R. L. Poynter		

Lines Listed:	1138	Q(300.0)=	430.923
Freq. (GHz) <	2998	Q(225.0)=	280.931
Max. J:	20	Q(150.0)=	153.426
LOGSTR0=	-11.3	Q(75.00)=	54.752
LOGSTR1=	-9.3	Q(37.50)=	19.756
Isotope Corr.:	-3.523	Q(18.75)=	7.291
Egy. (cm^{-1}) >	0.0	Q(9.375)=	2.829
μ_a =	0.470	A=	292351.302
μ_b =	0.974	B=	147861.801
μ_c =		C=	96704.120

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. **40**, 125. The experimental measurements were taken from: R. E. Hillger and M. W. P. Strandberg, 1951, Phys. Rev. **83**, 575. P. Thaddeus, L. C. Krisher, and J. H. N. Loubser, 1964, J. Mol. Spect. **40**, 125. P. Helminger, F. C. De Lucia, and W. H. Kirchhoff, 1973, J. Phys. Chem. Ref. Data **2**, 215. G. Steenbeckeliers, quoted in F. J. Lovas, 1978, J. Phys. Chem. Ref. Data **7**, 1445.

The dipole moment was reported by R. E. Hillger and M. W. P. Strandberg, 1951, Phys. Rev. **83**, 575.

Species Tag:	36001	Name:	HCl
Version:	2		Hydrochloric acid
Date:	Jan. 1989		
Contributor:	H. M. Pickett		

Lines Listed:	137	Q(300.0)=	83.387
Freq. (GHz) <	9760	Q(225.0)=	63.358
Max. J:	18	Q(150.0)=	43.341
LOGSTR0=	-8.2	Q(75.00)=	23.372
LOGSTR1=	-11.3	Q(37.50)=	13.437
Isotope Corr.:	-0.122	Q(18.75)=	8.584
Egy. (cm^{-1}) >	0.0	Q(9.375)=	6.488
μ_a =	1.109	A=	
μ_b =		B=	312989.3
μ_c =		C=	

The experimental measurements were reported by I. G. Nolt *et al.*, 1987, J. Mol. Spect. **125**, 274. The dipole moment was measured by F. H. De Leeuw and A. Dymanus, 1971, 26th Symposium on Molecular Spectroscopy, Columbus, Ohio.

Species Tag:	37001	Name:	DCl
Version:	1		Hydrochloric acid,
Date:	Dec. 1990		deuterium isotope
Contributor:	H. M. Pickett		
Lines Listed:	228	Q(300.0)=	156.315
Freq. (GHz) <	8405	Q(225.0)=	117.517
Max. J:	29	Q(150.0)=	78.759
LOGSTR0=	-9.6	Q(75.00)=	40.050
LOGSTR1=	-12.4	Q(37.50)=	20.730
Isotope Corr.:	-3.9460	Q(18.75)=	11.122
Egy. (cm^{-1}) >	0.0	Q(9.375)=	6.434
μ_a =	1.1033	A=	
μ_b =		B=	163356.2
μ_c =		C=	

The experimental frequency measurements and dipole moment were reported by F. C. De Lucia, P. Helminger, and W. Gordy, 1971, Phys. Rev. A **3**, 1849.

Species Tag:	37002	Name:	C3H
Version:	1		2-Propynylidyne
Date:	Apr. 1995		ground $^2\Pi$ state
Contributor:	H. M. Pickett M. L. Delitsky		and $\nu_4 = 1$ $^2\Sigma^\mu$ state
Lines Listed:	4990	Q(300.0)=	6283.6523
Freq. (GHz) <	3438.1	Q(225.0)=	4622.2113
Max. J:	60	Q(150.0)=	2960.9861
LOGSTR0=	-10.	Q(75.00)=	1323.4710
LOGSTR1=	-100	Q(37.50)=	546.9895
Isotope Corr.:		Q(18.75)=	210.2441
Egy. (cm^{-1}) >	0.0,20.3	Q(9.375)=	84.0073
μ_a =	3.10	A=	
μ_b =		B=	11189.059
μ_c =		C=	

The observed lines and dipole moment are from: S. Yamamoto, S. Saito and M. Ohishi, 1990, Astrophys. J. **348**,363. C. A. Gottlieb, E. W. Gottlieb, P. Thaddeus and J. M. Vrtilek, 1986, Astrophys. J. **303**, 446.

The $\nu_4 = 1$ state is only 610 GHz above the ground state and is strongly coupled with the ground state. The form of the interaction is given in J. T. Hougen, 1962, J. Chem. Phys. **36**, 519. The dipole moment for the $\nu_4 = 1$ state is assumed to be the same as the ground state. There is a 0.5 Debye b symmetry moment between the ground state and $\nu_4 = 1$.

Species Tag:	37003	Name:	c-C3H
Version:	1		Cyclopropynylidyne,
Date:	Apr. 1995		X $^2B_2$
Contributor:	H. M. Pickett M. L. Delitsky		
Lines Listed:	2973	Q(300.0)=	10356.193
Freq. (GHz) <	1618	Q(225.0)=	6813.967
Max. J:	31	Q(150.0)=	3739.383
LOGSTR0=	-8.0	Q(75.00)=	1345.860
LOGSTR1=	-9.5	Q(37.50)=	497.050
Isotope Corr.:	0.0	Q(18.75)=	192.176
Egy. (cm^{-1}) >	0.0	Q(9.375)=	81.302
μ_a =	2.40	A=	44516.8
μ_b =		B=	34016.3
μ_c =		C=	19188.9

The observed lines and dipole moment are from: S. Yamamoto and S. Saito, 1994, J. Chem. Phys. **101**, 5484.S. Yamamoto and S. Saito, 1994, AIP document No. PAPS-JCPSA-101-5484-14. S. Yamamoto, *et al.*, 1987, Astrophys. J. **322**, L55.

A more recent dipole moment of 2.30(10) was reported by F. J. Lovas, R. D. Suenram, T. Ogata and S. Yamamoto, 1992, Astrophys. J. **399**, 325.

Species Tag:	38001	Name:	HCl-37
Version:	2		Hydrochloric acid,
Date:	Jan. 1989		^{37}Cl isotope
Contributor:	H. M. Pickett		
Lines Listed:	137	Q(300.0)=	83.522
Freq. (GHz) <	9746	Q(225.0)=	63.445
Max. J:	18	Q(150.0)=	43.401
LOGSTR0=	-8.2	Q(75.00)=	23.399
LOGSTR1=	-11.2	Q(37.50)=	13.452
Isotope Corr.:	-0.611	Q(18.75)=	8.590
Egy. (cm^{-1}) >	0.0	Q(9.375)=	6.491
μ_a =	1.109	A=	
μ_b =		B=	312519.12
μ_c =		C=	

The experimental measurements were reported by I. G. Nolt *et al.*, 1987, J. Mol. Spect. **125**, 274. The dipole moment was measured by F. H. De Leeuw and A. Dymanus, 1971, 26th Symposium on Molecular Spectroscopy, Columbus, Ohio.

Species Tag:	38002	Name:	c-C3H2
Version:	2		Cyclopropenylidene,
Date:	Jan. 1996		X $^1\Sigma^+$,
Contributor:	J. C. Pearson		ground state, ν_6, ν_5,
			ν_3, and ν_2 states
Lines Listed:	30436	Q(300.0)=	13229.4772
Freq. (GHz) <	9999	Q(225.0)=	8368.2600
Max. J:	50	Q(150.0)=	4516.4097
LOGSTR0=	-8	Q(75.00)=	1597.8914
LOGSTR1=	-8	Q(37.50)=	566.8561
Isotope Corr.:		Q(18.75)=	201.8429
Egy. (cm^{-1}) >	0.0	Q(9.375)=	72.4029
μ_a =		A=	35092.6
μ_b =	3.43	B=	32212.8
μ_c =		C=	16749.1

The observed lines are from: P. Thaddeus, J. M. Vrtilek and C. A. Gottlieb,1985, Astrophys. J. **299**, L63. M. Bogey, C. Demuynck and J. L. Destombes, 1986, Chem. Phys. Lett. **125**, 383. J. M. Vrtilek, C. A. Gottlieb and P. Thaddeus, 1987, Astrophys. J. **314**, 716. R. Mollaaghababa, C. A. Gottlieb, J. M. Vrtilek and P. Thaddeus, 1993, J. Chem. Phys. **99**, 890. Y. Hirahara, A. Masuda and K. Kawaguchi, 1991, J. Chem. Phys. **95**, 3975.

The vibrational quantum number 0 corresponds to the ground state, 1 to $\nu_6 = 1$ (Out-of-plane in phase CH bend), 2 to $\nu_5 = 1$ (Out-of-plane out of phase CH bend), 3 to $\nu_3 = 1$ (symmetric CC stretch + in-plane symmetric CC stretch), and 4 to $\nu_2 = 1$ (C=C stretch).

The dipole moment was measured by: H. Kanata, S. Yamamoto and S. Saito, 1987, Chem. Phys. Lett. **140**, 221.

Species Tag:	38003	Name:	C3D
Version:	1		2-Propynylidyne
Date:	Apr. 1995		deuterium isotope,
Contributor:	H. M. Pickett		ground $^2\Pi$ state
	M. L. Delitsky		and $\nu_4\,^2\Sigma$ state
Lines Listed:	1560	Q(300.0)=	3579.9410
Freq. (GHz) $<$	2650	Q(225.0)=	2661.2498
Max. J:	60	Q(150.0)=	1736.0584
LOGSTR0=	-10.	Q(75.00)=	814.1121
LOGSTR1=	-100	Q(37.50)=	361.2093
Isotope Corr.:		Q(18.75)=	147.2941
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	55.9382
μ_a =	3.10	A=	
μ_b =		B=	10097.38
μ_c =		C=	

The observed lines were measured by S. Yamamoto, S. Saito and M. Ohishi, 1990, Astrophys. J. **348**, 363. The dipole has been assumed to be the same as for the ground state.

The $\nu_4 = 1$ state is only 119 GHz above the ground state and is strongly coupled with the ground state. The form of the interaction is given in J. T. Hougen, 1962, J. Chem. Phys. **36**, 519. The dipole moment for the $\nu_4 = 1$ state is assumed to be the same as the ground state. There is a 0.5 Debye b–symmetry dipole moment between the ground state and $\nu_4 = 1$.

Species Tag:	38004	Name:	c-CCC-13-H
Version:	1		Cyclopropynylidyne,
Date:	May 1995		X $^2B_2$
Contributor:	H. M. Pickett		symmetric ^{13}C isotope
	M. L. Delitsky		
Lines Listed:	6541	Q(300.0)=	15508.4824
Freq. (GHz) <	2426	Q(225.0)=	11648.3337
Max. J:	20	Q(150.0)=	7197.9279
LOGSTR0=	-5	Q(75.00)=	2757.2417
LOGSTR1=	-100	Q(37.50)=	1021.5879
Isotope Corr.:	-1.955	Q(18.75)=	394.7191
Egy. (cm^{-1}) >	0.0	Q(9.375)=	166.7827
μ_a =	2.40	A=	44539.8
μ_b =		B=	32821.1
μ_c =		C=	18801.8

The observed lines and dipole moment are from: S. Yamamoto and S. Saito, 1994, J. Chem. Phys. **101**, 5484. S. Yamamoto and S. Saito, 1994, AIP document No. PAPS-JCPSA-101-5484-14. The dipole is assumed to be the same as the parent species.

A more recent dipole moment of 2.30(10) was reported by F. J. Lovas, R. D. Suenram, T. Ogata and S. Yamamoto, 1992, Astrophys. J. **399**, 325.

Species Tag:	38005	Name:	c-C-13-CCH
Version:	1		Cyclopropynylidyne,
Date:	May 1995		X $^2B_2$
Contributor:	M. L. Delitsky		asymmetric ^{13}C
	H. M. Pickett		isotope
Lines Listed:	9753	Q(300.0)=	31038.445
Freq. (GHz) <	2306	Q(225.0)=	23259.482
Max. J:	21	Q(150.0)=	14285.652
LOGSTR0=	-5.0	Q(75.00)=	5357.968
LOGSTR1=	-6.6	Q(37.50)=	1904.145
Isotope Corr.:	-1.654	Q(18.75)=	677.953
Egy. (cm^{-1}) >	1.7	Q(9.375)=	243.389
μ_a =	2.40	A=	42896.6
μ_b =		B=	33514.7
μ_c =		C=	18720.9

The observed lines and dipole moment are from: S. Yamamoto and S. Saito, 1994, J. Chem. Phys. **101**, 5484. S. Yamamoto and S. Saito, 1994, AIP document No. PAPS-JCPSA-101-5484-14. The dipole is assumed to be the same as the parent species.

A more recent dipole moment of 2.30(10) was reported by F. J. Lovas, R. D. Suenram, T. Ogata and S. Yamamoto, 1992, Astrophys. J. **399**, 325.

Species Tag:	38006	Name:	c-C3D Cyclopropynylidyne, X $^2B_2$ deuterium isotope
Version:	1		
Date:	July 1995		
Contributor:	H. M. Pickett M. L. Delitsky		
Lines Listed:	6001	Q(300.0)=	6057.0702
Freq. (GHz) <	2274	Q(225.0)=	5237.1339
Max. J:	13	Q(150.0)=	4000.4438
LOGSTR0=	-8	Q(75.00)=	2063.3289
LOGSTR1=	-100	Q(37.50)=	856.9516
Isotope Corr.:	-3.824	Q(18.75)=	334.7762
Egy. (cm^{-1}) >	0.0	Q(9.375)=	140.6562
μ_a =	2.40	A=	44517.2
μ_b =		B=	27917.1
μ_c =		C=	17080.7

The observed lines and dipole moment are from: S. Yamamoto and S. Saito, 1990, Astrophys. J. **363**, L13. F. J. Lovas, R. D. Suenram, T. Ogata and S. Yamamoto, 1992, Astrophys. J. **399**, 325. The dipole is assumed to be the same as the parent species.

A more recient dipole moment of 2.30(10) was reported by F. J. Lovas, R. D. Suenram, T. Ogata and S. Yamamoto, 1992, Astrophys. J. **399**, 325.

Species Tag:	39001	Name:	c-HC-13-CCH Cyclopropenylidene, X $^1\Sigma^+$, asymmetric ^{13}C isotope
Version:	2		
Date:	Jan. 1996		
Contributor:	J. C. Pearson		
Lines Listed:	17768	Q(300.0)=	6554.7149
Freq. (GHz) <	9999	Q(225.0)=	4258.7312
Max. J:	50	Q(150.0)=	2318.6532
LOGSTR0=	-8	Q(75.00)=	820.8744
LOGSTR1=	-8	Q(37.50)=	291.1880
Isotope Corr.:	-1.654	Q(18.75)=	103.6708
Egy. (cm^{-1}) >	0.0	Q(9.375)=	37.1776
μ_a =	0.51	A=	34857.2
μ_b =	3.39	B=	31288.5
μ_c =		C=	16443.0

The observed lines are from M. Bogey, C. Demuynck, J. L. Destombes and H. Dubus, 1987, J. Mol. Spect. **122**, 313.

The dipole moment for C_3H_2 was determined by H. Kanata, S. Yamamoto and S. Saito, 1987, Chem. Phys. Lett. **140**, 221. The dipole has been rotated according to the structure of Bogey *et al.* to get the a and b components.

Species Tag:	39002	Name:	c-HCC-13-CH
Version:	2		Cyclopropenylidene,
Date:	Jan. 1996		X $^1\Sigma^+$,
Contributor:	J. C. Pearson		symmetric ^{13}C
			isotope
Lines Listed:	6892	Q(300.0)=	6632.0611
Freq. (GHz) <	9999	Q(225.0)=	4308.6785
Max. J:	50	Q(150.0)=	2345.6810
LOGSTR0=	-8.0	Q(75.00)=	830.3995
LOGSTR1=	-8.0	Q(37.50)=	294.5571
Isotope Corr.:	-1.955	Q(18.75)=	104.8650
Egy. (cm^{-1}) >	0.0	Q(9.375)=	37.6022
μ_a =		A=	33310.5
μ_b =	3.43	B=	32212.6
μ_c =		C=	16331.3

The observed lines are from M. Bogey, C. Demuynck, J. L. Destombes and H. Dubus, 1987, J. Mol. Spect. **122**, 313.

The dipole moment for C_3H_2 was determined by H. Kanata, S. Yamamoto and S. Saito, 1987, Chem. Phys. Lett. **140**, 221.

Species Tag:	39003	Name:	c-C3HD
Version:	2		Mono-deutero
Date:	Jan. 1996		cyclopropenylidene,
Contributor:	J. C. Pearson		X $^1\Sigma^+$,
Lines Listed:	21610	Q(300.0)=	7401.0283
Freq. (GHz) <	9999	Q(225.0)=	4810.1694
Max. J:	50	Q(150.0)=	2618.8773
LOGSTR0=	-8	Q(75.00)=	927.0252
LOGSTR1=	-8	Q(37.50)=	328.7466
Isotope Corr.:	-3.523	Q(18.75)=	116.9743
Egy. (cm^{-1}) >	0.0	Q(9.375)=	41.8988
μ_a =	1.29	A=	34517.5
μ_b =	3.18	B=	26965.8
μ_c =		C=	15098.5

The observed lines are from M. Bogey, C. Demuynck, J. L. Destombes and H. Dubus, 1987, J. Mol. Spect. **122**, 313.

The dipole moment for C_3H_2 was determined by H. Kanata, S. Yamamoto and S. Saito, 1987, Chem. Phys. Lett. **140**, 221. The dipole has been rotated according to the structure of Bogey *et al.* to get the a and b components.

Species Tag:	39004	Name:	DCl-37
Version:	1		Hydrochloric acid,
Date:	Dec. 1990		deuterium ^{37}Cl
Contributor:	H. M. Pickett		isotope

Lines Listed:	228	Q(300.0)=	156.783
Freq. (GHz) <	8382	Q(225.0)=	117.869
Max. J:	29	Q(150.0)=	78.995
LOGSTR0=	-9.6	Q(75.00)=	40.161
LOGSTR1=	-12.4	Q(37.50)=	20.787
Isotope Corr.:	-4.4350	Q(18.75)=	11.151
Egy. (cm^{-1}) >	0.0	Q(9.375)=	6.448
μ_a =	1.1033	A=	
μ_b =		B=	161183.122
μ_c =		C=	

The experimental frequency measurements and dipole moment were reported by F. C. De Lucia, P. Helminger, and W. Gordy, 1971, Phys. Rev. A **3**, 1849.

Species Tag:	40001	Name:	CH3CCH
Version:	1		Propyne
Date:	Dec. 1979		
Contributor:	R. L. Poynter		

Lines Listed:	813	Q(300.0)=	5428.751
Freq. (GHz) <	1345	Q(225.0)=	3524.521
Max. J:	79	Q(150.0)=	1920.879
LOGSTR0=	-6.7	Q(75.00)=	679.673
LOGSTR1=	-5.8	Q(37.50)=	241.268
Isotope Corr.:	0.	Q(18.75)=	88.267
Egy. (cm^{-1}) >	0.0	Q(9.375)=	34.419
μ_a =	0.75	A=	158590.
μ_b =		B=	8545.86
μ_c =		C=	B

The experimental measurements were obtained from A. Dubrulle, D. Boucher, J. Burie, and J. Demaison, 1978, J. Mol. Spect. **72**, 158. The A rotational constant was estimated from the structure. The dipole moment was measured by J. S. Muenter and V. W. Laurie, 1966, J. Chem. Phys. **45**, 855.

Species Tag:	40002	Name:	NaOH
Version:	1		Sodium hydroxide
Date:	Aug. 1987		
Contributor:	R. L. Poynter		

Lines Listed:	91	Q(300.0)=	498.884
Freq. (GHz) <	2201	Q(225.0)=	374.025
Max. J:	91	Q(150.0)=	249.345
LOGSTR0=	-6.3	Q(75.00)=	124.767
LOGSTR1=	-8.0	Q(37.50)=	62.532
Isotope Corr.:	0.0	Q(18.75)=	31.427
Egy. (cm^{-1}) >	0.0	Q(9.375)=	15.882
μ_a =	1.0	A=	
μ_b =		B=	12567.0590(120)
μ_c =		C=	

The measured lines were taken from E. F. Pearson and M. B. Trueblood, 1973, Astrophys. J. Lett. Ed. **179**, L146, and P. Kuipers *et al.*, 1976, Chem. Phys. **15**, 457. Because no dipole moment measurement has been reported, we assumed a value of unity in our calculation. Two theoretical estimates have been published: N. G. Rambidi, Yu. G. Abashkin, and A. I. Dement'ev, 1984, Russ. J. Inorg. Chem. **29**, 12–22, and G. A. Long, J. F. Capitani, and L. Pedersen, 1983, J. Mol. Struct. **105**, 229–230. Of these, the Rambidi *et al.* value is closer to our estimate of 6.63 Debye with an estimated error of maybe 1 Debye, which is based upon extrapolations from the dipole moments of Li, Cs, and Na fluorides and the Cs and Li hydroxides. The Rambidi *et al.* value is 6.706 debye, while the Long *et al.* value ranges between 6.30 and 5.42 debye, depending on the basis set used in their calculations. The line intensities should be multiplied by a factor of about 44 to get something closer to the right value. The theoretical calculations suggest that this molecule is linear. A measurement is needed.

Species Tag:	40003	Name:	SiC
Version:	1		X $^3\Pi$, v = 0 state
Date:	Dec. 1994		
Contributor:	H. M. Pickett		
Lines Listed:	982	Q(300.0)=	1567.7215
Freq. (GHz) <	9999	Q(225.0)=	1105.7351
Max. J:	90	Q(150.0)=	667.1014
LOGSTR0=	-7.0	Q(75.00)=	265.0090
LOGSTR1=	-9.0	Q(37.50)=	103.4726
Isotope Corr.:	0.0	Q(18.75)=	46.3133
Egy. (cm^{-1}) >	0.0	Q(9.375)=	24.9717
μ_a =	1.7	A=	
μ_b =		B=	20297.582
μ_c =		C=	

The millimeter lines are from J. Cernicharo, C. A. Gottlieb, M. Guelin, P. Thaddeus, and J. M. Vrtilek, 1989, Astrophys. J. Lett. Ed. **341**, L25-28. The dipole moment is a theoretical one quoted in this reference. The partition functions are based on a sum of states for the ground and first vibrationally excited state. The spectra were fitted to a Hunds case (b) Hamiltonian. The correlation of states in case (b) with those for case (a) are:

N = J $\Omega = 0$
N = J + 1 $\Omega = 1$
N = J − 1 $\Omega = 2$

Species Tag:	40004	Name:	SiC
Version:	1		X $^3\Pi$, v = 1 state
Date:	Dec. 1994		
Contributor:	H. M. Pickett		
Lines Listed:	703	Q(300.0)=	1567.7215
Freq. (GHz) $<$	9999	Q(225.0)=	1105.7351
Max. J:	90	Q(150.0)=	667.1014
LOGSTR0=	-7.0	Q(75.00)=	265.0090
LOGSTR1=	-9.0	Q(37.50)=	103.4726
Isotope Corr.:	0.0	Q(18.75)=	46.3133
Egy. (cm^{-1}) $>$	950.0	Q(9.375)=	24.9717
μ_a =	1.7	A=	
μ_b =		B=	20297.582
μ_c =		C=	

The millimeter lines are from R. Mollaaghababa, C. A. Gottlieb, J. M. Vrtilek, and P. Thaddeus, 1990, Astrophys. J. Lett. Ed. **352**, L21-23. The dipole moment is a theoretical one. (See ground state species.) The partition functions are based on a sum of states for the ground and first vibrationally excited state. The spectra were fitted to a Hunds case (b) Hamiltonian. The correlation of states in case (b) with those for case (a) are:

$$\begin{array}{ll} N = J & \Omega = 0 \\ N = J + 1 & \Omega = 1 \\ N = J - 1 & \Omega = 2 \end{array}$$

Species Tag:	40005	Name:	KH
Version:	1		Potassium hydride,
Date:	Sept 1995		$\nu = 0, 1$
Contributor:	M. L. Delitsky H. M. Pickett		
Lines Listed:	40	Q(300.0)=	63.101
Freq. (GHz) <	3894	Q(225.0)=	46.995
Max. J:	20	Q(150.0)=	31.331
LOGSTR0=	-20	Q(75.00)=	15.810
LOGSTR1=	-100	Q(37.50)=	8.072
Isotope Corr.:	-0.030	Q(18.75)=	4.215
Egy. (cm^{-1}) >	0.0	Q(9.375)=	2.303
$\mu_a =$	8.136	A=	
$\mu_b =$		B=	101152.1
$\mu_c =$		C=	

No rotational transitions were available. The IR transitions were taken from: Haese, Liu and Altman, 1984, J. Chem. Phys. **81**, 3766. Additional information on excited vibrational states and the electronic states is reviewed in Stwalley, W. C., *et al.*, 1991, J. Phys. Chem. Ref. Data **20**, 153.

The dipole moment was from: Langhoff, *et al.*, 1986, J. Chem. Phys. **85**, 5158.

Species Tag:	40006	Name:	C2O
Version:	1		Dicarbon monoxide
Date:	April 1996		X $^3\Sigma^-$
Contributor:	H. S. P. Müller		
Lines Listed:	354	Q(300.0)=	1625.5036
Freq. (GHz) <	1632	Q(225.0)=	1219.2029
Max. J:	70	Q(150.0)=	812.8704
LOGSTR0=	-9.0	Q(75.00)=	406.6471
LOGSTR1=	-8.0	Q(37.50)=	203.5847
Isotope Corr.:		Q(18.75)=	102.0790
Egy. (cm^{-1}) >	0.0	Q(9.375)=	51.3580
μ_a =	1.305	A=	
μ_b =		B=	11545.597
μ_c =		C=	

The data were taken from (1) C. Yamada, S. Saito, H. Kanamori, and E. Hirota, 1985, Astrophys. J. **290**, L65, and (2) Y. Ohshima, Y. Endo, and T. Ogata, 1995, J. Chem. Phys. **102** 1493.

The dipole moment is from an *ab initio* calculation: (3) C. Thomson and B. J. Wishart, 1973, Theor. Chim. Acta **31**, 347.

Species Tag:	40007	Name:	MgO, v = 0, 1
Version:	1		Magnesium oxide,
Date:	Sep. 1997		X $^{1}\Sigma^{+}$
Contributor:	H. S. P. Müller		

Lines Listed:	44	Q(300.0)=	374.621
Freq. (GHz) $<$	1500	Q(225.0)=	276.000
Max. J:	44	Q(150.0)=	182.838
LOGSTR0=	-6.0	Q(75.00)=	91.495
LOGSTR1=	-3.5	Q(37.50)=	45.906
Isotope Corr.:	-0.1051	Q(18.75)=	23.120
Egy. (cm^{-1}) $>$	0.0, 774.74	Q(9.375)=	11.731
μ_a =	6.88	A=	
μ_b =		B=	17149.38, 16989.58
μ_c =		C=	

The lines of the $v = 0$, 1, 2 were taken from (1) T. Törring and J. Hoeft, 1986, Chem. Phys. Lett. **126**, 477. Infrared transitions reported by (2) S. Civiš, H. G. Hedderich, and C. G. Blom, 1991, Chem. Phys. Lett. **176**, 489, were also used in the fit. The dipole moment is taken from an *ab initio* calculation by (3) P. W. Fowler and A. J. Sedlej, 1991, Mol. Phys. **73**, 43.

Species Tag:	41001	Name:	CH3CN
Version:	3		Acetonitrile
Date:	Jan. 1997		Methyl Cyanide
Contributor:	J. C. Pearson		nu_8=0,1
Lines Listed:	29304	Q(300.0)=	41079.2740
Freq. (GHz) <	1832	Q(225.0)=	23622.3423
Max. J:	99	Q(150.0)=	11400.2610
LOGSTR0=	-12.0	Q(75.00)=	3803.0012
LOGSTR1=	-10.0	Q(37.50)=	1347.2433
Isotope Corr.:	0.	Q(18.75)=	492.9504
Egy. (cm^{-1}) >	0.0	Q(9.375)=	192.2864
μ_a =	3.92197(13)	A=	158099.0
μ_b =		B=	9198.9
μ_c =		C=	B

The experimental measurements are from: D. Boucher, J. Burie, J. Demaison, A. Dubrulle, J. Legrand, and B. Segard, 1977, J. Mol. Spect. **64**, 290; A. Bauer and S. Maes, 1969, J. Phys. **30**, 169; S. G. Kukolich, D. J. Ruben, J. H. S. Wang, and J. R. Williams, 1973, J. Chem. Phys. **58**, 3155; S. G. Kukolich, G. Lind, M. Barfield, L. Faehl and J. L. Marshall, 1978, J. Am. Chem. Soc. **100**, 7155; S. G. Kukolich, 1982, J. Chem. Phys. **76**, 97; P. Venkateswarlu, J. G. Baker and W. Gordy, 1961, J. Mol. Spectrosc. **6**, 215. D. Boucher, J. Burie, A. Bauer, A. Dubrulle and J. Demaison, 1980, J. Phys. Chem. Ref. Data **9**, 659; F. S. Pavone, L. R. Zink, M. Prevedelli, M. Inguscio and L. Fusina, 1990, J. Mol. Spectrosc. **144**, 45; W. Chen, R. Bocquet, D. Boucher, J. Demaison and G. Wlodarczak, 1991, J. Mol. Spectrosc. **150**, 470; F. X. Brown, D. Dangoisse, and J. Demaison, 1988, J. Mol. Spectrosc. **129**, 483; R. Bocquet, G. Wlodarczak, A. Bauer and J. Demaison, 1988, J. Mol. Spectrosc. **127**, 382; F. Lewen, S. P. Belov, F. Maiwald, Th. Klaus and G. Winnewisser, 1995, Z. Naturforsch. **50a**, 1182; and J. C. Pearson and H. S. P. Müller, 1996, Astrophys. J. **471**, 1067.

The constants A, DK, HK cannot be determined from the microwave spectra and were fixed to the IR measurements of: R. Anttila, V.-M. Horneman, M. Koivussaari and R. Paso, 1993, J. Mol. Spectrosc. **157**, 198. M. Koivussaari, V.-M. Horneman and R. Anttila, 1992, J. Mol. Spectrosc. **152**, 377.

The dipole moment for the ground state was reported by J. Gadhi, A. Lahrouni, J. Legrand and J. Demaison, 1995, J. Chim. Phys. **92**, 1984. The nu_8 dipole was scaled from the ground state value by the amount in J. K. Messer and J. A. Roerts, 1982, J. Mol. Spectrosc. **96**, 351.

The v quantum numbers assign the following: 0 is the ground state, 1 is the K*l¡0 l doublet of nu_8=1, 2 is the K*l¿/=0 doublet of nu_8=1. The v8=1 (CCN bending) band energy of 365.015965(12) cm^{-1} (Koivusaari *et al.*) has been included in the calculation. The constants Pz^3 and Pz^5 off diagonal were fixed to the values of Koivusaari *et al.*.

Species Tag:	41002	Name:	CH3CC-13-H
Version:	1		Propyne,
Date:	Dec. 1979		^{13}C isotope
Contributor:	R. L. Poynter		on atom 1

Lines Listed:	822	Q(300.0)=	5596.288
Freq. (GHz) <	1323	Q(225.0)=	3633.290
Max. J:	80	Q(150.0)=	1979.703
LOGSTR0=	-6.7	Q(75.00)=	700.648
LOGSTR1=	-5.8	Q(37.50)=	248.657
Isotope Corr.:	-1.955	Q(18.75)=	90.970
Egy. (cm^{-1}) >	0.0	Q(9.375)=	35.465
μ_a =	0.750	A=	158590.
μ_b =		B=	8290.3
μ_c =		C=	B

The experimental measurements are from: D. Boucher, J. Burie, J. Demaison, A. Dubrulle, J. Legrand, and B. Segard, 1977, J. Mol. Spect. **64**, 290. A. Bauer and S. Maes, 1969, J. Phys. **30**, 169. S. G. Kukolich, D. J. Ruben, J. H. S. Wang, and J. R. Williams, 1973, J. Chem. Phys. **58**, 3155.

The dipole moment was reported by P. A. Steiner and W. Gordy, 1966, J. Mol. Spect. **21**, 291.

Species Tag:	41003	Name:	CH3C-13-CH Propyne, ^{13}C isotope on atom 2
Version:	1		
Date:	Dec. 1979		
Contributor:	R. L. Poynter H. M. Pickett		

Lines Listed:	813	Q(300.0)=	5431.252
Freq. (GHz) <	1344	Q(225.0)=	3526.145
Max. J:	79	Q(150.0)=	1921.764
LOGSTR0=	-6.7	Q(75.00)=	679.986
LOGSTR1=	-5.8	Q(37.50)=	241.324
Isotope Corr.:	-1.955	Q(18.75)=	88.308
Egy. (cm^{-1}) >	0.0	Q(9.375)=	34.435
μ_a =	0.75	A=	158590.
μ_b =		B=	8542.3
μ_c =		C=	B

The experimental measurements are from: D. Boucher, J. Burie, J. Demaison, A. Dubrulle, J. Legrand, and B. Segard, 1977, J. Mol. Spect. **64**, 290. A. Bauer and S. Maes, 1969, J. Phys. **30**, 169. S. G. Kukolich, D. J. Ruben, J. H. S. Wang, and J. R. Williams, 1973, J. Chem. Phys. **58**, 3155.

The dipole moment was reported by P. A. Steiner and W. Gordy, 1966, J. Mol. Spect. **21**, 291.

Species Tag:	41004	Name:	C-13-H3CCH
Version:	1		Propyne,
Date:	Dec. 1979		^{13}C isotope
Contributor:	R. L. Poynter		on atom 3
Lines Listed:	821	Q(300.0)=	5580.846
Freq. (GHz) <	1325	Q(225.0)=	3623.263
Max. J:	80	Q(150.0)=	1974.240
LOGSTR0=	-6.7	Q(75.00)=	698.715
LOGSTR1=	-5.8	Q(37.50)=	247.970
Isotope Corr.:	-1.955	Q(18.75)=	90.719
Egy. (cm^{-1}) >	0.0	Q(9.375)=	35.375
μ_a =	0.750	A=	158590.
μ_b =		B=	8313.24
μ_c =		C=	B

The experimental measurements are from: D. Boucher, J. Burie, J. Demaison, A. Dubrulle, J. Legrand, and B. Segard, 1977, J. Mol. Spect. **64**, 290. A. Bauer and S. Maes, 1969, J. Phys. **30**, 169. S. G. Kukolich, D. J. Ruben, J. H. S. Wang, and J. R. Williams, 1973, J. Chem. Phys. **58**, 3155.

The dipole moment was reported by P. A. Steiner and W. Gordy, 1966, J. Mol. Spect. **21**, 291.

Species Tag:	41005	Name:	CH3CCD
Version:	2		Propyne,
Date:	Jan. 1984		D isotope
Contributor:	R. L. Poynter		on C atom 1

Lines Listed:	822	Q(300.0)=	17190.957
Freq. (GHz) <	623	Q(225.0)=	11168.629
Max. J:	40	Q(150.0)=	6140.446
LOGSTR0=	-7.7	Q(75.00)=	2243.365
LOGSTR1=	-5.2	Q(37.50)=	795.243
Isotope Corr.:	-3.824	Q(18.75)=	290.469
Egy. (cm^{-1}) >	0.0	Q(9.375)=	113.162
μ_a =	0.77	A=	158590.
μ_b =		B=	7788.170
μ_c =		C=	B

The experimental measurements are from: J. S. Muenter and V. W. Laurie, 1966, J. Chem. Phys. **45**, 855. L. F. Thomas, E. I. Sherrard, and J. Sheridan, 1955, Trans. Farady. Soc. **51**, 619. C. D. Cogley, L. M. Tack, and S. G. Kukolich, 1982, J. Chem. Phys. **76**, 5669. The dipole moment was taken from Muenter and Laurie, above.

Species Tag:	41006	Name:	CH2DCCH
Version:	2		Propyne,
Date:	Aug. 1983		deuterium isotope
Contributor:	R. L. Poynter		on methyl carbon
Lines Listed:	223	Q(300.0)=	4428.943
Freq. (GHz) <	244	Q(225.0)=	2874.750
Max. J:	15	Q(150.0)=	1633.428
LOGSTR0=	-9.2	Q(75.00)=	904.899
LOGSTR1=	-5.1	Q(37.50)=	410.299
Isotope Corr.:	-3.347	Q(18.75)=	156.171
Egy. (cm^{-1}) >	0.0	Q(9.375)=	55.873
μ_a =	0.750	A=	117744.370
μ_b =		B=	8155.784
μ_c =		C=	8025.577

The experimental measurements are from L. F. Thomas, E. I. Sherrard, and J. Sheridan, 1955, Trans. Farady. Soc. **54**, 619. The dipole moment was assumed to be the same as for the parent species for this calculation.

Species Tag:	41007	Name:	Si^{13}C
Version:	1		X $^3\Pi$, v = 0 state
Date:	Dec. 1994		^{13}C isotope
Contributor:	H. M. Pickett		
Lines Listed:	2417	Q(300.0)=	3277.5992
Freq. (GHz) <	9999	Q(225.0)=	2330.4095
Max. J:	90	Q(150.0)=	1408.5707
LOGSTR0=	-7.0	Q(75.00)=	559.0332
LOGSTR1=	-9.0	Q(37.50)=	217.8318
Isotope Corr.:	0.0	Q(18.75)=	97.1513
Egy. (cm^{-1}) >	0.0	Q(9.375)=	52.0619
μ_a =	1.7	A=	
μ_b =		B=	19203.84
μ_c =		C=	

The millimeter lines are from R. Mollaaghababa, C. A. Gottlieb, J. M. Vrtilek, and P. Thaddeus, 1990, Astrophys. J. Lett. Ed. **352**, L21-23. The dipole moment is a theoretical one. (See normal isotope.) The spectra were fitted to a Hunds case (b) Hamiltonian. The correlation of states in case (b) with those for case (a) are:

N = J	$\Omega = 0$
N = J + 1	$\Omega = 1$
N = J − 1	$\Omega = 2$

Species Tag:	41008	Name:	CaH
Version:	1		$X^2\Sigma^+$ state
Date:	Mar. 1995		^{40}Ca isotope
Contributor:	H. M. Pickett		

Lines Listed:	387	Q(300.0)=	199.434
Freq. (GHz) <	9726	Q(225.0)=	149.727
Max. J:	36	Q(150.0)=	100.161
LOGSTR0=	-16.6	Q(75.00)=	50.711
LOGSTR1=	-19.4	Q(37.50)=	26.044
Isotope Corr.:	-0.0137	Q(18.75)=	13.753
Egy. (cm^{-1}) >	0.0	Q(9.375)=	7.693
μ_a =	1.0	A=	
μ_b =		B=	126772.9
μ_c =		C=	

The rotational data are from C. I. Frum, J. J. Oh, E. A. Cohen, and H. M. Pickett, 1993, Ap. J. **408**, L61-64. These data were fitted with vibrational data from C. I. Frum and H. M. Pickett, 1993, J. Mol. Spect. **159**, 329-336. The dipole moment used is arbitrary.

Species Tag:	41009	Name:	CH3NC
Version:	1		Methyl isocyanide
Date:	Apr. 1995		
Contributor:	M. L. Delitsky		
	H. M. Pickett		
Lines Listed:	1798	Q(300.0)=	9283.0358
Freq. (GHz) <	1972	Q(225.0)=	6028.9376
Max. J:	98	Q(150.0)=	3281.9883
LOGSTR0=	-8.0	Q(75.00)=	1161.2742
LOGSTR1=	-100	Q(37.50)=	412.2614
Isotope Corr.:	0.0	Q(18.75)=	150.8351
Egy. (cm^{-1}) >	0.0	Q(9.375)=	58.8524
μ_a =	3.890	A=	157151.
μ_b =		B=	10052.9
μ_c =		C=	B

The observed lines are from A. Bauer and M. Bogey, 1970, C. R. Acad. Sc. Ser. B. **271**, 892.

The dipole moment is from J. Cernicharo *et al.*, 1988, Astron. Astrophys. **189**, L1.

Species Tag:	42001	Name:	CH3CN-15
Version:	2		Acetonitrile,
Date:	April 1996		^{15}N isotope
Contributor:	J. C. Pearson		
Lines Listed:	2755	Q(300.0)=	10431.6539
Freq. (GHz) <	1753	Q(225.0)=	6774.0689
Max. J:	99	Q(150.0)=	3687.0984
LOGSTR0=	-10.0	Q(75.00)=	1304.3304
LOGSTR1=	-10.0	Q(37.50)=	462.9494
Isotope Corr.:	-2.432	Q(18.75)=	169.3726
Egy. (cm^{-1}) >	0.0	Q(9.375)=	66.0525
μ_a =	3.9256(7)	A=	158107.7
μ_b =		B=	8922.0
μ_c =		C=	B

The experimental measurements are from: D. Boucher, J. Burie, A. Bauer, A. Dubrulle and J. Demaison, 1980, J. Phys. Chem. Ref. Data **9**, 659., J. C. Pearson and H. S. P. Müller, 1996, Astrophys J. 471, in press, and B. Gatehouse and T. Brupbacher, 1996, private communication.

The details of the analysis are presented in the Pearson and Müller paper. The constants A, D$_K$, H$_K$ cannot be determined from the microwave spectra and were determined by scaling the IR measurements of: R. Anttila, V.-M. Horneman, M. Koivussaari and R. Paso, 1993, J. Mol. Spect. **157**, 198, and M. Koivussaari, V.-M. Horneman and R. Anttila, 1992, J. Mol. Spect. **152**, 377 by the ground state average (r$_z$) structure differences from normal species. Other higher order constants (H$_J$, L$_{JJK}$, L$_{JK}$, L$_{KKJ}$) were fixed to scaled from the normal species (tag 41001).

The dipole moment was reported by A. Mito, J. Sakai, and M. Katayama, 1984, J. Mol. Spect. **103**, 26.

Species Tag:	42002	Name:	CH2CO
Version:	1		Ketene
Date:	Jan. 1980		
Contributor:	R. L. Poynter		

Lines Listed:	835	Q(300.0)=	10322.862
Freq. (GHz) <	592	Q(225.0)=	6634.375
Max. J:	29	Q(150.0)=	3433.998
LOGSTR0=	-16.7	Q(75.00)=	1285.879
LOGSTR1=	-17.1	Q(37.50)=	457.088
Isotope Corr.:	0.	Q(18.75)=	157.217
Egy. (cm^{-1}) >	0.0	Q(9.375)=	47.577
μ_a =	1.422	A=	282473.
μ_b =		B=	10293.80
μ_c =		C=	9916.38

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. **41**, 333. The measurements were taken from: B. Fabricant, D. Krieger, and J. S. Muenter, 1977, J. Chem. Phys. **67**, 1576. J. W. C. Johns, J. M. R. Stone, and G. Winnewisser, 1972, J. Mol. Spect. **42**, 523. H. R. Johnson and M. W. P. Strandberg, 1952, J. Chem. Phys. **20**, 687.

The dipole moment was reported by Johnson (above) and B. Fabricant *et al.* (above).

Species Tag:	42003	Name:	NH2CN
Version:	1		Cyanamide
Date:	Jan. 1991		
Contributor:	E. A. Cohen		
Lines Listed:	13898	Q(300.0)=	17902.305
Freq. (GHz) <	9299	Q(225.0)=	11228.962
Max. J:	90	Q(150.0)=	5730.062
LOGSTR0=	-9.0	Q(75.00)=	1730.290
LOGSTR1=	-8.0	Q(37.50)=	506.222
Isotope Corr.:	0.0	Q(18.75)=	152.887
Egy. (cm^{-1}) >	0.0	Q(9.375)=	44.101
μ_a =	4.3269	A=	312141.88
μ_b =		B=	10129.758
μ_c =	-0.9612	C=	9865.924

The fit is based on microwave data reported by W. Read *et al.*, 1986, J. Mol. Spect. **115**, 316, and several far-infrared laser sideband measurements near 2.6 THz and far-infrared FT measurements of H. Birk, 1988, Thesis, Justus Liebig-Universit at Gießen. The data include transitions with $J \leq 70,\ K_a \leq 9$. The partition function includes both inversion states for $J < 90, K_a < 17$. Nitrogen quadrupole splittings are not given. The rotational constants and μ_a given above are for the lower inversion state. μ_c connects the two states. For $K_a > 9$ there is a perturbation from another vibrational state and the predictions have been truncated at that point. Frequencies for which the experimental uncertainty is greater than 200 kHz have not been merged with the calculated frequencies.

Species Tag:	42004	Name:	CaD
Version:	1		^{40}Ca^{2}H isotope
Date:	Mar. 1995		X$^2\Sigma^+$ state
Contributor:	H. M. Pickett		

Lines Listed:	501	Q(300.0)=	579.162
Freq. (GHz) <	4650	Q(225.0)=	434.410
Max. J:	39	Q(150.0)=	290.001
LOGSTR0=	-7.7	Q(75.00)=	145.848
LOGSTR1=	-8.0	Q(37.50)=	73.909
Isotope Corr.:	-3.8376	Q(18.75)=	37.993
Egy. (cm^{-1}) >	0.0	Q(9.375)=	20.100
μ_a =	1.0	A=	
μ_b =		B=	625623.19
μ_c =		C=	

The rotational data are from C. I. Frum, J. J. Oh, E. A. Cohen, and H. M. Pickett, 1993, Astrophys. J. **408**, L61-64. The dipole moment used is arbitrary.

Species Tag:	42005	Name:	K-41-H
Version:	1		Potassium hydride,
Date:	Oct. 1995		^{41}K isotope
Contributor:	M.L. Delitsky		$\nu = 0$, 1
	H.M. Pickett		
Lines Listed:	40	Q(300.0)=	63.097
Freq. (GHz) <	3899	Q(225.0)=	46.993
Max. J:	20	Q(150.0)=	31.331
LOGSTR0=	-20	Q(75.00)=	15.811
LOGSTR1=	-100	Q(37.50)=	8.073
Isotope Corr.:	-1.167	Q(18.75)=	4.215
Egy. (cm^{-1}) >	0.0	Q(9.375)=	2.303
μ_a =	8.136	A=	
μ_b =	8.136	B=	101141.3
μ_c =		C=	

No rotational transitions were available. The IR transitions were taken from: Haese, Liu and Altman, 1984, J. Chem. Phys. **81**, 3766. Additional information on excited vibrational states and the electronic states is reviewed in W. Stwalley *et al.*, 1991, J. Phys. Chem. Ref. Data **20**,153.

The dipole moment for the parent species of Langhoff *et al.*, 1986, J. Chem. Phys. **85**, 5158 was assumed.

The values of Y_{12}, Y_{03}, and Y_{13} were constrained by isotope relations to values from the main isotope.

Species Tag:	42006	Name:	C-13-H3CN
Version:	1		Acetonitrile,
Date:	April 1996		^{13}C on methyl isotope
Contributor:	J. C. Pearson		

Lines Listed:	9015	Q(300.0)=	31255.7307
Freq. (GHz) <	1773	Q(225.0)=	20296.6968
Max. J:	99	Q(150.0)=	11047.3940
LOGSTR0=	-10.0	Q(75.00)=	3908.0709
LOGSTR1=	-10.0	Q(37.50)=	1387.1037
Isotope Corr.:	-1.955	Q(18.75)=	507.4819
Egy. (cm^{-1}) >	0.0	Q(9.375)=	197.9113
μ_a =	3.92197(13)	A=	158107.7
μ_b =		B=	8933.3
μ_c =		C=	B

The experimental measurements are from: D. Boucher, J. Burie, A. Bauer, A. Dubrulle and J. Demaison, 1980, J. Phys. Chem. Ref. Data **9**, 659., J. C. Pearson and H. S. P. Müller, 1996, Astrophys J. Lett., submitted., and B. Gatehouse and T. Brupbacher, 1996, private communication.

The details of the analysis are presented in the Pearson and Müller paper. The constants A, D$_K$, H$_K$ cannot be determined from the microwave spectra and were determined by scaling the IR measurements of: R. Anttila, V.-M. Horneman, M. Koivussaari and R. Paso, 1993, J. Mol. Spect. **157**, 198, and M. Koivussaari, V.-M. Horneman and R. Anttila, 1992, J. Mol. Spect. **152**, 377 by the ground state average (r$_z$) structure differences from normal species. Other higher order constants (H$_J$, L$_{JJK}$, L$_{JK}$, L$_{KKJ}$) were fixed to scaled from the normal species (tag 41001).

The dipole moment was fixed to the main isotope reported by J. Gadhi, A. Lahrouni, J. Legrand, and J. Demaison, 1995, J. Chem. Phys. **92**, 1984.

Species Tag:	42007	Name:	CH3C-13-N
Version:	1		Acetonitrile,
Date:	April 1996		^{13}C on cyanide isotope
Contributor:	J. C. Pearson		

Lines Listed:	8951	Q(300.0)=	30370.2787
Freq. (GHz) <	1824	Q(225.0)=	19721.7674
Max. J:	99	Q(150.0)=	10734.5468
LOGSTR0=	-10.0	Q(75.00)=	3797.4978
LOGSTR1=	-10.0	Q(37.50)=	1347.9284
Isotope Corr.:	-1.955	Q(18.75)=	493.1997
Egy. (cm^{-1}) >	0.0	Q(9.375)=	192.3824
μ_a =	3.92197(13)	A=	158093.3
μ_b =		B=	9194.35
μ_c =		C=	B

The experimental measurements are from: D. Boucher, J. Burie, A. Bauer, A. Dubrulle and J. Demaison, 1980, J. Phys. Chem. Ref. Data **9**, 659., S. G. Kukolich, G. Lind, M. Barfield, L. Faehl, and J. L. Marshall, 1978, J. Am. Chem. Soc. **100**, 7155., S. G. Kukolich, 1982, J. Chem. Phys. **76**, 97., and J. C. Pearson and H. S. P. Müller, 1996, Astrophys J. Lett., submitted.

The details of the analysis are presented in the Pearson and Müller paper. The constants A, D_K, H_K cannot be determined from the microwave spectra and were determined by scaling the IR measurements of: R. Anttila, V.-M. Horneman, M. Koivussaari and R. Paso, 1993, J. Mol. Spect. **157**, 198, and M. Koivussaari, V.-M. Horneman and R. Anttila, 1992, J. Mol. Spect. **152**, 377 by the ground state average (r_z) structure differences from normal species. Other higher order constants (H_J, L_{JJK}, L_{JK}, L_{KKJ}) were fixed to scaled from the normal species (tag 41001).

The dipole moment was fixed to the main isotope reported by J. Gadhi, A. Lahrouni, J. Legrand, and J. Demaison, 1995, J. Chem. Phys. **92**, 1984.

Species Tag:	42008	Name:	CH2DCN
Version:	1		Acetonitrile,
Date:	June 1996		^{2}H isotope
Contributor:	J. C. Pearson		

Lines Listed:	19256	Q(300.0)=	9187.2850
Freq. (GHz) <	6443	Q(225.0)=	5965.7607
Max. J:	99	Q(150.0)=	3246.9912
LOGSTR0=	-10.0	Q(75.00)=	1148.5542
LOGSTR1=	-10.0	Q(37.50)=	406.7303
Isotope Corr.:	-3.347	Q(18.75)=	144.3101
Egy. (cm^{-1}) >	0.0	Q(9.375)=	51.3918
μ_a =	3.9201	A=	121074.5
μ_b =	0.1735	B=	8759.2
μ_c =		C=	8608.5

The experimental lines are from L. F. Thomas, E. J. Sherrard and J. Sheridan, 1955, Trans. Faraday Soc. **51**, 619; M. Le Guennec, G. Wlodarczak, J. Burie and J. Demaison, 1992, J. Mol. Spectrosc. **154**, 305.

The molecule was first observed in the interstellar medium by M. Gerin, F. Combs, G. Wlodarczak, T. Jacq, M Guelin, P Encrenaz, and C. Laurent, 1992, Astron. Astrophys. **259) L35.**

The dipole moment was calculated by axis rotation from the main isotope value reported by J. Gadhi, A. Lahrouni, J. Legrand, and J. Demaison, 1995, J. Chim, Phys. 92, 1984.

Species Tag:	**42009**	**Name:**	**H2CSi**
Version:	**1**		**Silylidene**
Date:	**Oct. 1996**		**Si-28 isotope**
Contributor:	**H. S. P. Müller**		
Lines Listed:	**670**	**Q(300.0)=**	**6256.484**
Freq. (GHz) <	**1700**	**Q(225.0)=**	**4070.529**
Max. J:	**60**	**Q(150.0)=**	**2214.889**
LOGSTR0=	**-11.0**	**Q(75.00)=**	**783.014**
LOGSTR1=	**-6.0**	**Q(37.50)=**	**278.008**
Isotope Corr.:	**-0.035**	**Q(18.75)=**	**102.907**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**42.781**
μ_a =	**0.3**	**A=**	**304797**
μ_b =		**B=**	**16586.997**
μ_c =		**C=**	**15633.072**

The measurements were taken from (1) M. Izuha, S. Yamamoto, and S. Saito, 1996, J. Chem. Phys. 105, 4923. The dipole moment is taken from an *ab initio* calculation mentioned in (1).

Species Tag:	**42010**	**Name:**	**SiN**
Version:	**1**		**$^2\Sigma^+$ State**
Date:	**Jan. 1996**		
Contributor:	**J. C. Pearson**		
Lines Listed:	**614**	**Q(300.0)=**	**1715.9354**
Freq. (GHz) <	**1780**	**Q(225.0)=**	**1290.9121**
Max. J:	**40**	**Q(150.0)=**	**861.5120**
LOGSTR0=	**-10.0**	**Q(75.00)=**	**431.6578**
LOGSTR1=	**-8.0**	**Q(37.50)=**	**216.8063**
Isotope Corr.:	**-0.035**	**Q(18.75)=**	**109.4063**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**55.7288**
μ_a =	**1.0**	**A=**	
μ_b =		**B=**	**21827.8**
μ_c =		**C=**	

The experimental measurements were reported by S. Saito, Y. Endo and E. Hirota, 1983, J. Chem. Phys. 78, 6447. The dipole moment has not been measured so unit dipole was used in the calculation.

Species Tag:	43001	Name:	CHDCO
Version:	1		Ketene,
Date:	Jan. 1980		mono deuterium
Contributor:	R. L. Poynter		isotope
Lines Listed:	886	Q(300.0)=	6683.440
Freq. (GHz) <	552	Q(225.0)=	4340.103
Max. J:	29	Q(150.0)=	2344.228
LOGSTR0=	-22.2	Q(75.00)=	828.705
LOGSTR1=	-22.7	Q(37.50)=	295.801
Isotope Corr.:	-3.523	Q(18.75)=	105.148
Egy. (cm^{-1}) >	0.0	Q(9.375)=	37.497
μ_a =		A=	194313.
μ_b =	1.422	B=	9647.396
μ_c =		C=	9174.975

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333. The measurements were taken from L. Nemes and M. Winnewisser, 1976, Z. Naturforsch. 31a, 272. The dipole moment is assumed to be the same as for the parent species.

Species Tag:	**43002**	**Name:**	**HNCO**
Version:	**1**		**Isocyanic acid**
Date:	**July 1987**		
Contributor:	**R. L. Poynter**		

Lines Listed:	**6078**	**Q(300.0)=**	**7785.741**
Freq. (GHz) <	**2997**	**Q(225.0)=**	**5123.892**
Max. J:	**47**	**Q(150.0)=**	**2802.206**
LOGSTR0=	**-10.0**	**Q(75.00)=**	**992.888**
LOGSTR1=	**-10.0**	**Q(37.50)=**	**352.614**
Isotope Corr.:	**0.0**	**Q(18.75)=**	**129.479**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**56.351**
μ_a =	**1.6020**	**A=**	**912711.435(197)**
μ_b =	**1.3500**	**B=**	**11071.0098(9)**
μ_c =		**C=**	**10910.5763(10)**

The line measurements and dipole moment were taken from W. H. Hocking *et al.*, 1975, Can. J. Phys. 53, 1869. Molecular beam measurements of the quadrupole components of the J = 1-0 rotational transition were taken from S. G. Kukolich *et al.*, 1971, J. Am. Chem. Soc. 93, 6769.

Species Tag:	43003	Name:	AlO Aluminum monoxide, X $^2\Sigma^+$
Version:	1		
Date:	July 1990		
Contributor:	E. A. Cohen		

Lines Listed:	1023	Q(300.0)=	3926.450
Freq. (GHz) $<$	2121	Q(225.0)=	2945.100
Max. J:	57	Q(150.0)=	1963.813
LOGSTR0=	-4.8	Q(75.00)=	983.105
LOGSTR1=	-5.0	Q(37.50)=	493.174
Isotope Corr.:	0.0	Q(18.75)=	248.142
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	125.719
μ_a =	4.6	A=	
μ_b =		B=	19141.572
μ_c =		C=	

The data have been taken from C. Yamada *et al.*, 1990, J. Chem. Phys. 92, 2146. The dipole moment is from a calculation by B. H. Lengsfield and B. Liu, 1982, J. Chem. Phys. 77, 6083.

Species Tag:	**43004**	**Name:**	**CP**
Version:	**1**		^2Sigma
Date:	**Jan. 1997**		
Contributor:	**J. C. Pearson**		
Lines Listed:	**397**	**Q(300.0)=**	**1050.1389**
Freq. (GHz) <	**2413**	**Q(225.0)=**	**787.8041**
Max. J:	**50**	**Q(150.0)=**	**525.5325**
LOGSTR0=	**-10.0**	**Q(75.00)=**	**263.3758**
LOGSTR1=	**-8.0**	**Q(37.50)=**	**132.3437**
Isotope Corr.:	**0.0**	**Q(18.75)=**	**66.8446**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**34.1103**
μ_a =	**1.0**	**A=**	
μ_b =		**B=**	**23859.9**
μ_c =		**C=**	

The experimental measurements were reported by S. Saito, S. Yamamoto, K. Kawaguchi, M. Ohishi, H. Suzuki, S.-I. Ishikawa and N. Kaifu, 1989, Astrophys. J. 341, 1114. There are a number of X to A electronic band (2100 cm^{-1}) measurements which were not included in this analysis.

The dipole moment has not been measured so unit dipole was used in the calculation.

Species Tag:	**44001**	**Name:**	**CS**
Version:	**2**		**Carbon monosulfide**
Date:	**Jan. 1984**		
Contributor:	**R. L. Poynter**		
Lines Listed:	**51**	**Q(300.0)=**	**255.505**
Freq. (GHz) <	**2476**	**Q(225.0)=**	**191.823**
Max. J:	**51**	**Q(150.0)=**	**127.968**
LOGSTR0=	**-3.6**	**Q(75.00)=**	**64.150**
LOGSTR1=	**-4.7**	**Q(37.50)=**	**32.240**
Isotope Corr.:	**-0.022**	**Q(18.75)=**	**16.285**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**8.316**
$\mu_a =$	**1.957**	**A=**	
$\mu_b =$		**B=**	**24495.562**
$\mu_c =$		**C=**	

The experimental data were taken from: R. Kewley, K. V. L. N. Sastry, M. Winnewisser, and W. Gordy, 1963, J. Chem. Phys. 39, 2856. R. C. Mockler and G. R. Bird, 1955, Phys. Rev. 98, 1837. M. Bogey, C. Demuynck, and J. L. Destombes, 1982, J. Mol. Spect. 95, 35.

The maximum J and frequency were limited by the estimated uncertainty in the predicted lines. The dipole moment is from G. Winnewisser and R. L. Cook, 1968, J. Mol. Spect. 28, 266.

Species Tag:	44002	Name:	SiO
Version:	2		Silicon monoxide,
Date:	Jan. 1984		^{28}Si isotope
Contributor:	R. L. Poynter		

Lines Listed:	31	Q(300.0)=	287.210
Freq. (GHz) $<$	1342	Q(225.0)=	215.874
Max. J:	31	Q(150.0)=	144.344
LOGSTR0=	-3.4	Q(75.00)=	72.327
LOGSTR1=	-1.7	Q(37.50)=	36.325
Isotope Corr.:	-0.035	Q(18.75)=	18.332
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	9.339
μ_a =	3.098	A=	
μ_b =		B=	21711.967
μ_c =		C=	

The experimental data were taken from T. Törring, 1968, Z. Naturforsch. 23a, 77, and E. L. Manson, W. W. Clark, F. C. De Lucia, and W. Gordy, 1977, Phys. Rev. A15, 223. The dipole moment was reported by W. A. Raymonda, J. S. Muenter, and W. A. Klemperer, 1970, J. Chem. Phys. 52, 3458.

Species Tag:	44003	Name:	CH3CHO-a
Version:	1		Acetaldehyde
Date:	Jan. 1980		ground torsional state,
Contributor:	R. L. Poynter		A species
Lines Listed:	1347	Q(300.0)=	12111.557
Freq. (GHz) <	1898	Q(225.0)=	7866.836
Max. J:	20	Q(150.0)=	4282.526
LOGSTR0=	-8.4	Q(75.00)=	1513.910
LOGSTR1=	-7.7	Q(37.50)=	535.303
Isotope Corr.:	0.	Q(18.75)=	190.283
Egy. (cm^{-1}) >	0.0	Q(9.375)=	67.764
μ_a =	2.550	A=	56609.474
μ_b =	0.870	B=	10162.766
μ_c =		C=	9100.412

The data set used is referenced by A. Bauder, F. J. Lovas, and D. R. Johnson, 1976, J. Phys. Chem. Ref. Data 5, 53. The lines were fit to a rigid rotor with centrifugal distortion.

Species Tag:	**44004**	**Name:**	**N2O**
Version:	**1**		**Nitrous oxide**
Date:	**Jan. 1980**		
Contributor:	**R. L. Poynter** **H. M. Pickett**		
Lines Listed:	**61**	**Q(300.0)=**	**497.966**
Freq. (GHz) <	**1528**	**Q(225.0)=**	**373.594**
Max. J:	**61**	**Q(150.0)=**	**249.173**
LOGSTR0=	**-6.7**	**Q(75.00)=**	**124.738**
LOGSTR1=	**-6.0**	**Q(37.50)=**	**62.546**
IsoIsotope Corr.:	**0.**	**Q(18.75)=**	**31.434**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**15.889**
μ_a =	**0.1608**	**A=**	
μ_b =		**B=**	**12561.637**
μ_c =		**C=**	

The experimental data were taken from the summary given in F. J. Lovas, 1978, J. Phys. Chem. Ref. Data 7, 1445. The dipole moment was measured by L. H. Scharpen, J. S. Muenter, and V. W. Laurie, 1970, J. Chem. Phys. 53, 2513.

Species Tag:	44005	Name:	CH3CHO-e
Version:	1		Acetaldehyde
Date:	Dec. 1980		ground torsional state,
Contributor:	H. M. Pickett		E state

Lines Listed:	691	Q(300.0)=	12111.557
Freq. (GHz) <	2995	Q(225.0)=	7866.836
Max. J:	15	Q(150.0)=	4282.526
LOGSTR0=	-9.0	Q(75.00)=	1513.910
LOGSTR1=	-10.8	Q(37.50)=	535.303
Isotope Corr.:	0.0	Q(18.75)=	189.452
Egy. (cm^{-1}) >	0.069	Q(9.375)=	67.298
μ_a =	2.55	A=	56448.5
μ_b =	0.87	B=	10160.1
μ_c =		C=	9101.3

The data set used is referenced by A. Bauder, F. J. Lovas, and D. R. Johnson, 1976, J. Phys. Chem. Ref. Data 5, 53. The lines were fit to a Hamiltonian that included terms up to the sixth power in angular momentum as well as P_a, P_aP^2, P_aP^4, P_a^3, $P_a^3P^2$, and P_a^5 terms. The fit produced observed–calculated frequencies that were 3.5 times the experimental uncertainties in an RMS sense. The calculated line strengths agree with those of Bauder *et al.*

Species Tag:	**44006**	**Name:**	**DNCO**
Version:	**1**		**Isocyanic acid,**
Date:	**July 1987**		**deuterium isotope**
Contributor:	**R. L. Poynter**		
Lines Listed:	**5504**	**Q(300.0)=**	**9451.486**
Freq. (GHz) <	**2997**	**Q(225.0)=**	**6706.562**
Max. J:	**32**	**Q(150.0)=**	**3918.322**
LOGSTR0=	**-8.0**	**Q(75.00)=**	**1428.236**
LOGSTR1=	**-8.0**	**Q(37.50)=**	**507.108**
Isotope Corr.:	**-3.824**	**Q(18.75)=**	**180.884**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**68.030**
μ_a =	**1.602**	**A=**	**510971.766(51)**
μ_b =	**1.350**	**B=**	**10313.7156(6)**
μ_c =		**C=**	**10079.6763(10)**

The measured lines and dipole moment were taken from W. H. Hocking *et al.*, 1975, Can. J. Phys. 53, 1869.

Species Tag:	**44007**	**Name:**	**HN-15-CO**
Version:	**1**		**Isocyanic acid,**
Date:	**July 1987**		**^{15}N isotope**
Contributor:	**R. L. Poynter**		
Lines Listed:	**888**	**Q(300.0)=**	**2580.477**
Freq. (GHz) <	**2989**	**Q(225.0)=**	**1738.601**
Max. J:	**40**	**Q(150.0)=**	**964.939**
LOGSTR0=	**-8.0**	**Q(75.00)=**	**342.610**
LOGSTR1=	**-7.0**	**Q(37.50)=**	**121.423**
Isotope Corr.:	**-2.432**	**Q(18.75)=**	**44.320**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**19.024**
$\mu_a =$	**1.602**	**A=**	**903185.4(14.6)**
$\mu_b =$	**1.350**	**B=**	**10737.8252(58)**
$\mu_c =$		**C=**	**10585.4602(58)**

The line measurements were taken from W. H. Hocking *et al.*, 1975, Can. J. Phys. 53, 1869. The dipole moment was assumed to be the same as for the parent molecular species.

Species Tag:	44008	Name:	HNC-13-O
Version:	1		Isocyanic acid,
Date:	July 1987		^{13}C isotope
Contributor:	R. L. Poynter		

Lines Listed:	4332	Q(300.0)=	7450.750
Freq. (GHz) <	2999	Q(225.0)=	5030.372
Max. J:	39	Q(150.0)=	2796.404
LOGSTR0=	-8.0	Q(75.00)=	994.031
LOGSTR1=	-8.0	Q(37.50)=	353.021
Isotope Corr.:	-1.955	Q(18.75)=	129.599
Egy. (cm^{-1}) >	0.0	Q(9.375)=	56.364
μ_a =	1.602	A=	910499.80(1.41)
μ_b =	1.350	B=	11071.4817(14)
μ_c =		C=	10910.7321(14)

The measurements were taken from W. H. Hocking *et al.*, 1975, Can. J. Phys. 53, 1869. The dipole moment was assumed to be the same as for the parent molecular species.

Species Tag:	**44009**	**Name:**	**N2O-v2**
Version:	**1**		**Nitrous oxide,**
Date:	**Aug. 1989**		$\nu_2 = 1$ **state**
Contributor:	**E. A. Cohen**		

Lines Listed:	**146**	**Q(300.0)=**	**497.966**
Freq. (GHz) <	**1855**	**Q(225.0)=**	**373.594**
Max. J:	**74**	**Q(150.0)=**	**249.173**
LOGSTR0=	**-7.1**	**Q(75.00)=**	**124.738**
LOGSTR1=	**-8.6**	**Q(37.50)=**	**62.546**
Isotope Corr.:	**0.0**	**Q(18.75)=**	**31.434**
Egy. (cm^{-1}) >	**589.6**	**Q(9.375)=**	**15.889**
μ_a =	**0.1608**	**A=**	
μ_b =		**B=**	**12578.5114**
μ_c =		**C=**	

The data were taken from: B. A. Andreev, 1976, J. Mol. Spect. 62, 125. R. Pearson *et al.*, **1970, J. Mol. Spect. 34, 440. J. LeMaire** *et al.*, **1971, J. Phys. Paris 32, 1971.**

Hyperfine splittings are not calculated. The dipole moment was assumed to be equal to that of the ground state.

Species Tag:	**44010**	**Name:**	**HCP** **Methylidynephosphine, X $^1\Sigma^+$**
Version:	**1**		
Date:	**April 1994**		
Contributor:	**H. M. Pickett**		

Lines Listed:	**34**	**Q(300.0)=**	**312.033**
Freq. (GHz) <	**1355**	**Q(225.0)=**	**234.963**
Max. J:	**34**	**Q(150.0)=**	**156.856**
LOGSTR0=	**-5.3**	**Q(75.00)=**	**78.578**
LOGSTR1=	**-3.6**	**Q(37.50)=**	**39.455**
Isotope Corr.:	**0.0**	**Q(18.75)=**	**19.898**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**10.120**
μ_a =	**0.039**	**A=**	
μ_b =		**B=**	**19976.0**
μ_c =		**C=**	

The rotational transitions and dipole moment are from J. K. Tyler, 1964, J. Chem. Phys. 40, 1170. Additional rotational lines are from J. W. C. Johns, J. M. R. Stone, and G. Winnewisser, 1971, J. Mol. Spect. 38, 437.

Species Tag:	**44011**	**Name:**	**AlOH**
Version:	**1**		**Aluminum hydroxide,**
Date:	**Jan. 1996**		**X $^1\Sigma^+$**
Contributor:	**J. C. Pearson**		

Lines Listed:	**766**	**Q(300.0)=**	**2387.766**
Freq. (GHz) $<$	**2230**	**Q(225.0)=**	**1790.771**
Max. J:	**70**	**Q(150.0)=**	**1194.141**
LOGSTR0=	**-8.0**	**Q(75.00)=**	**597.886**
LOGSTR1=	**-8.0**	**Q(37.50)=**	**299.903**
Isotope Corr.:	**0.0**	**Q(18.75)=**	**150.952**
Egy. (cm^{-1}) $>$	**0.0**	**Q(9.375)=**	**76.498**
$\mu_a =$	**1.040**	**A=**	
$\mu_b =$		**B=**	**15740.3**
$\mu_c =$		**C=**	

The experimental measurements were reported by A. J. Apponi, W. L. Barclay, Jr. and L. M. Ziurys, 1993, Astrophys. J. 414, L129. The dipole moment has been calculated to be 1.040 Debye by G. Vacek, B. J. DeLeeuw and H. F. Schaefer, 1993, J. Chem. Phys. 98, 8704.

Species Tag:	44012	Name:	N2O-2v2
Version:	1		Nitrous oxide,
Date:	July 1996		$\nu_2 = 2$ state
Contributor:	E. A. Cohen		

Lines Listed:	194	Q(300.0)=	497.966
Freq. (GHz) $<$	1658	Q(225.0)=	373.594
Max. J:	65	Q(150.0)=	249.173
LOGSTR0=	-10.0	Q(75.00)=	124.738
LOGSTR1=	-9.0	Q(37.50)=	62.546
Isotope Corr.:	0.0	Q(18.75)=	31.434
Egy. (cm^{-1}) $>$	1168.3	Q(9.375)=	15.889
μ_a =	0.1608	A=	
μ_b =		B=	12588.8857
μ_c =		C=	

Species Tag:	**45001**	**Name:**	**C-13-S**
Version:	**2**		**Carbon monosulfide,**
Date:	**Jan. 1984**		**^{13}C isotope**
Contributor:	**R. L. Poynter**		
Lines Listed:	**29**	**Q(300.0)=**	**270.645**
Freq. (GHz) <	**1337**	**Q(225.0)=**	**203.236**
Max. J:	**29**	**Q(150.0)=**	**135.550**
LOGSTR0=	**-3.7**	**Q(75.00)=**	**67.936**
LOGSTR1=	**-2.1**	**Q(37.50)=**	**34.127**
Isotope Corr.:	**-1.977**	**Q(18.75)=**	**17.235**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**8.790**
μ_a =	**1.957**	**A=**	
μ_b =		**B=**	**23123.856**
μ_c =		**C=**	

The experimental measurements were reported by R. C. Mockler and G. R. Bird, 1955, Phys. Rev. 98, 1837, and M. Bogey, C. Demuynck, and J. L. Destombes, 1982, J. Mol. Spect. 95, 35. The dipole moment was assumed to be the same as for the parent species. The maximum J and frequency were limited by the estimated uncertainty in the predicted lines.

Species Tag:	45002	Name:	Si-29-O
Version:	1		Silicon monoxide,
Date:	Dec. 1979		^{29}Si isotope
Contributor:	R. L. Poynter		

Lines Listed:	66	Q(300.0)=	290.871
Freq. (GHz) <	2797	Q(225.0)=	219.180
Max. J:	66	Q(150.0)=	146.184
LOGSTR0=	-4.4	Q(75.00)=	73.232
LOGSTR1=	-6.3	Q(37.50)=	36.779
Isotope Corr.:	-1.327	Q(18.75)=	18.561
Egy. (cm^{-1}) >	0.0	Q(9.375)=	9.451
μ_a =	3.098	A=	
μ_b =		B=	21514.07
μ_c =		C=	

The experimental data were taken from E. Tiemann, 1974, J. Phys. Chem. Ref. Data 3, 245, and T. Törring, 1968, Z. Naturforsch. 23a, 777. The dipole moment was reported by J. W. Raymonda, J. S. Muenter, and W. A. Klemperer, 1970, J. Chem. Phys. 52, 3458.

Species Tag:	**45003**	**Name:**	**NH2CHO**
Version:	**2**		**Formamide**
Date:	**Jan. 1981**		
Contributor:	**R. L. Poynter**		
Lines Listed:	**3476**	**Q(300.0)=**	**29154.139**
Freq. (GHz) <	**1931**	**Q(225.0)=**	**18479.908**
Max. J:	**29**	**Q(150.0)=**	**10313.357**
LOGSTR0=	**-9.0**	**Q(75.00)=**	**3633.290**
LOGSTR1=	**-8.1**	**Q(37.50)=**	**1293.302**
Isotope Corr.:	**0.**	**Q(18.75)=**	**459.198**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**163.719**
μ_a =	**3.616**	**A=**	**72716.954**
μ_b =	**0.852**	**B=**	**11373.453**
μ_c =		**C=**	**9833.903**

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333. The measurements were taken from: C. C. Costain and J. M. Dowling, 1960, J. Chem. Phys. 32, 290. D. R. Johnson, F. J. Lovas, and W. H. Kirchhoff, 1972, J. Phys. Chem. Ref. Data 1, 1011. W. H. Kirchhoff and D. R. Johnson, 1973, J. Mol. Spect. 45, 159. S. G. Kukolich and A. C. Nelson, 1971, Chem. Phys. Lett. 11, 383. R. J. Kurland and E. B. Wilson, Jr., 1957, J. Chem. Phys. 27, 585.

The dipole moment was reported in the paper by Kurland and Wilson.

Species Tag:	**45005**	**Name:**	**HCS+**
Version:	**1**		**Thioformyl cation /**
Date:	**Jan. 1990**		**Thioxomethylium,**
Contributor:	**R. L. Poynter**		**X $^1\Sigma^+$**
Lines Listed:	**64**	**Q(300.0)=**	**293.495**
Freq. (GHz) <	**2709**	**Q(225.0)=**	**220.141**
Max. J:	**64**	**Q(150.0)=**	**146.859**
LOGSTR0=	**-4.4**	**Q(75.00)=**	**73.587**
LOGSTR1=	**-6.3**	**Q(37.50)=**	**36.957**
Isotope Corr.:	**-0.022**	**Q(18.75)=**	**18.647**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**9.495**
μ_a =	**1.86**	**A=**	**10691.406(43)**
μ_b =		**B=**	
μ_c =		**C=**	

The measured lines were taken from P. Thaddeus *et al.*, 1981, Astrophys. J. Lett. Ed. 246, L41, and C.S. Gudeman *et al.*, 1981, Astrophys. J. Lett. Ed. 246, L47. The dipole moment was obtained from a CI calculation reported in the Gudeman paper.

Species Tag:	45006	Name:	HNCO-18
Version:	1		Isocyanic acid,
Date:	Sept. 1988		^{18}O isotope
Contributor:	R. L. Poynter		

Lines Listed:	4929	Q(300.0)=	8122.691
Freq. (GHz) $<$	2991	Q(225.0)=	5390.140
Max. J:	45	Q(150.0)=	2960.056
LOGSTR0=	-7.9	Q(75.00)=	1049.059
LOGSTR1=	-7.9	Q(37.50)=	372.563
Isotope Corr.:	-2.690	Q(18.75)=	136.741
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	59.443
μ_a =	1.602	A=	912631.43(1.50)
μ_b =	1.350	B=	10470.9010(18)
μ_c =		C=	10327.2476(18)

The measurements were taken from W. H. Hocking *et al.*, 1975, Can. J. Phys. 53, 1869. The dipole moment was assumed to be the same as for the parent molecular species.

Species Tag:	45007	Name:	NN-15-O
Version:	1		Nitrous oxide,
Date:	Aug. 1989		central ^{15}N
Contributor:	E. A. Cohen		

Lines Listed:	85	Q(300.0)=	498.196
Freq. (GHz) $<$	2123	Q(225.0)=	373.680
Max. J:	85	Q(150.0)=	249.230
LOGSTR0=	-7.2	Q(75.00)=	124.767
LOGSTR1=	-8.9	Q(37.50)=	62.546
Isotope Corr.:	-2.432	Q(18.75)=	31.441
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	15.889
μ_a =	0.1608	A=	
μ_b =		B=	12560.732
μ_c =		C=	

The data were taken from B. A. Andreev, 1976, J. Mol. Spect. 62, 125, and M. W. P. Strandberg, 1949, Phys. Rev. 75, 827. The dipole moment was assumed to be the same as for the normal species.

Species Tag:	**45008**	**Name:**	**N-15-NO**
Version:	**1**		**Nitrous oxide,**
Date:	**Aug. 1990**		**end ^{15}N**
Contributor:	**E. A. Cohen**		
Lines Listed:	**87**	**Q(300.0)=**	**515.585**
Freq. (GHz) <	**2099**	**Q(225.0)=**	**386.723**
Max. J:	**87**	**Q(150.0)=**	**257.870**
LOGSTR0=	**-7.3**	**Q(75.00)=**	**129.092**
LOGSTR1=	**-8.9**	**Q(37.50)=**	**64.714**
Isotope Corr.:	**-2.432**	**Q(18.75)=**	**32.524**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**16.432**
μ_a =	**0.1608**	**A=**	
μ_b =		**B=**	**12137.311**
μ_c =		**C=**	

The data were taken from B. A. Andreev, 1976, J. Mol. Spect. 62, 125, and D. K. Coles, 1948, Phys. Rev. 72, 973. The dipole moment was assumed to be the same as for the normal species.

Species Tag:	**45009**	**Name:**	**DCP** **Methylidyne-phosphine,** **X $^1\Sigma^+$,** **Deuterium isotope**
Version:	**1**		
Date:	**April 1994**		
Contributor:	**H. M. Pickett**		
Lines Listed:	**34**	**Q(300.0)=**	**364.754**
Freq. (GHz) <	**1154**	**Q(225.0)=**	**275.867**
Max. J:	**34**	**Q(150.0)=**	**184.374**
LOGSTR0=	**-5.5**	**Q(75.00)=**	**92.363**
LOGSTR1=	**-3.6**	**Q(37.50)=**	**46.345**
Isotope Corr.:	**-3.824**	**Q(18.75)=**	**23.340**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**11.841**
μ_a =	**0.397**	**A=**	
μ_b =		**B=**	**16984.4**
μ_c =		**C=**	

The rotational lines are from J. W. C. Johns, J. M. R. Stone, and G. Winnewisser, 1971, J. Mol. Spect. 38, 437. The dipole moment is assumed to be the same as the parent isotopic species.

Species Tag:	**45010**	**Name:**	**HOCO+**
Version:	**1**		**Protonated CO_2**
Date:	**March 1995**		
Contributor:	**H. M. Pickett**		

Lines Listed:	**1745**	**Q(300.0)=**	**2370.828**
Freq. (GHz) <	**9994**	**Q(225.0)=**	**1693.558**
Max. J:	**30**	**Q(150.0)=**	**997.700**
LOGSTR0=	**-7.9**	**Q(75.00)=**	**365.595**
LOGSTR1=	**-8.0**	**Q(37.50)=**	**129.599**
Isotope Corr.:	**0.0**	**Q(18.75)=**	**46.698**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**19.262**
μ_a =	**2.0**	**A=**	**789950.574**
μ_b =	**2.8**	**B=**	**10773.736**
μ_c =		**C=**	**10609.432**

The line measurements are from M. Bogey, C. Demuynk, J. L. Destombes, and A. Krupnov, 1988, J. Mol. Struct. 190, 465. The dipole moments are based on calculations by S. Green *et al.*, 1976, Chem. Phys. 17, 479.

Species Tag:	**45011**	**Name:**	**AlOD**
Version:	**1**		**Aluminum**
Date:	**Jan. 1996**		**deuteroxide,**
Contributor:	**J. C. Pearson**		**X $^1\Sigma^+$**
Lines Listed:	**70**	**Q(300.0)=**	**441.449**
Freq. (GHz) <	**3675**	**Q(225.0)=**	**331.073**
Max. J:	**70**	**Q(150.0)=**	**220.759**
LOGSTR0=	**-8.0**	**Q(75.00)=**	**110.513**
LOGSTR1=	**-8.0**	**Q(37.50)=**	**55.416**
Isotope Corr.:	**-3.824**	**Q(18.75)=**	**27.874**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**14.107**
μ_a =	**1.040**	**A=**	
μ_b =		**B=**	**14187.9**
μ_c =		**C=**	

The experimental measurements were reported by A. J. Apponi, W. L. Barclay, Jr. and L. M. Ziurys, 1993, Astrophys. J. 414, L129. The dipole moment has been calculated to be 1.040 Debye by G. Vacek, B. J. DeLeeuw and H. F. Schaefer, 1993, J. Chem. Phys. 98, 8704. Hyperfine structure will be observed at low J values, but was not included in this analysis.

Species Tag:	45012	Name:	O-17-CO
Version:	1		Carbon dioxide
Date:	Jan. 1996		mono ^{17}O isotope
Contributor:	H. S. P. Müller		

Lines Listed:	285	Q(300.0)=	3307.5365
Freq. (GHz) <	600	Q(225.0)=	2480.9245
Max. J:	26	Q(150.0)=	1654.4650
LOGSTR0=	-14.0	Q(75.00)=	828.1587
LOGSTR1=	-12.0	Q(37.50)=	415.0647
Isotope Corr.:	-3.126	Q(18.75)=	208.5364
Egy. (cm^{-1}) >	0.0	Q(9.375)=	105.2847
$\mu_a =$	0.0005	A=	
$\mu_b =$		B=	11350.548
$\mu_c =$		C=	

The data were taken from (1) J. Gripp, H. Mäder, H. Dreizler, and J. L. Teffo, 1995, J. Mol. Spect. 172, 430. A value $D = 0.003790$ (100) MHz was taken from (2) L. S. Rothman, R. L. Hawkins, R. B. Wattson, and R. R. Gamache, 1992, J. Quant. Spectrosc. Radiat. Transfer 48, 537. The uncertainty is three times that of ^{18}OCO tag no. 46013.

A dipole moment of 0.000605 D was calculated in (1). This value was corrected as described for ^{18}OCO tag no. 46013.

Species Tag:	**45013**	**Name:**	**PN**
Version:	**1**		nu**=0,1,2,3,4**
Date:	**Dec. 1996**		$^1\Sigma^+$
Contributor:	**J. C. Pearson**		

Lines Listed:	**1637**	**Q(300.0)=**	**801.1685**
Freq. (GHz) <	**3290**	**Q(225.0)=**	**600.0817**
Max. J:	**70**	**Q(150.0)=**	**400.2305**
LOGSTR0=	**-14.0**	**Q(75.00)=**	**200.5798**
LOGSTR1=	**-14.0**	**Q(37.50)=**	**100.7852**
Isotope Corr.:	**0.0**	**Q(18.75)=**	**50.8994**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**25.9677**
μ_a =	**2.7471**	**A=**	
μ_b =		**B=**	**23578.2**
μ_c =		**C=**	

The data were taken from: J. Hoeft, E. Tiemann and Törring, 1972, Z. Naturforsch. 27a, 703. F. C. Wyse, E. L. Manson and W. Gordy, 1972, J. Chem. Phys. 57, 1106. I. K. Ahmad and P. A. Hamilton, 1995, J. Mol. Spectrosc. 169, 286.

The value of the nitrogen nuclear quadrupole (eqQ_N) and the nirtogen magnetic interaction (C_N) were fixed to the molecular beam electric resonance value of J. Raymonda and W. Klemperer, 1971, J. Chem. Phys. 55, 232. The phosphorus magnetic interaction (C_P) of -78.2 kHz was not included in the analysis. The vibrational energies for nu¿1 were fixed to the values given by Ahmad and Hamilton.

A dipole moment of 2.7514-0.0086(nu+1/2) Debye was determined by Raymonda and Klemperer and corrected by Wyse, Manson and Gordy.

PN was first observed in the interstellar medium by L. M. Ziurys, 1987, Astrophys. J. 321, L81.

Species Tag:	46001	Name:	CS-34
Version:	2		Carbon monosulfide,
Date:	Jan. 1984		^{34}S isotope
Contributor:	R. L. Poynter		

Lines Listed:	34	Q(300.0)=	259.657
Freq. (GHz) <	1633	Q(225.0)=	194.940
Max. J:	34	Q(150.0)=	130.047
LOGSTR0=	-3.6	Q(75.00)=	65.178
LOGSTR1=	-2.5	Q(37.50)=	32.757
Isotope Corr.:	-1.376	Q(18.75)=	16.546
Egy. (cm^{-1}) >	0.0	Q(9.375)=	8.447
μ_a =	1.957	A=	
μ_b =		B=	24103.541
μ_c =		C=	

The experimental measurements were reported by R. C. Mockler and G. R. Bird, 1955, Phys. Rev. 98, 1837, and M. Bogey, C. Demuynck, and J. L. Destombes, 1982, J. Mol. Spect. 95, 35. The dipole moment was assumed to be the same as for the parent species. The maximum J and frequency were limited by the estimated uncertainty in the predicted lines.

Species Tag:	46002	Name:	Si-30-O
Version:	1		Silicon monoxide,
Date:	Dec. 1979		^{30}Si isotope
Contributor:	R. L. Poynter		

Lines Listed:	67	Q(300.0)=	294.374
Freq. (GHz) <	2805	Q(225.0)=	221.258
Max. J:	67	Q(150.0)=	147.911
LOGSTR0=	-4.5	Q(75.00)=	74.114
LOGSTR1=	-6.4	Q(37.50)=	37.222
Isotope Corr.:	-1.506	Q(18.75)=	18.776
Egy. (cm^{-1}) >	0.0	Q(9.375)=	9.561
μ_a =	1.957	A=	
μ_b =		B=	24103.541
μ_c =		C=	

The experimental data were taken from E. Tiemann, 1974, J. Phys. Chem. Ref. Data 3, 245, and T. Törring, 1968, Z. Naturforsch. 23a, 777. The dipole moment was reported by J. W. Raymonda, J. S. Muenter, and W. A. Klemperer, 1970, J. Chem. Phys. 52, 3458.

Species Tag:	46003	Name:	H2CS
Version:	1		Thioformaldehyde
Date:	Jan. 1980		
Contributor:	R. L. Poynter		
Lines Listed:	517	Q(300.0)=	5984.115
Freq. (GHz) <	938	Q(225.0)=	3760.971
Max. J:	27	Q(150.0)=	2088.815
LOGSTR0=	-9.1	Q(75.00)=	750.067
LOGSTR1=	-10.0	Q(37.50)=	265.644
Isotope Corr.:	-0.022	Q(18.75)=	91.180
Egy. (cm^{-1}) >	0.0	Q(9.375)=	27.523
$\mu_a =$	1.649	A=	291291.641
$\mu_b =$		B=	17699.628
$\mu_c =$		C=	16651.830

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333. The measurements and other references were taken from D. R. Johnson, F. J. Lovas, and W. H. Kirchhoff, 1972, J. Phys. Chem. Ref. Data 1, 1011. The dipole moment was taken from B. Fabricant, D. Krieger, and J. S. Muenter, 1977, J. Chem. Phys. 67, 1576.

Species Tag:	46004	Name:	C2H5OH
Version:	3		Ethyl alcohol,
Date:	Sept. 1995		*trans, gauche* states
Contributor:	J. C. Pearson		

Lines Listed:	12557	Q(300.0)=	36443.575
Freq. (GHz) $<$	600	Q(225.0)=	24885.120
Max. J:	34	Q(150.0)=	13631.512
LOGSTR0=	-10.0	Q(75.00)=	3997.639
LOGSTR1=	-8.0	Q(37.50)=	1070.023
Isotope Corr.:	0.	Q(18.75)=	291.575
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	95.618
μ_a =	0.046	A=	34891.7707
μ_b =	1.438	B=	9350.6776
μ_c =	0.000	C=	8135.2352

Trans State: The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333. The measurements were taken from: J. Michielson-Effinger, 1969, J. Phys. (Paris) 30, 333, Y. Sasada, M. Takano, and T. Satoh, 1971, J. Mol. Spect. 38, 33, H. Takano, Y. Sasada, and T. Satoh, 1968, J. Mol. Spect. 26, 157, F. J. Lovas, 1982, J. Phys. Chem. Ref. Data 11, 251, and J. C. Pearson, K. V. L. N. Sastry, M. Winnewisser, E. Herbst, and F. De Lucia, 1995, J. Phys. Chem. Ref. Data 24, 1-32. The dipole moment was reported by Takano *et al.*, above. The *trans* state transitions are designated as v = 2. The dipoles and rotation constants listed are for the *trans* state.

Gauche States: The analysis used here is based on the Fixed Frame Axis Method (FFAM) which is described in C. R. Quade and Chun C. Lin, 1963, J. Chem. Phys. 38, 540-550. Measurements were taken from: E. A. Cohen, 1979, unpublished, R. K. Kakar and C. R. Quade, 1980, J. Chem. Phys. 78, 4300-4307, and J. C. Pearson, K. V. L. N. Sastry, E. Herbst and F. C. De Lucia, 1995, submitted to J. Mol. Spect. The dipole moment was reported by Kakar and Quade, above. The dipoles are μ_a = 1.264, μ_b = 0.104, and μ_c = 1.101. The vibrational quantum number v = 0 is used to designate the lower *gauche+* state and v = 1 to designate the *gauche-* state.

Both States: No *trans-gauche* interactions are included in this analysis. It should be noted that the *trans* and *gauche* states are strongly coupled so that at the high end of the J and K_a values given the lines will often be significantly perturbed. An approximate set of limits for separate analysis is given in Table 4 of Pearson *et al.* J. Mol. Spect. It should also be noted that some predicted intensities and line positions may be significantly dif-

ferent due to neglecting the effects of the other state(s). These effects are more severe in the *gauche* states since the interactions begin at lower K_a values. The estimated 39.2 cm^{-1} energy of the v = 0 has been included in the calculation.

Species Tag:	46005	Name:	HCOOH
Version:	1		Formic acid,
Date:	Jan. 1980		ground *trans* state
Contributor:	R. L. Poynter		

Lines Listed:	1888	Q(300.0)=	8883.826
Freq. (GHz) $<$	2986	Q(225.0)=	5770.321
Max. J:	20	Q(150.0)=	3141.233
LOGSTR0=	-9.2	Q(75.00)=	1085.676
LOGSTR1=	-8.8	Q(37.50)=	393.459
Isotope Corr.:	0.	Q(18.75)=	139.991
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	49.934
μ_a =	1.396	A=	77512.25
μ_b =	0.260	B=	12055.11
μ_c =		C=	10416.12

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333. The measurements were taken from: J. Bellet, C. Samson, G. Steenbeckeliers, and R. Wertheimer, 1971, J. Mol. Struc. 9, 49. R. G. Lerner, B. P. Dailey, and J. P. Friend, 1957, J. Chem. Phys. 26, 680. R. Trambarulo, A. Clark, and C. Hearns, 1958, J. Chem. Phys. 28, 736.

The dipole moment used in the present work was measured by H. Kim, R. Keller, and W. D. Gwinn, 1962, J. Chem. Phys. 37, 2748, and was adjusted to the new OCS standard (J. S. Muenter, 1968, J. Chem. Phys. 48, 4544). Improved values [$\mu_a = 1.4214(21)$D and $\mu_b = 0.2096(65)$D] have been reported recently by H. Kuze, T. Kuga, and T. Shimizu, 1982, J. Mol. Spect. 93, 248.

Species Tag:	46006	Name:	NO2
Version:	2		NO_2,
Date:	Jan. 1991		Nitrogen dioxide
Contributor:	H. M. Pickett		X $^2A_1$

Lines Listed:	16444	Q(300.0)=	13508.277
Freq. (GHz) $<$	6448	Q(225.0)=	8761.935
Max. J:	71	Q(150.0)=	4764.310
LOGSTR0=	-9.0	Q(75.00)=	1683.837
LOGSTR1=	-8.0	Q(37.50)=	596.348
Isotope Corr.:	0.0	Q(18.75)=	211.836
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	75.701
μ_a =		A=	239904.
μ_b =	0.316	B=	13002.
μ_c =		C=	12305.

The data were taken from W. C. Bowman and F. C. De Lucia, 1982, J. Chem. Phys. 77, 92, and N. Semmoud-Monnanteuil *et al.*, 1989, J. Mol. Spect. 134, 176. Additional data from A. Perrin *et al.*, 1988, Mol. Phys. 63, 791, also were used, and high-order constants were fixed to the values in this reference. The spectra were calculated using a full diagonalization of the Hamiltonian. The partition function was calculated by direct summation to F = 90.

Species Tag:	**46007**	**Name:**	**N2O-18**
Version:	**1**		**Nitrous oxide,**
Date:	**Aug. 1989**		**^{18}O species**
Contributor:	**E. A. Cohen**		
Lines Listed:	**88**	**Q(300.0)=**	**527.716**
Freq. (GHz) <	**2075**	**Q(225.0)=**	**395.822**
Max. J:	**88**	**Q(150.0)=**	**263.937**
LOGSTR0=	**-7.3**	**Q(75.00)=**	**132.130**
LOGSTR1=	**-8.9**	**Q(37.50)=**	**66.222**
Isotope Corr.:	**-2.690**	**Q(18.75)=**	**33.281**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**16.811**
μ_a =	**0.1608**	**A=**	
μ_b =		**B=**	**11859.111**
μ_c =		**C=**	

The data were taken from B. A. Andreev, 1976, J. Mol. Spect. 62, 125. The dipole moment was assumed to be the same as for the normal species.

Species Tag:	**46008**	**Name:**	**CH3OCH3**
Version:	**1**		**Dimethyl Ether**
Date:	**Oct. 1992**		**ground state,**
Contributor:	**H. M. Pickett**		**AA, EE, EA, AE**

Lines Listed:	**21735**	**Q(300.0)=**	**228016.**
Freq. (GHz) <	**9999**	**Q(225.0)=**	**152698.**
Max. J:	**50**	**Q(150.0)=**	**84188.**
LOGSTR0=	**-9.0**	**Q(75.00)=**	**29828.**
LOGSTR1=	**-7.0**	**Q(37.50)=**	**10563.**
Isotope Corr.:	**0.0**	**Q(18.75)=**	**3748.**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**1334.**
μ_a =		**A=**	**38788.2**
μ_b =	**1.302**	**B=**	**10056.5**
μ_c =		**C=**	**8886.8**

The data set used is referenced by F. J. Lovas, H. Lutz, and H. Dreizler, 1979, J. Phys. Chem. Ref. Data 8, 1051 and W. Neustock, A. Guarnieri, J. Demaison, and G. Wlodarczak, 1990, Z. Naturforsch. 45a, 702. The v designations of 0, 1, 2, 3 represent the AA, EE, EA, and AE states, respectively. In order to keep the degeneracies within bounds, the standard spin degeneracies were reduced by 2 and the partition function was also reduced by 2. The weights used are 3, 8, 2, 1 for the ee and oo rotational states, and 5, 8, 2, 3 for the oe and eo states. Note that there are numerous errors or inconsistencies in the literature. The convention used here follows that of R. Myers and E. B. Wilson, Jr., 1960, J. Chem. Phys. 33, 186. The lines were fit to a Hamiltonian that included terms up to the sixth power in angular momentum as well as appropriate odd powers of angular momentum. Dependence on K expected from an IAM treatment was incorporated using sine and cosine terms in $2\pi\rho_a K/3$. The quality of the fit was, on the average, twice the experimental uncertainty. The EE and EA states have both b and c type lines, while the AA and AE states have only b type lines.

Species Tag:	46009	Name:	AlF
Version:	1		Aluminum monofluoride
Date:	Feb. 1995		
Contributor:	M. L. Delitsky H. M. Pickett		
Lines Listed:	1188	Q(300.0)=	2279.9824
Freq. (GHz) <	3113.1	Q(225.0)=	1709.8675
Max. J:	99	Q(150.0)=	1140.1672
LOGSTR0=	-10.0	Q(75.00)=	570.8811
LOGSTR1=	-100.0	Q(37.50)=	286.3956
Isotope Corr.:		Q(18.75)=	144.1978
Egy. (cm^{-1}) >	0	Q(9.375)=	73.1215
μ_a =	1.53	A=	
μ_b =		B=	16488.35
μ_c =		C=	

The observed laboratory frequency measurements and dipoles were taken from: F. Lovas and E. Tiemann, 1974, J. Phys. Chem. Ref. Data 3, 609 and references therein.

Species Tag:	46010	Name:	NS
Version:	1		X $^{2}\Pi$ state
Date:	Feb. 1995		
Contributor:	H. M. Pickett		
Lines Listed:	2510	Q(300.0)=	2180.0701
Freq. (GHz) <	9999	Q(225.0)=	1509.7872
Max. J:	60	Q(150.0)=	907.0784
LOGSTR0=	-10	Q(75.00)=	410.9976
LOGSTR1=	-10	Q(37.50)=	202.1829
Isotope Corr.:	0.0	Q(18.75)=	100.5265
Egy. (cm^{-1}) >	0.0	Q(9.375)=	49.7175
μ_a =	1.81	A=	
μ_b =		B=	23155.43
μ_c =		C=	

The experimental frequencies are from F. J. Lovas and R. J. Suenram, 1982, J. Mol. Spect. 93, 416. The dipole moment is from T. Amano, S. Saito, E. Hirota, and Y. Moreno, 1969, J. Mol. Spect. 32, 97.

Species Tag:	**46011**	**Name:**	**DOCO+**
Version:	**1**		**Deuteronated CO_2**
Date:	**March 1995**		
Contributor:	**H. M. Pickett**		

Lines Listed:	**677**	**Q(300.0)=**	**3301.413**
Freq. (GHz) <	**2313**	**Q(225.0)=**	**2377.388**
Max. J:	**30**	**Q(150.0)=**	**1415.142**
LOGSTR0=	**-8.0**	**Q(75.00)=**	**522.878**
LOGSTR1=	**-8.0**	**Q(37.50)=**	**185.439**
Isotope Corr.:	**0.0**	**Q(18.75)=**	**65.826**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**24.027**
μ_a =	**2.0**	**A=**	**437487.793**
μ_b =		**B=**	**10163.999**
μ_c =		**C=**	**9908.687**

The line measurements are from M. Bogey, C. Demuynk, J. L. Destombes, and A. Krupnov, 1988, J. Mol. Struct. 190, 465 and M. Bogey, C. Demuynk, and J. L. Destombes, 1986, J. Chem. Phys. 84, 10. The dipole moment is based on calculations by S. Green *et al.*, 1976, Chem. Phys. 17, 479. The b–dipole transitions are not calculated because the experimental data do not include lines that allow confident prediction of the b–dipole transitions.

Species Tag:	46012	Name:	HOC-13-O+
Version:	1		Protonated $^{13}CO_2$
Date:	March 1995		
Contributor:	H. M. Pickett		
Lines Listed:	1735	Q(300.0)=	2372.466
Freq. (GHz) <	9983	Q(225.0)=	1694.338
Max. J:	30	Q(150.0)=	998.160
LOGSTR0=	-7.9	Q(75.00)=	365.763
LOGSTR1=	-8.0	Q(37.50)=	129.658
Isotope Corr.:	0.0	Q(18.75)=	46.720
Egy. (cm^{-1}) >	0.0	Q(9.375)=	19.266
μ_a =	2.0	A=	789184.928
μ_b =	2.8	B=	10772.897
μ_c =		C=	10608.499

The line measurements are from M. Bogey, C. Demuynk, J. L. Destombes, and A. Krupnov, 1988, J. Mol. Struct. 190, 465 and M. Bogey, C. Demuynk, and J. L. Destombes, 1986, J. Chem. Phys. 84, 10. The dipole moments are based on calculations by S. Green *et al.*, 1976, Chem. Phys. 17, 479, but have not been corrected for any shift in inertial axes with substitution.

Species Tag:	**46013**	**Name:**	**O-18-CO**
Version:	**1**		**Carbon dioxide,**
Date:	**Jan. 1996**		**mono ^{18}O isotope**
Contributor:	**H. S. P. Müller**		
Lines Listed:	**91**	**Q(300.0)=**	**566.8598**
Freq. (GHz) <	**2000**	**Q(225.0)=**	**425.1894**
Max. J:	**91**	**Q(150.0)=**	**283.5449**
LOGSTR0=	**-12.0**	**Q(75.00)=**	**141.9266**
LOGSTR1=	**-14.0**	**Q(37.50)=**	**71.9266**
Isotope Corr.:	**-2.390**	**Q(18.75)=**	**35.7310**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**18.0348**
μ_a =	**0.0009**	**A=**	
μ_b =		**B=**	**11037.894**
μ_c =		**C=**	

The data were taken from (1) Y. Endo, K. Yoshida, S. Saito, and E. Hirota, 1980, J. Chem. Phys. 73, 3511 and from (2) J. Gripp, H. Mäder, H. Dreizler, and J. L. Teffo, 1995, J. Mol. Spect. 172, 430. The *H* value was taken from (3) L. S. Rothman, R. L. Hawkins, R. B. Wattson, and R. R. Gamache, 1992, J. Quant. Spect. Radiat. Transfer 48, 537.

A dipole moment of 0.00070 (15) D was estimated in (1). A value of 0.00115 D was calculated in (4) F. A. Gangemi, 1963, J. Chem. Phys. 39, 3490. The choosen value is an average.

Species Tag:	47001	Name:	H2C-13-S
Version:	1		Thioformaldehyde,
Date:	Jan. 1980		^{13}C isotope
Contributor:	R. L. Poynter		

Lines Listed:	110	Q(300.0)=	6220.139
Freq. (GHz) <	336	Q(225.0)=	4040.174
Max. J:	10	Q(150.0)=	2114.949
LOGSTR0=	-8.7	Q(75.00)=	777.678
LOGSTR1=	-4.6	Q(37.50)=	264.363
Isotope Corr.:	-1.977	Q(18.75)=	94.254
Egy. (cm^{-1}) >	0.0	Q(9.375)=	28.615
μ_a =	1.649	A=	291660.0
μ_b =		B=	16998.342
μ_c =		C=	16030.791

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333. The measurements and other references were taken from D. R. Johnson, F. J. Lovas, and W. H. Kirchhoff, 1972, J. Phys. Chem. Ref. Data 1, 1011. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	**47002**	**Name:**	**HC-13-OOH**
Version:	**1**		**Formic acid,**
Date:	**Jan. 1980**		**^{13}C isotope**
Contributor:	**R. L. Poynter**		

Lines Listed:	**1194**	**Q(300.0)=**	**8896.105**
Freq. (GHz) $<$	**1709**	**Q(225.0)=**	**6672.676**
Max. J:	**20**	**Q(150.0)=**	**3144.851**
LOGSTR0=	**-9.9**	**Q(75.00)=**	**1094.208**
LOGSTR1=	**-8.5**	**Q(37.50)=**	**399.209**
Isotope Corr.:	**-1.955**	**Q(18.75)=**	**142.037**
Egy. (cm^{-1}) $>$	**0.0**	**Q(9.375)=**	**50.664**
μ_a =	**1.396**	**A=**	**77580.494**
μ_b =	**0.260**	**B=**	**12053.567**
μ_c =		**C=**	**10378.997**

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333. The measurements were taken from J. Bellet, A. Deldalle, C. Samson, G. Steenbeckeliers, and R. Wertheimer, 1971, J. Mol. Struc. 9, 65, and R. G. Lerner, B. P. Dailey, and J. P. Friend, 1957, J. Chem. Phys. 26, 680. The dipole moment was assumed to be the same as for the parent species, tag no. 46005.

Species Tag:	47003	Name:	DCOOH Formic acid, deuterium isotope on C atom
Version:	1		
Date:	Jan. 1980		
Contributor:	R. L. Poynter		

Lines Listed:	628	Q(300.0)=	10529.310
Freq. (GHz) <	1196	Q(225.0)=	6840.690
Max. J:	20	Q(150.0)=	3626.603
LOGSTR0=	-8.8	Q(75.00)=	1251.411
LOGSTR1=	-7.0	Q(37.50)=	466.122
Isotope Corr.:	-3.824	Q(18.75)=	165.882
Egy. (cm^{-1}) >	0.0	Q(9.375)=	59.156
μ_a =	1.396	A=	57709.33
μ_b =	0.260	B=	12055.971
μ_c =		C=	9955.609

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333. The measurements were taken from J. Bellet, A. Deldalle, C. Samson, G. Steenbeckeliers, and R. Wertheimer, 1971, J. Mol. Struc. 9, 65, and R. G. Lerner, B. P. Dailey, and J. P. Friend, 1957, J. Chem. Phys. 26, 680. The dipole moment was assumed to be the same as for the parent species, tag no. 46005.

Species Tag:	47004	Name:	HCOOD Formic acid, deuterium isotope on O atom
Version:	1		
Date:	Jan. 1980		
Contributor:	R. L. Poynter		

Lines Listed:	612	Q(300.0)=	9954.052
Freq. (GHz) <	1319	Q(225.0)=	6465.469
Max. J:	20	Q(150.0)=	3519.654
LOGSTR0=	-8.9	Q(75.00)=	1213.109
LOGSTR1=	-7.0	Q(37.50)=	440.555
Isotope Corr.:	-3.824	Q(18.75)=	156.819
Egy. (cm^{-1}) >	0.0	Q(9.375)=	55.911
$\mu_a =$	1.396	A=	66100.14
$\mu_b =$	0.260	B=	11762.577
$\mu_c =$		C=	9969.943

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333. The measurements were taken from J. Bellet, A. Deldalle, C. Samson, G. Steenbeckeliers, and R. Wertheimer, 1971, J. Mol. Struc. 9, 65, and R. G. Lerner, B. P. Dailey, and J. P. Friend, 1957, J. Chem. Phys. 26, 680. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	47005	Name:	PO+
Version:	1		Phosphorus Oxide Ion
Date:	Dec. 1996		nu=0,1,2,3,4
Contributor:	J. C. Pearson		$^1\Sigma^+$
Lines Listed:	239	Q(300.0)=	266.6863
Freq. (GHz) <	2337	Q(225.0)=	199.8550
Max. J:	50	Q(150.0)=	133.3087
LOGSTR0=	-14.0	Q(75.00)=	66.8106
LOGSTR1=	-14.0	Q(37.50)=	33.5707
Isotope Corr.:	0.0	Q(18.75)=	16.9544
Egy. (cm^{-1}) >	0.0	Q(9.375)=	8.6499
μ_a =	3.44	A=	
μ_b =		B=	23593.5
μ_c =		C=	

The data were taken from: R. H. Petrmichl, K. A. Peterson and R. C. Woods, 1990, J. Chem. Phys. 94, 3504. Data through nu=11 was used in the analysis, but predictions were made only through nu=4. The vibrational energies were fixed to the values calculated from the Dunham relationships.

A dipole moment of 3.44 Debye was calculated by Petrmichl, Peterson and Woods. It has been assumed for all the vibrational states.

Species Tag:	47006	Name:	P0
Version:	1		Ground
Date:	Jan. 1997		$^2\Pi_r$ State
Contributor:	J. C. Pearson		

Lines Listed:	743	Q(300.0)=	1539.8440
Freq. (GHz) $<$	2631	Q(225.0)=	1067.6214
Max. J:	60	Q(150.0)=	643.0602
LOGSTR0=	-10.0	Q(75.00)=	293.6296
LOGSTR1=	-10.0	Q(37.50)=	146.5057
Isotope Corr.:	-0.0	Q(18.75)=	74.8963
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	39.1587
$\mu_a =$	1.0	A=	
$\mu_b =$		B=	21899.5
$\mu_c =$		C=	

The data were taken from: K. Kawaguchi, S. Saito and E. Hirota, 1983, J. Chem. Phys. 79, 629. The ground state A value was fixed to the electronic value of R. D. Verma and S. R. Singhal, 1975, Can. J. Phys 53, 411. The frequency of the $Pi_{3/2}$ J=2.5-1.5, F=3-2 given at 109823.923 is believed to be the 109829.923 used in the analysis.

The dipole is unknown so a unit dipole (1.0 Debye) was used in the calculations.

Species Tag:	48001	Name:	SO
Version:	1		Sulfur monoxide
Date:	Dec. 1979		X $^3\Sigma$
Contributor:	H. M. Pickett		

Lines Listed:	330	Q(300.0)=	850.159
Freq. (GHz) <	2992	Q(225.0)=	632.266
Max. J:	51	Q(150.0)=	414.477
LOGSTR0=	-6.0	Q(75.00)=	197.515
LOGSTR1=	-7.8	Q(37.50)=	90.344
Isotope Corr.:	-0.022	Q(18.75)=	38.878
Egy. (cm^{-1}) >	0.0	Q(9.375)=	15.904
μ_a =	1.55	A=	
μ_b =		B=	21523.02
μ_c =		C=	

The calculational method is described in T. Amano and E. Hirota, 1974, J. Mol. Spect. 53, 346. The data used are from W. W. Clark and F. C. De Lucia, 1976, J. Mol. Spect. 60, 332. Both electric dipole and magnetic dipole transitions are listed. The electric dipole moment is from F. X. Powell and D. R. Lide, Jr., 1964, J. Chem. Phys. 41, 1413.

Species Tag:	**48002**	**Name:**	**SO-v1**
Version:	**1**		**X $^3\Sigma$, $\nu = 1$**
Date:	**Dec. 1979**		
Contributor:	**H. M. Pickett**		
Lines Listed:	**261**	**Q(300.0)=**	**850.159**
Freq. (GHz) <	**2969**	**Q(225.0)=**	**632.266**
Max. J:	**51**	**Q(150.0)=**	**414.477**
LOGSTR0=	**-7.7**	**Q(75.00)=**	**197.515**
LOGSTR1=	**-9.4**	**Q(37.50)=**	**90.344**
Isotope Corr.:	**-0.022**	**Q(18.75)=**	**38.878**
Egy. (cm^{-1}) >	**1111.5**	**Q(9.375)=**	**15.904**
μ_a =	**1.55**	**A=**	
μ_b =		**B=**	**21351.0**
μ_c =		**C=**	

The calculational method is described in T. Amano and E. Hirota, 1974, J. Mol. Spect. 53, 346. The data are from T. Amano, E. Hirota, and Y. Morino, 1967, J. Phys. Soc. Jap. 22, 399. All centrifugal distortion constants were fixed to their ground state values. Magnetic and electric dipole transitions are included. The electric dipole moment is from F. X. Powell and D. R. Lide, 1964, J. Chem. Phys. 41, 1413. This state is 1111.5 cm^{-1} above ν=0 (G. Herzberg, 1950, Spectra of Diatomic Molecules, Van Nostrands, New York).

Species Tag:	**48003**	**Name:**	**H2CS-34**
Version:	**1**		**Thioformaldehyde,**
Date:	**Jan. 1980**		**^{34}S isotope**
Contributor:	**R. L. Poynter**		

Lines Listed:	**111**	**Q(300.0)=**	**6084.150**
Freq. (GHz) $<$	**343**	**Q(225.0)=**	**4563.521**
Max. J:	**10**	**Q(150.0)=**	**2150.801**
LOGSTR0=	**-8.6**	**Q(75.00)=**	**760.501**
LOGSTR1=	**-4.6**	**Q(37.50)=**	**259.239**
Isotope Corr.:	**-1.376**	**Q(18.75)=**	**92.300**
Egy. (cm^{-1}) $>$	**0.0**	**Q(9.375)=**	**28.009**
μ_a =	**1.647**	**A=**	**291660.**
μ_b =		**B=**	**17387.949**
μ_c =		**C=**	**16376.922**

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333. The measurements and other references were taken from D. R. Johnson, F. J. Lovas and W. H. Kirchhoff, 1972, J. Phys. Chem. Ref. Data 1, 1011. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	48004	Name:	O3
Version:	3		Ozone,
Date:	May 1990		ground vibrational
Contributor:	H. M. Pickett		state
Lines Listed:	7089	Q(300.0)=	3553.040
Freq. (GHz) <	8908	Q(225.0)=	2230.489
Max. J:	80	Q(150.0)=	1198.671
LOGSTR0=	-9.8	Q(75.00)=	423.448
LOGSTR1=	-10.0	Q(37.50)=	150.038
Isotope Corr.:	0.0	Q(18.75)=	53.297
Egy. (cm^{-1}) >	0.0	Q(9.375)=	19.037
μ_a =		A=	106536.24
μ_b =	0.5324	B=	13349.26
μ_c =		C=	11834.36

The ozone spectrum was fitted using the microwave, millimeter, far-infrared, and infrared transitions given in H. M. Pickett *et al.*, 1985, J. Mol. Spect. 110, 186, and H. M. Pickett *et al.*, 1988, J. Mol. Spect. 128, 151. The dipole moment is from M. Lichtenstein *et al.*, 1971, J. Mol. Spect. 40, 10. Line strengths were calculated using a model Hamiltonian in which the ground state and the three fundamentals were coupled with theoretical matrix elements, and infrared transition dipoles were allowed to mix with the permanent dipole. This treatment gives the correct perturbation of the rotational intensities due to centrifugal distortion. The partition includes contributions from all vibrational states.

Species Tag:	**48005**	**Name:**	**O3-v2**
Version:	**3**		**(010) or ν_2 state**
Date:	**March 1990**		
Contributor:	**H. M. Pickett**		
Lines Listed:	**4947**	**Q(300.0)=**	**3553.040**
Freq. (GHz) <	**5945**	**Q(225.0)=**	**2230.489**
Max. J:	**86**	**Q(150.0)=**	**1198.671**
LOGSTR0=	**-10.0**	**Q(75.00)=**	**423.448**
LOGSTR1=	**-10.0**	**Q(37.50)=**	**150.038**
Isotope Corr.:	**0.0**	**Q(18.75)=**	**53.297**
Egy. (cm^{-1}) >	**700.9**	**Q(9.375)=**	**19.037**
μ_a =		**A=**	**108137.91**
μ_b =	**0.5324**	**B=**	**13311.44**
μ_c =		**C=**	**11765.03**

The ozone spectrum was fitted using the microwave, millimeter, far-infrared, and infrared transitions given in H. M. Pickett *et al.*, 1988, J. Mol. Spect. 128, 151. The dipole moment was assumed to be the same as for the ground state.

Species Tag:	48006	Name:	O3-v1,3
Version:	3		Ozone,
Date:	March 1990		(100) and (001) states
Contributor:	H. M. Pickett		or ν_1 and ν_3 states

Lines Listed:	9685	Q(300.0)=	3553.040
Freq. (GHz) $<$	5163	Q(225.0)=	2230.489
Max. J:	81	Q(150.0)=	1198.671
LOGSTR0=	-9.9	Q(75.00)=	423.448
LOGSTR1=	-10.0	Q(37.50)=	150.038
Isotope Corr.:	0.0	Q(18.75)=	53.297
Egy. (cm^{-1}) $>$	1042.9	Q(9.375)=	19.037
μ_a =		A=	104943.93
μ_b =	0.5324	B=	13229.74
μ_c =		C=	11726.61

The ozone spectrum was fitted using the microwave, millimeter, far-infrared, and infrared transitions given in H. M. Pickett *et al.*, 1985, J. Mol. Spect. 110, 186. The dipole moment was assumed to be the same as for the ground state.

Species Tag:	48007	Name:	O3-2v2
Version:	2		Ozone,
Date:	March 1990		(020) or $2\nu_2$
Contributor:	H. M. Pickett		vibrational state

Lines Listed:	3031	Q(300.0)=	3553.040
Freq. (GHz) <	4861	Q(225.0)=	2230.489
Max. J:	74	Q(150.0)=	1198.671
LOGSTR0=	-9.9	Q(75.00)=	423.448
LOGSTR1=	-10.0	Q(37.50)=	150.038
Isotope Corr.:	0.0	Q(18.75)=	53.297
Egy. (cm^{-1}) >	1399.3	Q(9.375)=	19.037
μ_a =		A=	109796.18
μ_b =	0.5324	B=	13273.15
μ_c =		C=	11694.07

The ozone spectrum was fitted using the microwave, millimeter, far-infrared, and infrared transitions given in H. M. Pickett *et al.*, 1988, J. Mol. Spect. 128, 151. The dipole moment was assumed to be the same as for the ground state.

Species Tag:	48008	Name:	O3-v1,3+v2
Version:	1		Coriolis coupled
Date:	Nov. 1990		states $\nu_1 + \nu_2$
Contributor:	E. A. Cohen		and $\nu_2 + \nu_3$
			or (110) and (011)
Lines Listed:	10912	Q(300.0)=	3553.040
Freq. (GHz) $<$	7404	Q(225.0)=	2230.489
Max. J:	70	Q(150.0)=	1198.671
LOGSTR0=	-10.0	Q(75.00)=	423.448
LOGSTR1=	-12.8	Q(37.50)=	150.038
Isotope Corr.:	0.0	Q(18.75)=	53.297
Egy. (cm^{-1}) $>$	1727.3	Q(9.375)=	19.037
μ_a =		A=	106495.52
μ_b =	0.5324	B=	13187.79
μ_c =		C=	11651.21

The predictions are based on the infrared work of V. Malathy Devi *et al.*, 1987, J. Mol. Spect. 125, 174. There are no measured pure rotational lines reported for these states. The dipole moment was assumed to be the same as for the ground state.

Species Tag:	48009	Name:	NS
Version:	1		X $^{2}\Pi$
Date:	Feb. 1995		^{34}S isotope
Contributor:	H. M. Pickett		

Lines Listed:	2364	Q(300.0)=	2219.7541
Freq. (GHz) <	9999	Q(225.0)=	1537.2488
Max. J:	60	Q(150.0)=	923.5649
LOGSTR0=	-10	Q(75.00)=	418.4686
LOGSTR1=	-10	Q(37.50)=	205.8667
Isotope Corr.:	-1.376	Q(18.75)=	102.3679
Egy. (cm^{-1}) >	0.0	Q(9.375)=	50.6385
μ_a =	1.81	A=	
μ_b =		B=	23155.43
μ_c =		C=	

The experimental frequencies are from F. J. Lovas and R. J. Suenram, 1982, J. Mol. Spect. 93, 416. The dipole moment is from T. Amano, S. Saito, E. Hirota, and Y. Moreno, 1969, J. Mol. Spect. 32, 97.

Species Tag:	48010	Name:	SO+
Version:	1		Ground
Date:	Dec. 1996		$^2\Pi_r$ States
Contributor:	J. C. Pearson		

Lines Listed:	194	Q(300.0)=	624.3847
Freq. (GHz) <	2291	Q(225.0)=	445.1934
Max. J:	50	Q(150.0)=	279.3410
LOGSTR0=	-8.0	Q(75.00)=	136.5347
LOGSTR1=	-8.0	Q(37.50)=	69.0386
Isotope Corr.:	-0.022	Q(18.75)=	35.3709
Egy. (cm^{-1}) >	0.0	Q(9.375)=	18.5670
μ_a =	1.0	A=	
μ_b =		B=	23249.1
μ_c =		C=	

The data were taken from: T. Amano, T. Amano and H. E. Warner, 1992, J. Mol. Spectrosc. 146, 519. The A value was fixed to the electronic emmission value of I. W. Milkman, J. C. Ghoi, J. L. Hardwick and J. T. Moseley, 1988, J. Mol. Spectrosc. 130, 20.

The dipole is unknown so a unit dipole was used in the calculations.

There have been several tentitively reportes of SO+ in the interstellar medium, however no convincing assignment has been published to date.

Species Tag:	49001	Name:	O3-sym-O-17
Version:	2		Ozone,
Date:	Mar. 1995		symmetric ^{17}O isotope
Contributor:	E. A. Cohen		

Lines Listed:	26092	Q(300.0)=	20803.525
Freq. (GHz) $<$	4603	Q(225.0)=	13507.522
Max. J:	76	Q(150.0)=	7352.785
LOGSTR0=	-8.5	Q(75.00)=	2605.615
LOGSTR1=	-8.0	Q(37.50)=	928.081
Isotope Corr.:	-3.432	Q(18.75)=	334.464
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	123.884
μ_a =		A=	102351.
μ_b =	0.5337	B=	13350.8
μ_c =		C=	11781.7

The spectra are from E. A. Cohen, K. W. Hillig II, and H. M. Pickett, 1995, J. Mol. Struct. 352/353, 273. The calculation fixes centrifugal distortion constants beyond the sextic terms to those of the parent species with the exception of the coefficients of P_a^{2n} which are assumed to be proportional to A^n. The dipole moment was assumed to be the same as for the parent species, however centrifugal corrections have not been applied. Where several experimental lines have the same frequency, the uncertainties refer to the center of a blended feature, not to the individual components.

Species Tag:	49002	Name:	O3-asym-O-17
Version:	2		Ozone,
Date:	Mar. 1984		asymmetric
Contributor:	E. A. Cohen		^{17}O isotope

Lines Listed:	52613	Q(300.0)=	42098.453
Freq. (GHz) $<$	4681	Q(225.0)=	27331.975
Max. J:	77	Q(150.0)=	14876.039
LOGSTR0=	-8.6	Q(75.00)=	5268.769
LOGSTR1=	-8.3	Q(37.50)=	1873.796
Isotope Corr.:	-3.131	Q(18.75)=	672.414
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	246.163
μ_a =	0.0037	A=	105491.1
μ_b =	0.5337	B=	12951.3
μ_c =		C=	11508.0

The spectra are from E. A. Cohen, K. W. Hillig II, and H. M. Pickett, 1995, J. Mol. Struct. 352/353, 273, as well as the more recently measured $32_{2,30} - 32_{1,31}$ transition near 426012 MHz. The calculation fixes centrifugal distortion constants beyond the sextic terms to those of the parent species with the exception of the coefficients of P_a^{2n} which are assumed to be proportional to A^n. The dipole moments are assumed values based on the structure and the value for the parent species, however centrifugal corrections have not been applied. Where several experimental lines have the same frequency, the uncertainties refer to the center of a blended feature, not to the individual components.

Species Tag:	**49003**	**Name:**	**C4H**
Version:	**1**		**Butadiynyl radical,**
Date:	**Apr. 1995**		**X $^2\Sigma^+$**
Contributor:	**M. L. Delitsky** **H. M. Pickett**		
Lines Listed:	**742**	**Q(300.0)=**	**5255.5819**
Freq. (GHz) <	**920.**	**Q(225.0)=**	**3943.3827**
Max. J:	**98**	**Q(150.0)=**	**2629.1571**
LOGSTR0=	**-8.0**	**Q(75.00)=**	**1315.0879**
LOGSTR1=	**-100**	**Q(37.50)=**	**658.1711**
Isotope Corr.:	**0.0**	**Q(18.75)=**	**329.7433**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**165.5392**
μ_a =	**0.900**	**A=**	
μ_b =		**B=**	**4758.6**
μ_c =		**C=**	

The observed lines are from: M. Guelin *et al.*, 1982, Astron. Astrophys. 109, 23. C.A. Gottlieb *et al.*, 1983, Astrophys. J. 275, 916. The dipole moment is from C.A. Olano *et al.*, 1988, Astron. Astrophys. 196, 194.

Species Tag:	**49004**	**Name:**	**MgCCH**
Version:	**1**		**Magnesium acetylide**
Date:	**Sept. 1995**		**X $^2\Sigma$**
Contributor:	**J. C. Pearson**		

Lines Listed:	**274**	**Q(300.0)=**	**2498.1078**
Freq. (GHz) <	**999**	**Q(225.0)=**	**1873.8091**
Max. J:	**99**	**Q(150.0)=**	**1249.0657**
LOGSTR0=	**-8.0**	**Q(75.00)=**	**624.6680**
LOGSTR1=	**-8.0**	**Q(37.50)=**	**312.6183**
Isotope Corr.:		**Q(18.75)=**	**156.6313**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**78.6485**
μ_a =	**1.000**	**A=**	
μ_b =		**B=**	**5010.38**
μ_c =		**C=**	

The observed lines are from:

M. A. Anderson and L. M. Ziurys, 1995, Astrophys. J. 439, L25 – L28.

The dipole moment is unknown and has been assumend to be unity. The molecule is in a $^2\Sigma$ electronic ground state.

Species Tag:	**50001**	**Name:**	**S-34-O**
Version:	**1**		**X $^3\Sigma$**
Date:	**Dec. 1979**		**^{34}S isotope**
Contributor:	**H. M. Pickett**		
Lines Listed:	**280**	**Q(300.0)=**	**866.962**
Freq. (GHz) <	**2934**	**Q(225.0)=**	**644.614**
Max. J:	**49**	**Q(150.0)=**	**422.669**
LOGSTR0=	**-6.0**	**Q(75.00)=**	**201.326**
LOGSTR1=	**-7.5**	**Q(37.50)=**	**92.045**
Isotope Corr.:	**-1.376**	**Q(18.75)=**	**39.555**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**16.147**
μ_a =	**1.55**	**A=**	
μ_b =		**B=**	**21102.72**
μ_c =		**C=**	

The calculational method is described in T. Amano and E. Hirota, 1974, J. Mol. Spect. 53, 346. The data used were reported in E. Tiemann, 1974, J. Phys. Chem. Ref. Data 3, 259. Both electric and magnetic dipole transitions are listed in the catalog. The dipole moments were assumed to be the same as for the parent species.

Species Tag:	**50002**	**Name:**	**SO-18**
Version:	**1**		**X $^{3}\Sigma$,**
Date:	**Dec. 1979**		**^{18}O isotope**
Contributor:	**H. M. Pickett**		

Lines Listed:	**179**	**Q(300.0)=**	**917.487**
Freq. (GHz) $<$	**2537**	**Q(225.0)=**	**675.461**
Max. J:	**33**	**Q(150.0)=**	**446.684**
LOGSTR0=	**-5.0**	**Q(75.00)=**	**212.814**
LOGSTR1=	**-6.8**	**Q(37.50)=**	**97.118**
Isotope Corr.:	**-2.712**	**Q(18.75)=**	**41.601**
Egy. (cm^{-1}) $>$	**0.0**	**Q(9.375)=**	**16.885**
μ_a =	**1.55**	**A=**	
μ_b =		**B=**	**19929.**
μ_c =		**C=**	

The calculational method is described in T. Amano and E. Hirota, 1974, J. Mol. Spect. 53, 346. The value of $\gamma(1)$ was fixed at -156.51 MHz and $\rho(1)$ was set to zero. Both electric dipole and magnetic dipole transitions are listed in the catalog. The dipole moments were assumed to be the same as for the parent species. The data used are listed in E. Tiemann, 1974, J. Phys. Chem. Ref. Data 3, 259.

Species Tag:	50003	Name:	O3-sym-O-18
Version:	2		Ozone, ground state,
Date:	Mar. 1984		symmetric ^{18}O isotope
Contributor:	H. M. Pickett R. L. Poynter		
Lines Listed:	3184	Q(300.0)=	3525.332
Freq. (GHz) $<$	6529	Q(225.0)=	2290.340
Max. J:	50	Q(150.0)=	1247.096
LOGSTR0=	-9.0	Q(75.00)=	441.875
LOGSTR1=	-9.0	Q(37.50)=	156.567
Isotope Corr.:	-2.690	Q(18.75)=	55.616
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	19.861
μ_a =		A=	98646.687
μ_b =	0.5324	B=	13352.732
μ_c =		C=	11731.767

The catalog of symmetric ^{18}O ozone is based on the work of J. Depannemaecker and J. Bellet, 1977, J. Mol. Spect. 66, 106. The $^{16}O_3$ dipole moment was assumed. This catalog version extends the line calculation in frequency and J.

Species Tag:	**50004**	**Name:**	**O3-asym-O-18**
Version:	**2**		**Asymmetric ^{18}O ozone**
Date:	**Mar. 1984**		
Contributor:	**H. M. Pickett** **R. L. Poynter**		

Lines Listed:	**7304**	**Q(300.0)=**	**7214.397**
Freq. (GHz) $<$	**6209**	**Q(225.0)=**	**4685.975**
Max. J:	**50**	**Q(150.0)=**	**2549.765**
LOGSTR0=	**-8.9**	**Q(75.00)=**	**904.065**
LOGSTR1=	**-9.0**	**Q(37.50)=**	**320.258**
Isotope Corr.:	**-2.389**	**Q(18.75)=**	**113.763**
Egy. (cm^{-1}) $>$	**0.0**	**Q(9.375)=**	**40.607**
μ_a =		**A=**	**104573.161**
μ_b =	**0.5324**	**B=**	**12591.48**
μ_c =		**C=**	**11212.5057**

The catalog of asymmetric ^{18}O ozone is based on the work of J. Depannemaecker and J. Bellet, 1977, J. Mol. Spect. 66, 106. The dipole moment used is the $^{16}O_3$ value rotated to the inertial axes of asymmetric ^{18}O ozone (based on the equilibrium structure). The new calculation extends the catalog in frequency and J.

Species Tag:	**50005**	**Name:**	**O3-s-O18-v2**
Version:	**1**		$\nu_2 = 1$
Date:	**Mar. 1984**		
Contributor:	**C. Chiu and E. A. Cohen**		

Lines Listed:	**2387**	**Q(300.0)=**	**3525.332**
Freq. (GHz) <	**4065**	**Q(225.0)=**	**2290.340**
Max. J:	**50**	**Q(150.0)=**	**1247.096**
LOGSTR0=	**-8.9**	**Q(75.00)=**	**441.875**
LOGSTR1=	**-8.9**	**Q(37.50)=**	**156.567**
Isotope Corr.:	**2.690**	**Q(18.75)=**	**55.616**
Egy. (cm^{-1}) >	**678.0**	**Q(9.375)=**	**19.861**
μ_a =		**A=**	**100177.**
μ_b =	**0.5324**	**B=**	**13316.**
μ_c =		**C=**	**11659.**

New spectra were measured at JPL and were fit to a Watson S set Hamiltonian. The dipole moments were assumed to be the same as for the ground state. The vibrational energy is an assumed value.

Species Tag:	50006	Name:	O3-a-O18-v2
Version:	1		^{18}O$_3$ $\nu_2 = 1$,
Date:	Mar. 1984		end atom substitution
Contributor:	C. Chiu		
	E. A. Cohen		

Lines Listed:	4213	Q(300.0)=	7214.397
Freq. (GHz) $<$	3944	Q(225.0)=	4685.975
Max. J:	50	Q(150.0)=	2549.765
LOGSTR0=	-9.0	Q(75.00)=	904.065
LOGSTR1=	-9.0	Q(37.50)=	320.258
Isotope Corr.:		Q(18.75)=	113.763
Egy. (cm^{-1}) $>$	693.0	Q(9.375)=	40.607
μ_a =	0.0068	A=	106071.8
μ_b =	0.5324	B=	12556.0
μ_c =		C=	11150.6

New spectra were measured at JPL and were fit to a Watson S set Hamiltonian. The dipole moments were assumed to be the same as for the ground state. The vibrational energy is an assumed value.

Species Tag:	50007	Name:	CH3Cl-35
Version:	1		Methyl chloride,
Date:	Mar. 1989		^{35}Cl isotope
Contributor:	E. A. Cohen		

Lines Listed:	6372	Q(300.0)=	28216.297
Freq. (GHz) $<$	2115	Q(225.0)=	18323.145
Max. J:	81	Q(150.0)=	9977.002
LOGSTR0=	-7.5	Q(75.00)=	3533.458
LOGSTR1=	-7.9	Q(37.50)=	1208.370
Isotope Corr.:	-.122	Q(18.75)=	447.816
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	178.608
μ_a =	1.899	A=	156051.
μ_b =		B=	13292.8767
μ_c =		C=	B

The data were taken from G. Wlodarczak *et al.*, 1986, J. Mol. Spect. 116, 251, and references cited therein. Additional measurements up to $K = 12$ were made at JPL for $J = 24 - 23$. The dipole moment is from J. A. Golby and R. J. Butcher, 1984, J. Mol. Spect. 107, 292, but see also G. Wlodarczak *et al.*, 1985, J. Mol. Spect. 112, 401.

Species Tag:	50008	Name:	C3N
Version:	1		Cyanoethynyl,
Date:	Apr. 1995		X $^{2}\Sigma^{+}$
Contributor:	M. L. Delitsky		
	H. M. Pickett		
Lines Listed:	1349	Q(300.0)=	7582.4199
Freq. (GHz) <	986.5	Q(225.0)=	5688.9037
Max. J:	99	Q(150.0)=	3793.0183
LOGSTR0=	-8.0	Q(75.00)=	1897.3279
LOGSTR1=	-100	Q(37.50)=	949.6199
Isotope Corr.:		Q(18.75)=	475.8020
Egy. (cm^{-1}) >	0.0	Q(9.375)=	238.9055
μ_a =	2.200	A=	
μ_b =		B=	4947.6
μ_c =		C=	

The observed lines are from: M. Guelin *et al.*, 1982, Astron. Astrophys. 109, 23. C. A. Gottlieb *et al.*, 1983, Astrophys.J. 275, 916.

The dipole moment is from M. Guelin *et al.*, above.

Species Tag:	50009	Name:	MgCN
Version:	1		Magnesium monocyanide,
Date:	Sept. 1995		X $^2\Sigma$
Contributor:	J. C. Pearson		

Lines Listed:	273	Q(300.0)=	2457.0064
Freq. (GHz) <	999	Q(225.0)=	1842.8710
Max. J:	99	Q(150.0)=	1228.4190
LOGSTR0=	-8.0	Q(75.00)=	614.3377
LOGSTR1=	-8.0	Q(37.50)=	307.4515
Isotope Corr.:		Q(18.75)=	154.0476
Egy. (cm^{-1}) >	0.0	Q(9.375)=	77.3566
μ_a =	1.000	A=	
μ_b =		B=	5094.80
μ_c =		C=	

The observed lines are from: M. A. Anderson, T. C. Steimle and L. M. Ziurys, 1994, Astrophys. J. 429, L41. The dipole moment is unknown and has been assumend to be unity. The molecule is in a $^2\Sigma$ electronic ground state.

Species Tag:	50010	Name:	MgNC Magnesium isocyanide, X $^2\Sigma$
Version:	1		
Date:	Sept. 1995		
Contributor:	J. C. Pearson		
Lines Listed:	269	Q(300.0)=	2098.7613
Freq. (GHz) <	999	Q(225.0)=	1573.8011
Max. J:	99	Q(150.0)=	1049.0468
LOGSTR0=	-8.0	Q(75.00)=	524.6652
LOGSTR1=	-8.0	Q(37.50)=	262.6184
Isotope Corr.:		Q(18.75)=	131.6319
Egy. (cm^{-1}) >	0.0	Q(9.375)=	66.1493
μ_a =	1.000	A=	
μ_b =		B=	5966.90
μ_c =		C=	

The observed lines are from: K. Kawaguchi, E. Kagi, T. Hirano, S. Takano, and S. Saito, 1993, Astrophys. J. 406, L39. The first astronomical observation was by M. Guelin, J. Cernicharo, C. Kahanem and J. Gomez-Gonzalez, 1986, Astron. Astrophys. 157, L17. The dipole moment is unknown and has been assumend to be unity. The molecule is in a $^2\Sigma$ electronic ground state.

Species Tag:	51001	Name:	HCCCN
Version:	3		Cyanoacetylene,
Date:	June 1996		or 2-Propynenitrile
Contributor:	H. S. P. Müller		

Lines Listed:	139	Q(300.0)=	4124.495
Freq. (GHz) <	1050	Q(225.0)=	3093.536
Max. J:	115	Q(150.0)=	2062.526
LOGSTR0=	-7.0	Q(75.00)=	1031.679
LOGSTR1=	-4.4	Q(37.50)=	516.319
Isotope Corr.:	0.	Q(18.75)=	258.656
Egy. (cm^{-1}) >	0.0	Q(9.375)=	129.830
μ_a =	3.724	A=	
μ_b =		B=	4549.058
μ_c =		C=	

The set of experimental lines used in the calculation was obtained from the references in W. J. Lafferty and F. J. Lovas, 1978, J. Phys. Chem. Ref. Data 7, 441. The dipole moment was also given in this reference. Additional lines were taken from K. M. T. Yamada, A. Moravec, and G. Winnewisser, 1996, Z. Naturforsch. 50a, 1179.

Quadrupole splittings due to the ^{14}N nucleus are small. They are only considered for $J \leq 5$. For all other J the spin multiplicity was considered.

Species Tag:	51002	Name:	ClO
Version:	3		Chlorine monoxide,
Date:	Jan. 1991		X $^2\Pi$ states, v = 0
Contributor:	E. A. Cohen		
Lines Listed:	2585	Q(300.0)=	3349.655
Freq. (GHz) <	2983	Q(225.0)=	2307.810
Max. J:	83	Q(150.0)=	1424.624
LOGSTR0=	-10.0	Q(75.00)=	689.287
LOGSTR1=	-11.5	Q(37.50)=	351.318
Isotope Corr.:	-0.122	Q(18.75)=	183.316
Egy. (cm^{-1}) >	0.0	Q(9.375)=	99.701
μ_a =	1.2974	A=	
μ_b =		B=	18601.791
μ_c =		C=	

The experimental lines are from R. K. Kakar, E. A. Cohen, and M. Geller, 1978, J. Mol. Spect. 70, 243, and E. A. Cohen, H. M. Pickett, and M. Geller, 1984, J. Mol. Spect. 106, 430. The millimeter and submillimeter data were combined with the FT infrared data of J. B. Burkholder *et al.*, 1987, J. Mol. Spect. 124, 139, in a simultaneous fit to both vibrational states. The partition function is a sum over the ground and first vibrational state up to F = 90 for both the $\Omega = 3/2$ and $\Omega = 1/2$ states. The dipole moment is from D. Yaron, K. Peterson, and W. Klemperer, 1988, J. Chem. Phys. 88, 4702.

Species Tag:	**51003**	**Name:**	**ClO-v1**
Version:	**1**		**Chlorine monoxide,**
Date:	**Jan. 1991**		**X $^2\Pi$ states, v = 1**
Contributor:	**E. A. Cohen**		
Lines Listed:	**2112**	**Q(300.0)=**	**3349.655**
Freq. (GHz) <	**2881**	**Q(225.0)=**	**2307.810**
Max. J:	**81**	**Q(150.0)=**	**1424.624**
LOGSTR0=	**-9.9**	**Q(75.00)=**	**689.287**
LOGSTR1=	**-11.6**	**Q(37.50)=**	**351.318**
Isotope Corr.:	**-0.122**	**Q(18.75)=**	**183.316**
Egy. (cm^{-1}) >	**844.2**	**Q(9.375)=**	**99.701**
μ_a =	**1.2758**	**A=**	
μ_b =		**B=**	**18423.566**
μ_c =		**C=**	

The experimental lines are from R. K. Kakar, E. A. Cohen, and M. Geller, 1978, J. Mol. Spect. 70, 243, and E. A. Cohen, H. M. Pickett and M. Geller, 1984, J. Mol. Spect. 106, 430. The millimeter and submillimeter data were combined with the FT infrared data of J. B. Burkholder *et al.*, 1987, J. Mol. Spect. 124, 139, in a simultaneous fit to both vibrational states. The partition function is a sum over the ground and first vibrational state up to F = 90 for both the $\Omega = 3/2$ and $\Omega = 1/2$ states. The dipole moment is from D. Yaron, K. Peterson, and W. Klemperer, 1988, J. Chem. Phys. 88, 4702.

Species Tag:	**51004**	**Name:**	**HCCNC**
Version:	**1**		**Ethynyl**
Date:	**Dec. 1994**		**isocyanide**
Contributor:	**M. L. Delitsky**		
	H. M. Pickett		
Lines Listed:	**563**	**Q(300.0)=**	**3775.7021**
Freq. (GHz) $<$	**991.05**	**Q(225.0)=**	**2832.7507**
Max. J:	**99**	**Q(150.0)=**	**1888.7322**
LOGSTR0=	**-10.0**	**Q(75.00)=**	**944.7917**
LOGSTR1=	**-100.0**	**Q(37.50)=**	**472.8781**
Isotope Corr.:	**0.0**	**Q(18.75)=**	**236.9363**
Egy. (cm^{-1}) $>$	**0.0**	**Q(9.375)=**	**118.9708**
μ_a =	**2.93**	**A=**	
μ_b =		**B=**	**4967.838**
μ_c =		**C=**	

The observed frequency measurements were taken from: A. Guarnieri, R. Hinze, M. Krüger and H. Zerbe-Foese, 1992, J. Mol. Spect. 156, 39. M. Krüger, W. Stahl and H. Dreizler, 1992, J. Mol. Spect. 158, 298. The quadrupole coupling values were investigated in M. Krüger, above. Detailed field gradients and quadrupole coupling constants are presented in D. Cremer and M. Krüger, 1991, J. Phys. Chem. 96, 3239.

The dipole moment was taken from M. Krüger, H. Dreizler, D. Preugschat and D. Lentz, 1991, Angew. Chem. Int. Ed. Engl. 30, 1644.

Species Tag:	**51005**	**Name:**	**HCCNC-v7**
Version:	**1**		**Ethynyl-isocyanide,**
Date:	**Jan. 1995**		ν_7 **vibrational state**
Contributor:	**M. L. Delitsky** **H. M. Pickett**		
Lines Listed:	**291**	**Q(300.0)=**	**3775.7021**
Freq. (GHz) <	**984.98**	**Q(225.0)=**	**2832.7507**
Max. J:	**99**	**Q(150.0)=**	**1888.7322**
LOGSTR0=	**-10.0**	**Q(75.00)=**	**944.7917**
LOGSTR1=	**-100.0**	**Q(37.50)=**	**472.8781**
Isotope Corr.:	**0.0**	**Q(18.75)=**	**236.9363**
Egy. $(\mathrm{cm}^{-1}) >$	**203.**	**Q(9.375)=**	**118.9708**
μ_a =	**2.93**	**A=**	
μ_b =		**B=**	**4983.493**
μ_c =		**C=**	

The observed frequency measurements were taken from A. Guarnieri, R. Hinze, M. Krüger and H. Zerbe-Foese, 1992, J. Mol. Spect. 156, 39. The ν_7 vibration is the lowest excited bending state at 203 cm^{-1}. It should be noted that the ν_7 is an l doubled state.

The dipole moment was assumed to be the same as for the ground state. M. Krüger, H. Dreizler, D. Preugschat and D. Lentz, 1991, Angew. Chem. Int. Ed. Engl. 30, 1644.

Species Tag:	51006	Name:	HCCNC-v6
Version:	1		Ethynyl-isocyanide,
Date:	Jan. 1995		ν_6 vibrational state
Contributor:	M. L. Delitsky		
	H. M. Pickett		
Lines Listed:	291	Q(300.0)=	3775.7021
Freq. (GHz) $<$	983.83	Q(225.0)=	2832.7507
Max. J:	99	Q(150.0)=	1888.7322
LOGSTR0=	-10.0	Q(75.00)=	944.7917
LOGSTR1=	-100.0	Q(37.50)=	472.8781
Isotope Corr.:	0.0	Q(18.75)=	236.9363
Egy. (cm^{-1}) $>$	424.0	Q(9.375)=	118.9708
μ_a =	2.93	A=	
μ_b =		B=	4978.500
μ_c =		C=	

The observed frequency measurements were taken from A. Guarnieri, R. Hinze, M. Krüger and H. Zerbe-Foese, 1992, J. Mol. Spect. 156, 39. The ν_6 vibration is a low lying excited bending state at 424 cm^{-1}. It should be noted that the ν_6 is an l doubled state.

The dipole moment was assumed to be the same as for the ground state. M. Krüger, H. Dreizler, D. Preugschat and D. Lentz, 1991, Angew. Chem. Int. Ed. Engl. 30, 1644.

Species Tag:	51007	Name:	HCCNC-v5
Version:	1		Ethynyl-isocyanide,
Date:	Jan. 1995		ν_5 vibrational state
Contributor:	M. L. Delitsky H. M. Pickett		
Lines Listed:	278	Q(300.0)=	3775.7021
Freq. (GHz) $<$	985.34	Q(225.0)=	2832.7507
Max. J:	99	Q(150.0)=	1888.7322
LOGSTR0=	-10.0	Q(75.00)=	944.7917
LOGSTR1=	-100.0	Q(37.50)=	472.8781
Isotope Corr.:	0.0	Q(18.75)=	236.9363
Egy. (cm^{-1}) $>$	634.0	Q(9.375)=	118.9708
μ_a =	2.93	A=	
μ_b =		B=	4970.517
μ_c =		C=	

The observed frequency measurements were taken from A. Guarnieri, R. Hinze, M. Krüger and H. Zerbe-Foese, 1992, J. Mol. Spect. 156, 39. The ν_5 vibration is the lowest excited bending state at 634 cm^{-1}. It should be noted that the ν_5 is an l doubled state.

The dipole moment was assumed to be the same as for the ground state. M. Krüger, H. Dreizler, D. Preugschat and D. Lentz, 1991, Angew. Chem. Int. Ed. Engl. 30, 1644.

Species Tag:	51008	Name:	HNCCC
Version:	1		3-Imino-
Date:	Jan. 1995		1,2-propa-
Contributor:	M. L. Delitsky		dienylidene
	H. M. Pickett		
Lines Listed:	574	Q(300.0)=	4017.0039
Freq. (GHz) <	931.415	Q(225.0)=	3014.3657
Max. J:	99	Q(150.0)=	2009.8453
LOGSTR0=	-10.0	Q(75.00)=	1005.3423
LOGSTR1=	-100.0	Q(37.50)=	503.1517
Isotope Corr.:	0.0	Q(18.75)=	252.0726
Egy. (cm^{-1}) >		Q(9.375)=	126.5386
μ_a =	5.665	A=	
μ_b =		B=	4668.338
μ_c =		C=	

The observed frequency measurements were taken from: Y. Hirahara, Y. Oshima and Y. Endo, 1993, Astrophys. J. 403, L83. Kawaguchi *et al.*, 1992, Astrophys. J. 396, L49.

The dipole moment was calculated by P. Botschwina, M. Horn, S. Seeger and J. Flügge, 1992, Chem. Phys. Lett. 195, 427.

Although quantum calculations of the structure indicate that the molecule may be non-linear, spectral measurements are available only for the $K = 0$ state. For the purposes of fitting the spectra and predicting frequencies and intensities, the $K = 0$ states are equivalent to a linear molecule. The catalog entries for this species are currently presented as a linear molecule, and the intensities are calculated for a unit concentration of $K = 0$ molecules in the ground vibrational state.

Species Tag:	**52001**	**Name:**	**HCCC-13-N**
Version:	**1**		**Cyanoacetylene,**
Date:	**Dec. 1979**		**^{13}C isotope**
Contributor:	**R. L. Poynter**		**on atom 1**

Lines Listed:	**152**	**Q(300.0)=**	**4139.998**
Freq. (GHz) <	**896**	**Q(225.0)=**	**3105.989**
Max. J:	**99**	**Q(150.0)=**	**2071.095**
LOGSTR0=	**-6.6**	**Q(75.00)=**	**1035.858**
LOGSTR1=	**-4.2**	**Q(37.50)=**	**518.442**
Isotope Corr.:	**-1.955**	**Q(18.75)=**	**259.717**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**130.377**
μ_a =	**3.724**	**A=**	
μ_b =		**B=**	**4530.2**
μ_c =		**C=**	

The set of experimental lines used in the calculation was obtained from the references in W. J. Lafferty and F. J. Lovas, 1978, J. Phys. Chem. Ref. Data 7, 441. The dipole moment was remeasured by the above authors.

Species Tag:	52002	Name:	HCC-13-CN Cyanoacetylene, ^{13}C isotope on atom 2
Version:	1		
Date:	Dec. 1979		
Contributor:	R. L. Poynter		

Lines Listed:	146	Q(300.0)=	4140.950
Freq. (GHz) $<$	895	Q(225.0)=	3106.705
Max. J:	99	Q(150.0)=	2071.095
LOGSTR0=	-6.6	Q(75.00)=	1036.096
LOGSTR1=	-4.2	Q(37.50)=	518.561
Isotope Corr.:	-1.955	Q(18.75)=	259.777
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	130.377
μ_a =	3.724	A=	
μ_b =		B=	4529.76
μ_c =		C=	

The set of experimental lines used in the calculation was obtained from the references in W. J. Lafferty and F. J. Lovas, 1978, J. Phys. Chem. Ref. Data 7, 441. The dipole moment was remeasured by the above authors.

Species Tag:	**52003**	**Name:**	**HC-13-CCN**
Version:	**1**		**Cyanoacetylene,**
Date:	**Dec. 1979**		**^{13}C isotope**
Contributor:	**R. L. Poynter**		**on atom 3**
Lines Listed:	**144**	**Q(300.0)=**	**4255.005**
Freq. (GHz) <	**872**	**Q(225.0)=**	**3192.273**
Max. J:	**99**	**Q(150.0)=**	**2128.139**
LOGSTR0=	**-6.6**	**Q(75.00)=**	**1064.633**
LOGSTR1=	**-4.2**	**Q(37.50)=**	**532.721**
Isotope Corr.:	**-1.955**	**Q(18.75)=**	**266.870**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**133.937**
μ_a =	**3.724**	**A=**	
μ_b =		**B=**	**4408.44**
μ_c =		**C=**	

The set of experimental lines used in the calculation was obtained from the references in W. J. Lafferty and F. J. Lovas, 1978, J. Phys. Chem. Ref. Data 7, 441. The dipole moment was remeasured by the above authors.

Species Tag:	**52004**	**Name:**	**HCCCN-15**
Version:	**1**		**Cyanoacetylene,**
Date:	**Dec. 1979**		**^{15}N isotope**
Contributor:	**R. L. Poynter**		
Lines Listed:	**99**	**Q(300.0)=**	**1415.467**
Freq. (GHz) <	**873**	**Q(225.0)=**	**1061.940**
Max. J:	**99**	**Q(150.0)=**	**708.109**
LOGSTR0=	**-5.3**	**Q(75.00)=**	**354.160**
LOGSTR1=	**-3.2**	**Q(37.50)=**	**177.256**
Isotope Corr.:	**-2.432**	**Q(18.75)=**	**88.797**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**44.566**
μ_a =	**3.724**	**A=**	
μ_b =		**B=**	**4416.75**
μ_c =		**C=**	

The set of experimental lines used in the calculation was obtained from the references in W. J. Lafferty and F. J. Lovas, 1978, J. Phys. Chem. Ref. Data 7, 441. The dipole moment was remeasured by the above authors.

Species Tag:	52005	Name:	DCCCN
Version:	1		Cyanoacetylene, deuterium isotope
Date:	Dec. 1979		
Contributor:	R. L. Poynter		

Lines Listed:	156	Q(300.0)=	4443.243
Freq. (GHz) <	835	Q(225.0)=	3332.729
Max. J:	99	Q(150.0)=	2222.287
LOGSTR0=	-6.7	Q(75.00)=	1111.732
LOGSTR1=	-4.2	Q(37.50)=	556.288
Isotope Corr.:	-3.824	Q(18.75)=	278.612
Egy. (cm^{-1}) >	0.0	Q(9.375)=	139.830
μ_a =	3.724	A=	
μ_b =		B=	4221.58
μ_c =		C=	

The set of experimental lines used in the calculation was obtained from the references in W. J. Lafferty and F. J. Lovas, 1978, J. Phys. Chem. Ref. Data 7, 441. The dipole moment was assumed to be the same as for the parent molecule.

Species Tag:	52006	Name:	HOCl
Version:	3		Hypochlorous acid
Date:	Jan. 1984		
Contributor:	H. M. Pickett		

Lines Listed:	6929	Q(300.0)=	9521.381
Freq. (GHz) $<$	9983	Q(225.0)=	6181.587
Max. J:	60	Q(150.0)=	3363.566
LOGSTR0=	-7.9	Q(75.00)=	1190.145
LOGSTR1=	-8.0	Q(37.50)=	421.891
Isotope Corr.:	-0.122	Q(18.75)=	150.626
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	58.371
μ_a =	0.3627	A=	613483.8
μ_b =	1.471	B=	15116.795
μ_c =		C=	14725.78

The data and calculational method are given in H. E. Singbeil *et al.*, 1984, J. Mol. Spect. 103, 466. The chlorine hyperfine structure is omitted in this version of the catalog for higher J, since the splittings are generally smaller than the width of lower stratospheric lines. The maximum value of K_a in the calculation is 20.

Species Tag:	**52007**	**Name:**	**SiCC**
Version:	**2**		**Silicon dicarbide**
Date:	**Mar. 1994**		
Contributor:	**H. M. Pickett**		

Lines Listed:	**304**	**Q(300.0)=**	**3032.042**
Freq. (GHz) <	**9999**	**Q(225.0)=**	**2364.275**
Max. J:	**22**	**Q(150.0)=**	**1550.871**
LOGSTR0=	**-10.0**	**Q(75.00)=**	**633.977**
LOGSTR1=	**-4.0**	**Q(37.50)=**	**229.198**
Isotope Corr.:	**0.0**	**Q(18.75)=**	**81.370**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**29.025**
μ_a =	**2.393**	**A=**	**52473.3**
μ_b =		**B=**	**13158.6**
μ_c =		**C=**	**10441.6**

Measurements of ground state transitions and the dipole moment are from R. D. Suenram, F. J. Lovas, and K. Matsumura, 1989, Astrophys. J. Lett. 342, L103. The other transitions are from C. A. Gottlieb, J. M. Vrtilek, and P. Thaddeus, 1989, Astrophys. J. Lett. 343, L29.

Species Tag:	**52008**	**Name:**	**CCCO**
Version:	**1**		**Tricarbon monoxide,**
Date:	**Jan. 1990**		**X $^1\Sigma^+$**
Contributor:	**R. L. Poynter**		

Lines Listed:	**51**	**Q(300.0)=**	**1297.777**
Freq. (GHz) $<$	**492**	**Q(225.0)=**	**974.541**
Max. J:	**51**	**Q(150.0)=**	**649.980**
LOGSTR0=	**-5.6**	**Q(75.00)=**	**325.162**
LOGSTR1=	**-2.6**	**Q(37.50)=**	**162.742**
Isotope Corr.:	**0.0**	**Q(18.75)=**	**81.545**
Egy. (cm^{-1}) $>$	**0.0**	**Q(9.375)=**	**40.935**
μ_a =		**A=**	
μ_b =	**2.391**	**B=**	**4810.8809(17)**
μ_c =		**C=**	

The line measurements were taken from R. D. Brown *et al.*, 1983, J. Am. Chem. Soc. 105, 6496, and R. D. Brown *et al.*, 1985, J. Am. Chem. Soc. 107, 4112. The dipole moment was reported in the first of these two papers.

Species Tag:	**52009**	**Name:**	**CH3Cl-37**
Version:	**1**		**Methyl chloride,**
Date:	**Mar. 1989**		**^{37}Cl isotope**
Contributor:	**E. A. Cohen**		
Lines Listed:	**6403**	**Q(300.0)=**	**28621.992**
Freq. (GHz) $<$	**2083**	**Q(225.0)=**	**18603.725**
Max. J:	**81**	**Q(150.0)=**	**10120.452**
LOGSTR0=	**-7.5**	**Q(75.00)=**	**3584.264**
LOGSTR1=	**-7.9**	**Q(37.50)=**	**1227.722**
Isotope Corr.:	**-0.611**	**Q(18.75)=**	**454.883**
Egy. (cm^{-1}) $>$	**0.0**	**Q(9.375)=**	**181.343**
μ_a =	**1.895**	**A=**	**156051.**
μ_b =		**B=**	**13088.1710**
μ_c =		**C=**	**B**

The data were taken from G. Wlodarczak *et al.*, 1986, J. Mol. Spect. 116, 251, and references cited therein. Additional measurements up to $K = 12$ were made at JPL for $J = 24 - 23$. The dipole moment is from J. A. Golby and R. J. Butcher, 1984, J. Mol. Spect. 107, 292, but see also G. Wlodarczak *et al.*, 1985, J. Mol. Spect. 112, 401.

Species Tag:	**52010**	**Name:**	**CH2F2**
Version:	**1**		**Difluoro methane**
Date:	**Nov. 1989**		
Contributor:	**H. M. Pickett**		
Lines Listed:	**11942**	**Q(300.0)=**	**55398.785**
Freq. (GHz) <	**3624**	**Q(225.0)=**	**34017.324**
Max. J:	**80**	**Q(150.0)=**	**17992.842**
LOGSTR0=	**-7.9**	**Q(75.00)=**	**6324.120**
LOGSTR1=	**-7.0**	**Q(37.50)=**	**2239.752**
Isotope Corr.:	**0.0**	**Q(18.75)=**	**794.877**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**283.270**
μ_a =		**A=**	**49142.867**
μ_b =	**1.9785**	**B=**	**10604.822**
μ_c =		**C=**	**9249.756**

Microwave transitions are from E. Hirota *et al.*, 1970, J. Mol. Spect. 34, 222. Millimeter and submillimeter transitions are from L. Martinache *et al.*, 1986, J. Mol. Spect. 119, 225. Far-infrared spectra are from M. Carlotti *et al.*, 1988, J. Mol. Spect. 132, 158. These frequencies were multiplied by 0.9999982 to bring the lines more in agreement with the microwave and submillimeter data. The dipole moment is from K. Kawaguchi and T. Tanaka, 1986, J. Mol. Spect. 68, 125. The partition function includes allowance for the vibrational states.

Species Tag:	**52011**	**Name:**	**CH2F2-v4**
Version:	**1**		**Difluoro methane,**
Date:	**Nov. 1989**		**ν_4 state**
Contributor:	**H. M. Pickett**		
Lines Listed:	**7808**	**Q(300.0)=**	**55398.785**
Freq. (GHz) <	**3189**	**Q(225.0)=**	**34017.324**
Max. J:	**79**	**Q(150.0)=**	**17992.842**
LOGSTR0=	**-8.0**	**Q(75.00)=**	**6324.120**
LOGSTR1=	**-7.0**	**Q(37.50)=**	**2239.752**
Isotope Corr.:	**0.0**	**Q(18.75)=**	**794.877**
Egy. (cm^{-1}) >	**528.5**	**Q(9.375)=**	**283.270**
μ_a =		**A=**	**49480.535**
μ_b =	**1.9785**	**B=**	**10582.942**
μ_c =		**C=**	**9216.495**

Far-infrared spectra are from M. Carlotti *et al.*, 1988, J. Mol. Spect. 132, 158. These frequencies were multiplied by 0.9999982 to bring the ground state lines more in agreement with the microwave and submillimeter data. The dipole moment is from K. Kawaguchi and T. Tanaka, 1986, J. Mol. Spect. 68, 125. The partition function includes allowance for the vibrational states.

Species Tag:	**52012**	**Name:**	**DNCCC**
Version:	**1**		
Date:	**Jan. 1995**		
Contributor:	**M. L. Delitsky** **H. M. Pickett**		
Lines Listed:	**3098**	**Q(300.0)=**	**12778.1637**
Freq. (GHz) <	**861.502**	**Q(225.0)=**	**9591.6915**
Max. J:	**99**	**Q(150.0)=**	**6395.7308**
LOGSTR0=	**-10.0**	**Q(75.00)=**	**3199.2303**
LOGSTR1=	**-100.0**	**Q(37.50)=**	**1601.0829**
Isotope Corr.:	**-3.824**	**Q(18.75)=**	**802.0379**
Egy. (cm^{-1}) >		**Q(9.375)=**	**402.5269**
μ_a =	**5.665**	**A=**	
μ_b =		**B=**	**4400.593**
μ_c =		**C=**	

The observed laboratory frequency measurements were taken from Y. Hirahara, Y. Oshima and Y. Endo, 1993, Astrophys. J. 403, L83.

The dipole moment for HNCCC was calculated by P. Botschwina, M. Horn, S. Seeger and J. Flügge, 1992, Chem. Phys. Lett. 195, 427. The same value was assumed for DNCCC.

Although quantum calculations of the structure indicate that the molecule may be non-linear, spectral measurements are available only for the $K = 0$ state. For the purposes of fitting the spectra and predicting frequencies and intensities, the $K = 0$ states are equivalent to a linear molecule. The catalog entries for this species are currently presented as a linear molecule, and the intensities are calculated for a unit concentration of $K = 0$ molecules in the ground vibrational state.

Species Tag:	52013	Name:	CNCN
Version:	2		Isocyanogen
Date:	Jan. 1998		
Contributor:	H. S. P. Müller		
	H. M. Pickett		
Lines Listed:	206	Q(300.0)=	10877.0116
Freq. (GHz) $<$	1022	Q(225.0)=	8159.7753
Max. J:	99	Q(150.0)=	5440.4711
LOGSTR0=	-9.0	Q(75.00)=	2721.5031
LOGSTR1=	-6.0	Q(37.50)=	1362.1960
Isotope Corr.:	0.	Q(18.75)=	682.5893
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	342.8030
μ_a =	0.7074	A=	
μ_b =		B=	5174.1377
μ_c =		C=	

The data is taken from M. C. L. Gerry, F. Stroh, and M. Winnewisser, 1990, J. Mol. Spectrosc. 140, 147. Quadrupole splittings have been resolved for $J = 1$-0 and 2-1. Predictions with quadrupole splittings have been included for all J even though the splittings are rather small.

Species Tag:	53001	Name:	C2H3CN
Version:	3		Acrylonitrile,
Date:	Oct. 1996		ground state, $\nu_{11} = 1$
Contributor:	H. S. P. Müller		and $\nu_{15} = 1$
	J. C. Pearson		
Lines Listed:	75697	Q(300.0)=	119380.376
Freq. (GHz) <	2000	Q(225.0)=	68141.227
Max. J:	99	Q(150.0)=	31738.832
LOGSTR0=	-10.0	Q(75.00)=	9958.401
LOGSTR1=	-9.0	Q(37.50)=	3481.779
Isotope Corr.:	0	Q(18.75)=	1232.852
Egy. (cm^{-1}) >	0.0, 239, 340	Q(9.375)=	437.499
μ_a =	3.815	A=	49850.697
μ_b =	0.894	B=	4971.1636
μ_c =		C=	4513.8773

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333. The measurements were taken from: (1) C. C. Costain and B. P. Stoicheff, 1959, J. Chem. Phys. 30, 777; (2) M. C. L. Gerry and G. Winnewisser, 1973, J. Mol. Spect. 48, 1; (3) M. C. L. Gerry, K. Yamada, and G. Winnewisser, 1979, J. Phys. Chem. Ref. Data 8, 107; (4) G. Cazzoli and Z. Kisiel, 1988, J. Mol. Spect. 130, 303; (5) M. Stolze and D. H. Sutter, 1985, Z. Naturforsch. 40a, 998; (6) J. Demaison, J. Cosléou, R. Bocquet, and A. G. Lesarri, 1994, J. Mol. Spect. 167, 400; (7) O. I. Baskakov, S. F. Dyubko, V. V. Ilyushin, M. N. Efimenko, V. A. Efremov, S. V. Podnos, and E. A. Alekseev, (1997) J. Mol. Spect. 179, 94; and J. M. Colmont, G. Wlodarczk, D. Priem, H. S. P. Müller, E. H. Tien, R. J. Richards, and M. C. L. Gerry, 1997, J. Mol. Spect. 181, .

For the ground vibrational state ^{14}N quadrupole splittings have been included in the catalog where they have been resolved experimentally; see e. g. (5), (7), (8).

The partition function given here includes the spin-multiplicity of the ^{14}N nucleus as well as the two low lying vibrational states.

The dipole moment is from (5). The ground state dipole moment was used for the excited states.

The vibrational states are 0 = ground state, 1 = in plane CCN bend, $\nu_{11} = 1$, at 239 cm^{-1} and 2 = CCN out of plane bend, $\nu_{15} = 1$, at 340 cm^{-1}.

Species Tag:	**53002**	**Name:**	**Cl-37-O**
Version:	**3**		**Chlorine monoxide,**
Date:	**Jan. 1991**		**X $^2\Pi$ states, v = 0**
Contributor:	**E. A. Cohen**		

Lines Listed:	**2624**	**Q(300.0)=**	**3409.573**
Freq. (GHz) <	**3000**	**Q(225.0)=**	**2347.470**
Max. J:	**85**	**Q(150.0)=**	**1449.105**
LOGSTR0=	**-10.0**	**Q(75.00)=**	**700.971**
LOGSTR1=	**-11.5**	**Q(37.50)=**	**357.108**
Isotope Corr.:	**-0.611**	**Q(18.75)=**	**186.209**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**101.135**
μ_a =	**1.2974**	**A=**	
μ_b =		**B=**	**18217.159**
μ_c =		**C=**	

The experimental lines are from R. K. Kakar, E. A. Cohen, and M. Geller, 1978, J. Mol. Spect. 70, 243, and E. A. Cohen, H. M. Pickett, and M. Geller, 1984, J. Mol. Spect. 106, 430. The millimeter and submillimeter data were combined with the FT infrared data of J. B. Burkholder *et al.*, **1987, J. Mol. Spect. 124, 139, in a simultaneous fit to both vibrational states. The partition function is a sum over the ground and first vibrational state up to F = 90 for both the $\Omega = 3/2$ and $\Omega = 1/2$ states. The dipole moment is from D. Yaron, K. Peterson, and W. Klemperer, 1988, J. Chem. Phys. 88, 4702, and was assumed to be unchanged for ^{37}ClO.**

Species Tag:	53003	Name:	C-13-CCO
Version:	1		Tricarbon monoxide,
Date:	Jan. 1990		X $^{1}\Sigma^{+}$,
Contributor:	R. L. Poynter		^{13}C isotope
			on carbon atom 3
Lines Listed:	99	Q(300.0)=	1350.206
Freq. (GHz) $<$	915	Q(225.0)=	1012.511
Max. J:	99	Q(150.0)=	675.150
LOGSTR0=	-5.6	Q(75.00)=	337.676
LOGSTR1=	-3.7	Q(37.50)=	169.005
Isotope Corr.:	-1.955	Q(18.75)=	84.664
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	42.501
μ_a =	2.391	A=	
μ_b =		B=	4632.8406(37)
μ_c =		C=	

The line measurements were taken from R. D. Brown *et al.*, 1985, J. Am. Chem. Soc. 107, 4112. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	53004	Name:	CC-13-CO
Version:	1		Tricarbon monoxide,
Date:	Jan. 1990		X $^{1}\Sigma^{+}$,
Contributor:	R. L. Poynter		^{13}C isotope
			on carbon atom 2
Lines Listed:	99	Q(300.0)=	1307.345
Freq. (GHz) <	945	Q(225.0)=	980.513
Max. J:	99	Q(150.0)=	653.731
LOGSTR0=	-5.6	Q(75.00)=	327.005
LOGSTR1=	-3.7	Q(37.50)=	163.662
Isotope Corr.:	-1.955	Q(18.75)=	81.997
Egy. (cm^{-1}) >	0.0	Q(9.375)=	41.166
μ_a =	2.391	A=	
μ_b =		B=	4784.2457(32)
μ_c =		C=	

The line measurements were taken from R. D. Brown *et al.*, 1985, J. Am. Chem. Soc. 107, 4112. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	53005	Name:	CCC-13-O
Version:	1		Tricarbon monoxide,
Date:	Jan. 1990		X $^1\Sigma^+$,
Contributor:	R. L. Poynter		^{13}C isotope
			on carbon atom 1
Lines Listed:	99	Q(300.0)=	1303.703
Freq. (GHz) <	947	Q(225.0)=	977.762
Max. J:	99	Q(150.0)=	651.884
LOGSTR0=	-5.6	Q(75.00)=	326.075
LOGSTR1=	-3.7	Q(37.50)=	163.196
Isotope Corr.:	-1.955	Q(18.75)=	81.763
Egy. (cm^{-1}) >	0.0	Q(9.375)=	41.049
μ_a =	2.391	A=	
μ_b =		B=	4797.9956(34)
μ_c =		C=	

The line measurements were taken from R. D. Brown *et al.*, 1985, J. Am. Chem. Soc. 107, 4112. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	**53006**	**Name:**	**Cl-37-O-v1**
Version:	**1**		**Chlorine monoxide,**
Date:	**Jan. 1991**		**X $^2\Pi$ states, v = 1**
Contributor:	**E. A. Cohen**		

Lines Listed:	**2132**	**Q(300.0)=**	**3409.573**
Freq. (GHz) <	**2834**	**Q(225.0)=**	**2347.470**
Max. J:	**81**	**Q(150.0)=**	**1449.105**
LOGSTR0=	**-9.9**	**Q(75.00)=**	**700.971**
LOGSTR1=	**-11.5**	**Q(37.50)=**	**357.108**
Isotope Corr.:	**-0.611**	**Q(18.75)=**	**186.209**
Egy. (cm^{-1}) >	**837.1**	**Q(9.375)=**	**101.135**
μ_a =	**1.2758**	**A=**	
μ_b =		**B=**	**18113.451**
μ_c =		**C=**	

The experimental lines are from R. K. Kakar, E. A. Cohen, and M. Geller, 1978, J. Mol. Spect. 70, 243, and E. A. Cohen, H. M. Pickett, and M. Geller, 1984, J. Mol. Spect. 106, 430. The millimeter and submillimeter data were combined with the FT infrared data of J. B. Burkholder *et al.*, **1987, J. Mol. Spect. 124, 139, in a simultaneous fit to both vibrational states. The partition function is a sum over the ground and first vibrational state up to F = 90 for both the $\Omega = 3/2$ and $\Omega = 1/2$ states. The dipole moment is from D. Yaron, K. Peterson, and W. Klemperer, 1988, J. Chem. Phys. 88, 4702, and assumed to be unchanged for ^{37}ClO.**

Species Tag:	53007	Name:	C2H3NC
Version:	1		Vinyl isocyanide
Date:	Sept. 1995		
Contributor:	J. C. Pearson		

Lines Listed:	9362	Q(300.0)=	22773.670
Freq. (GHz) $<$	1000	Q(225.0)=	15271.762
Max. J:	60	Q(150.0)=	8437.069
LOGSTR0=	-10.0	Q(75.00)=	2987.428
LOGSTR1=	-10.0	Q(37.50)=	1056.547
Isotope Corr.:	0	Q(18.75)=	374.187
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	132.824
μ_a =	3.47	A=	51479.46
μ_b =	0.79	B=	5386.65
μ_c =		C=	4868.94

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333. The measurements were taken from: K. Yamada and M. Winnewisser, 1975, Z. Naturforsch. 30a, 672-689. G. Bestmann and H. Dreizler, 1981, Z. Naturforsch. 37a, 58-63.

The dipole moment was measured by K. Bolton, N. L. Owen, and J. Sheridan, 1970, Spectrochim. Acta 26 A, 909.

Species Tag:	**53008**	**Name:**	**HNCCN+**
Version:	**1**		
Date:	**June 1996**		**(protonated Dicyane)**
Contributor:	**H. S. P. Müller**		**X $^1\Sigma^+$**
Lines Listed:	**99**	**Q(300.0)=**	**1408.1406**
Freq. (GHz) <	**880**	**Q(225.0)=**	**1056.8982**
Max. J:	**99**	**Q(150.0)=**	**704.7054**
LOGSTR0=	**-5.0**	**Q(75.00)=**	**352.4901**
LOGSTR1=	**-3.0**	**Q(37.50)=**	**176.4046**
Isotope Corr.:	**0.**	**Q(18.75)=**	**88.3677**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**44.3512**
μ_a =	**6.448**	**A=**	
μ_b =		**B=**	**4438.010**
μ_c =		**C=**	

The data is taken from T. Amano and F. Scappini, 1991, J. Chem. Phys. 95, 2280. Quadrupole splittings have not been resolved. The dipole moment is from an *ab initio* calculation of P. Botschwina and P. Sebald, 1990, Chem. Phys. 141, 311.

Species Tag:	**54001**	**Name:**	**CH2CHC-13-N**
Version:	**1**		**Acrylonitrile,**
Date:	**Jan. 1980**		**^{13}C isotope**
Contributor:	**R. L. Poynter**		**on atom 1**
Lines Listed:	**118**	**Q(300.0)=**	**26332.967**
Freq. (GHz) <	**349**	**Q(225.0)=**	**17104.088**
Max. J:	**10**	**Q(150.0)=**	**9311.081**
LOGSTR0=	**-8.4**	**Q(75.00)=**	**3291.547**
LOGSTR1=	**-6.5**	**Q(37.50)=**	**1163.858**
Isotope Corr.:	**-1.955**	**Q(18.75)=**	**358.509**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**138.325**
μ_a =	**3.68**	**A=**	**49781.**
μ_b =	**1.25**	**B=**	**4948.153**
μ_c =		**C=**	**4494.485**

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333. The measurements were taken from C. C. Costain and B. P. Stoicheff, 1959, J. Chem. Phys. 30, 77. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	**54002**	**Name:**	**CH2C-13-HCN**
Version:	**1**		**Acrylonitrile,**
Date:	**Jan. 1980**		**^{13}C isotope**
Contributor:	**R. L. Poynter**		**on atom 2**
Lines Listed:	**117**	**Q(300.0)=**	**26662.445**
Freq. (GHz) <	**178**	**Q(225.0)=**	**17318.096**
Max. J:	**10**	**Q(150.0)=**	**9427.576**
LOGSTR0=	**-8.5**	**Q(75.00)=**	**3332.729**
LOGSTR1=	**-6.5**	**Q(37.50)=**	**1178.420**
Isotope Corr.:	**-1.955**	**Q(18.75)=**	**362.911**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**140.023**
μ_a =	**3.68**	**A=**	**48645.**
μ_b =	**1.25**	**B=**	**4948.700**
μ_c =		**C=**	**4485.145**

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333.. The measurements were taken from C. C. Costain and B. P. Stoicheff, 1959, J. Chem. Phys. 30, 77. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	54003	Name:	C-13-H2CHCN
Version:	1		Acrylonitrile,
Date:	Jan. 1980		^{13}C isotope
Contributor:	R. L. Poynter		on atom 3

Lines Listed:	116	Q(300.0)=	27089.428
Freq. (GHz) $<$	180	Q(225.0)=	26631.754
Max. J:	10	Q(150.0)=	9578.558
LOGSTR0=	-8.6	Q(75.00)=	3386.102
LOGSTR1=	-6.4	Q(37.50)=	1197.292
Isotope Corr.:	-1.955	Q(18.75)=	366.860
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	141.710
μ_a =	3.68	A=	49180.
μ_b =	1.25	B=	4837.34
μ_c =		C=	4398.07

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333. The measurements were taken from C. C. Costain and B. P. Stoicheff, 1959, J. Chem. Phys. 30, 77. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	**54004**	**Name:**	**CH2CDCN**
Version:	**2**		**Acrylonitrile,**
Date:	**Dec. 1996**		**Deuterium isotope**
Contributor:	**H. S. P. Müller**		**on atom 2**

Lines Listed:	**6381**	**Q(300.0)=**	**29776.887**
Freq. (GHz) <	**800**	**Q(225.0)=**	**19346.390**
Max. J:	**70**	**Q(150.0)=**	**10523.606**
LOGSTR0=	**-8.5**	**Q(75.00)=**	**3718.695**
LOGSTR1=	**-5.0**	**Q(37.50)=**	**1315.326**
Isotope Corr.:	**-3.824**	**Q(18.75)=**	**465.793**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**165.282**
μ_a =	**3.815**	**A=**	**40196.55**
μ_b =	**0.894**	**B=**	**4934.352**
μ_c =		**C=**	**4388.387**

The measurements were taken from J. M. Colmont, G. Wlodarczak, D. Priem, H. S. P. Müller, E. H. Tien, R. J. Richards, and M. C. L. Gerry, 1997, J. Mol. Spectrosc. 181, 330. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	54005	Name:	HOCl-37
Version:	3		Hypochlorous acid,
Date:	Jan. 1984		^{37}Cl isotope
Contributor:	H. M. Pickett		
Lines Listed:	6925	Q(300.0)=	9689.470
Freq. (GHz) <	9999	Q(225.0)=	6290.716
Max. J:	60	Q(150.0)=	3422.946
LOGSTR0=	-7.9	Q(75.00)=	1211.156
LOGSTR1=	-8.0	Q(37.50)=	429.339
Isotope Corr.:	-0.611	Q(18.75)=	153.250
Egy. (cm^{-1}) >	0.0	Q(9.375)=	59.375
μ_a =	0.3627	A=	613461
μ_b =	1.471	B=	14850.441
μ_c =		C=	14472.895

The data and calculational method are given in H. E. Singbeil *et al.*, 1984, J. Mol. Spect. 103, 466. The chlorine hyperfine structure is omitted at higher J since the splittings are generally smaller than the width of lower stratospheric lines. The maximum value of K in the calculation is 20.

Species Tag:	54006	Name:	CCCO-18
Version:	1		Tricarbon monoxide,
Date:	Jan. 1990		X $^1\Sigma^+$,
Contributor:	R. L. Poynter		^{18}O isotope

Lines Listed:	99	Q(300.0)=	1368.044
Freq. (GHz) $<$	903	Q(225.0)=	1026.124
Max. J:	99	Q(150.0)=	684.069
LOGSTR0=	-5.6	Q(75.00)=	342.137
LOGSTR1=	-3.7	Q(37.50)=	171.238
Isotope Corr.:	-2.690	Q(18.75)=	85.783
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	43.063
μ_a =	2.391	A=	
μ_b =		B=	4572.2943(14)
μ_c =		C=	

The line measurements were taken from R. D. Brown *et al.*, 1985, J. Am. Chem. Soc. 107, 4112. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	54007	Name:	HCCCHO
Version:	1		Propynal or
Date:	Jan. 1996		Propiolic aldehyde
Contributor:	J. C. Pearson		

Lines Listed:	8407	Q(300.0)=	19562.548
Freq. (GHz) $<$	2000	Q(225.0)=	13737.474
Max. J:	50	Q(150.0)=	7922.005
LOGSTR0=	-8.0	Q(75.00)=	2856.363
LOGSTR1=	-8.0	Q(37.50)=	1010.200
Isotope Corr.:		Q(18.75)=	357.654
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	126.904
μ_a =	2.39	A=	68035.3
μ_b =	0.60	B=	4826.3
μ_c =		C=	4499.5

The experimental measurements were taken from: J. A. Howe and J. H. Goldstein, J. Chem. Phys. 23, 1223 (1955). C. C. Costain and R. J. Morton, J. Chem. Phys. 31, 389 (1959). G. Winnewisser, J. Mol. Spect. 46, 16 (1973). The dipole moment comes from Howe and Goldstein, above.

Propynal is a known interstellar molecule first detected in 1988 by W. M. Irvine, R. D. Brown, D. M. Cragg, P. Friberg, P. D. Godfrey *et al.*, Astrophys. J. 335, L89 (1988).

Species Tag:	55001	Name:	C2H5CN
Version:	4		Ethyl Cyanide or
Date:	Jan. 1997		Propionitrile
Contributor:	J. C. Pearson		
Lines Listed:	52883	Q(300.0)=	37389.7769
Freq. (GHz) <	3373	Q(225.0)=	24284.7664
Max. J:	99	Q(150.0)=	13209.5756
LOGSTR0=	-9.0	Q(75.00)=	4667.9360
LOGSTR1=	-9.0	Q(37.50)=	1651.0571
Isotope Corr.:	0	Q(18.75)=	584.6478
Egy. (cm^{-1}) >	0.0	Q(9.375)=	207.4255
μ_a =	3.85	A=	27663.7
μ_b =	1.23	B=	4714.2
μ_c =		C=	4235.1

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333, and W. H. Kirchhoff and D. R. Johnson, 1973, J. Mol. Spect. 45, 159. The measurements were taken from: J. Burie, J. Demaison, A. Dubrulle, and D. Boucher, 1978, J. Mol. Spect. 72, 275; D. R. Johnson, F. J. Lovas, C. A. Gottlieb, E. W. Gottlieb, M. M. Litvak, M. Guelin, and P. Thaddeus, 1977, Astrophys. J. 218, 370; F. J. Lovas, 1982, J. Phys. Chem. Ref. Data 11, 251; H. Mäder, H. M. Heise, and H. Dreizler, 1973, Z. Naturforsch. 29a, 164; J. C. Pearson, K. V. L. N. Sastry, E. Herbst and F. C. De Lucia, 1994, Astrophys. J. Suppl. 93, 589; Y. Fukuyama, H. Odashima, K. Takagi, S. Tsunekawa, 1996, Astrophys. J. Suppl. 104 329.

The dipole moment was taken from H. M. Heise, H. Lutz, and H. Dreizler, 1974, Z. Naturforsch. 29a, 1345.

The methyl torsion and the ^{14}N hyperfine have been resolved in ethyl cyanide, but were not included in the calculation since the effects are small and usually not observable in the millimeter and submillimeter. For analysis see Heise *et al.* and D. Boucher, A. Dubrulle, J. Demaison, and H. Dreizler, 1980, Z. Naturforsch. 35a, 1136.

Species Tag:	56001	Name:	CH3CH2C-13-N
Version:	2		Ethyl cyanide,
Date:	Jan. 1981		^{13}C isotope on atom 1
Contributor:	R. L. Poynter		

Lines Listed:	1183	Q(300.0)=	112460.531
Freq. (GHz) <	530	Q(225.0)=	71285.328
Max. J:	10	Q(150.0)=	39774.051
LOGSTR0=	-9.0	Q(75.00)=	12659.013
LOGSTR1=	-8.2	Q(37.50)=	4620.618
Isotope Corr.:	-1.955	Q(18.75)=	1414.165
Egy. (cm^{-1}) >	0.0	Q(9.375)=	654.486
μ_a =	3.84	A=	27634.94
μ_b =	1.37	B=	4689.805
μ_c =		C=	4214.746

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333, and W. H. Kirchhoff and D. R. Johnson, 1973, J. Mol. Spect. 45, 159. The measurements were taken from H. M. Heise, H. Lutz, and H. Dreizler, 1973, Z. Naturforsch. 29a, 1345. The dipole is an approximate value.

Species Tag:	**56002**	**Name:**	**CH3C-13-H2CN**
Version:	**2**		**Ethyl cyanide,**
Date:	**Jan. 1981**		**^{13}C isotope on atom 2**
Contributor:	**R. L. Poynter**		
Lines Listed:	**1252**	**Q(300.0)=**	**113684.125**
Freq. (GHz) <	**519**	**Q(225.0)=**	**72060.930**
Max. J:	**10**	**Q(150.0)=**	**40206.848**
LOGSTR0=	**-9.0**	**Q(75.00)=**	**12796.760**
LOGSTR1=	**-8.2**	**Q(37.50)=**	**4670.894**
Isotope Corr.:	**-1.955**	**Q(18.75)=**	**1429.552**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**661.607**
μ_a =	**3.84**	**A=**	**27045.40**
μ_b =	**1.37**	**B=**	**4697.868**
μ_c =		**C=**	**4207.046**

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333, and W. H. Kirchhoff and D. R. Johnson, 1973, J. Mol. Spect. 45, 159. The measurements were taken from H. M. Heise, H. Lutz, and H. Dreizler, 1973, Z. Naturforsch. 29a, 1345. The dipole moment is an approximate value.

Species Tag:	56003	Name:	C-13-H3CH2CN
Version:	2		Ethyl cyanide,
Date:	Jan. 1981		^{13}C isotope
Contributor:	R. L. Poynter		on atom 3
Lines Listed:	1183	Q(300.0)=	115292.219
Freq. (GHz) <	524	Q(225.0)=	73080.258
Max. J:	10	Q(150.0)=	40775.586
LOGSTR0=	-9.0	Q(75.00)=	12977.773
LOGSTR1=	-8.2	Q(37.50)=	4736.962
Isotope Corr.:	-1.955	Q(18.75)=	1449.439
Egy. (cm^{-1}) >	0.0	Q(9.375)=	670.965
$\mu_a =$	3.84	A=	27342.174
$\mu_b =$	1.37	B=	4597.939
$\mu_c =$		C=	4133.707

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333, and W. H. Kirchhoff and D. R. Johnson, 1973, J. Mol. Spect. 45, 159. The measurements were taken from H. M. Heise, H. Lutz, and H. Dreizler, 1973, Z. Naturforsch. 29a, 1345. The dipole is an approximate value.

Species Tag:	**56004**	**Name:**	**C2H5CN-15** **Ethyl cyanide,** **^{15}N isotope**
Version:	**1**		
Date:	**Jan. 1980**		
Contributor:	**R. L. Poynter**		
Lines Listed:	**1621**	**Q(300.0)=**	**38459.180**
Freq. (GHz) $<$	**1077**	**Q(225.0)=**	**24980.445**
Max. J:	**20**	**Q(150.0)=**	**13598.785**
LOGSTR0=	**-8.7**	**Q(75.00)=**	**3966.433**
LOGSTR1=	**-7.7**	**Q(37.50)=**	**1542.411**
Isotope Corr.:	**-2.432**	**Q(18.75)=**	**598.136**
Egy. (cm^{-1}) $>$	**0.0**	**Q(9.375)=**	**213.895**
$\mu_a =$	**3.84**	**A=**	**27541.953**
$\mu_b =$	**1.37**	**B=**	**4574.771**
$\mu_c =$		**C=**	**4119.430**

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333. The measurements were taken from H. M. Heise, H. Mäder, and H. Dreizler, 1976, Z. Naturforsch. 31a, 1228. The dipole is an approximate value.

Species Tag:	56005	Name:	CH2DCH2CN-s
Version:	2		Ethyl cyanide, deuterium isotope on methyl carbon *trans* to CN group
Date:	Jan. 1980		
Contributor:	R. L. Poynter		
Lines Listed:	1166	Q(300.0)=	118795.508
Freq. (GHz) <	530	Q(225.0)=	75300.883
Max. J:	10	Q(150.0)=	41995.227
LOGSTR0=	-9.0	Q(75.00)=	14849.096
LOGSTR1=	-8.3	Q(37.50)=	5250.493
Isotope Corr.:	-3.347	Q(18.75)=	1787.722
Egy. (cm^{-1}) >	0.0	Q(9.375)=	607.995
μ_a =	3.84	A=	27650.795
μ_b =	1.37	B=	4425.061
μ_c =		C=	4000.763

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333, and W. H. Kirchhoff and D. R. Johnson, 1973, J. Mol. Spect. 45, 159. The measurements were taken from H. Mäder, H. M. Heise, and H. Dreizler, 1973, Z. Naturforsch. 29a, 164. The dipole moment is an approximate value.

Species Tag:	**56006**	**Name:**	**CH2DCH2CN-a**
Version:	**2**		**Ethyl cyanide,**
Date:	**Jan. 1981**		**deuterium isotope on**
Contributor:	**R. L. Poynter**		**methyl carbon** *gauche*
			to the CN group
Lines Listed:	**1286**	**Q(300.0)=**	**121059.867**
Freq. (GHz) <	**480**	**Q(225.0)=**	**76736.188**
Max. J:	**10**	**Q(150.0)=**	**42815.391**
LOGSTR0=	**-9.0**	**Q(75.00)=**	**15132.134**
LOGSTR1=	**-8.2**	**Q(37.50)=**	**5350.569**
Isotope Corr.:	**-3.347**	**Q(18.75)=**	**1827.259**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**623.304**
μ_a =	**3.84**	**A=**	**25022.568**
μ_b =	**1.37**	**B=**	**4583.422**
μ_c =		**C=**	**4110.245**

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333, and W. H. Kirchhoff and D. R. Johnson, 1973, J. Mol. Spect. 45, 159. The measurements were taken from H. Mäder, N. M. Heise, and H. Dreizler, 1973, Z. Naturforsch. 29a, 164. The dipole moment is an approximate value.

Species Tag:	**56007**	**Name:**	**CCS**
Version:	**1**		**Dicarbon monosulfide,**
Date:	**Nov. 1993**		**CCS $^3\Sigma^-$ radical**
Contributor:	**E. A. Cohen**		

Lines Listed:	**563**	**Q(300.0)=**	**2844.129**
Freq. (GHz) <	**2032**	**Q(225.0)=**	**2020.090**
Max. J:	**99**	**Q(150.0)=**	**1396.403**
LOGSTR0=	**-8.0**	**Q(75.00)=**	**643.888**
LOGSTR1=	**-8.0**	**Q(37.50)=**	**314.781**
Isotope Corr.:	**0.0**	**Q(18.75)=**	**138.873**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**56.463**
μ_a =	**2.9**	**A=**	
μ_b =		**B=**	**6477.75036(27)**
μ_c =		**C=**	

The measurements were taken from S. Yamamoto *et al.*, 1990, Astrophys. J. 361, 318. The dipole moment was quoted in this paper from an *ab initio* calculation by A. Murakami. The relative weights of the reported measurements have been chosen to reproduce the molecular parameters in the referenced paper. An assigned uncertainty of 20 kHz for a line given unit weight in the paper produces approximately the same 1σ uncertainties for calculated transitions as reported in the reference. Note that N is not a good quantum number and that in this calculation the naming of the $N_J = 2_1$ and 0_1 is the reverse of that in the reference.

Species Tag:	**56008**	**Name:**	**C2H3CHO**
Version:	**1**		**s-trans and s-cis Acrolein**
Date:	**Jan. 1996**		
Contributor:	**J. C. Pearson**		
Lines Listed:	**24051**	**Q(300.0)=**	**19562.548**
Freq. (GHz) <	**2000**	**Q(225.0)=**	**13737.474**
Max. J:	**50**	**Q(150.0)=**	**7922.005**
LOGSTR0=	**-8.0**	**Q(75.00)=**	**2856.363**
LOGSTR1=	**-8.5**	**Q(37.50)=**	**1010.200**
Isotope Corr.:		**Q(18.75)=**	**357.654**
Egy. (cm^{-1}) >	**0.0, 594**	**Q(9.375)=**	**126.904**
μ_a =	**3.052**	**A=**	**47353.7**
μ_b =	**0.630**	**B=**	**4659.5**
μ_c =	**0**	**C=**	**4242.7**

Acrolein exists in two stable conformers, s-trans and s-cis. The s-trans state is more stable by 594 cm^{-1}. The dipole moments and rotational constants given are for the s-trans conformer.

The s-trans experimental measurements were taken from: R. Wagner, J. Fine, J. W. Simmons and J. H. Goldstein, J. Chem. Phys. 26, 634 (1957). E. A. Cherniak and C. C. Costain, J. Chem. Phys. 45, 104 (1966). M. Winnewisser, G. Winnewisser, T. Honda and E. Hirota, Z. Naturforsch. 30a, 1001 (1975).

The dipole moments and measurements for the s-cis state come from: C. E. Blom and A. Bauder, Chem. Phys. Lett. 88, 55 (1982). C. E. Blom, G. Grassi and A. Bauder, J. Am. Chem. Soc. 106, 7427 (1984).

The s-trans levels are denoted as state 0 and s-cis is state 1. The dipole moments for the s-cis form are $\mu_a = 2.010$D and $\mu_b = 1.573$D.

Species Tag:	56009	Name:	MgS
Version:	1		Magnesium sulfide,
Date:	Sep. 1997		X $^1\Sigma^+$
Contributor:	H. S. P. Müller		

Lines Listed:	99	Q(300.0)=	782.292
Freq. (GHz) $<$	1554	Q(225.0)=	586.566
Max. J:	99	Q(150.0)=	390.997
LOGSTR0=	-6.0	Q(75.00)=	195.586
LOGSTR1=	-5.0	Q(37.50)=	97.941
Isotope Corr.:	-0.1051	Q(18.75)=	49.133
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	24.734
μ_a =	6.88	A=	
μ_b =		B=	8006.927
μ_c =		C=	

The lines were taken from (1) S. Takano, S. Yamamoto, and S. Saito, 1989, Chem. Phys. Lett. 159, 563; and (2) K. A. Walker and M. C. L. Gerry, 1997, J. Mol. Spect. 182, 178. The dipole moment is taken from an *ab initio* calculation by (3) P. W. Fowler and A. J. Sedlej, 1991, Mol. Phys. 73, 43.

Species Tag:	57001	Name:	C-13CCS
Version:	1		Dicarbon monosulfide
Date:	Nov. 1993		^{13}CCS, X $^3\Sigma^-$
Contributor:	E. A. Cohen		
Lines Listed:	1013	Q(300.0)=	5953.713
Freq. (GHz) <	1232	Q(225.0)=	4438.003
Max. J:	99	Q(150.0)=	2922.894
LOGSTR0=	-8.0	Q(75.00)=	1410.246
LOGSTR1=	-6.0	Q(37.50)=	658.455
Isotope Corr.:	-1.955	Q(18.75)=	290.244
Egy. (cm^{-1}) >	0.0	Q(9.375)=	117.819
μ_a =	2.9	A=	
μ_b =		B=	6188.08655(51)
μ_c =		C=	

The measurements were taken from S. Yamamoto *et al.*, 1990, Astrophys. J. 361, 318. The dipole moment was quoted in this paper from an *ab initio* calculation by A. Murakami. Uniform weighting of the reported measurements reproduces the molecular parameters given in the referenced paper. An assigned uncertainty of 30 kHz for each measured line produces approximately the same 1σ uncertainties for calculated transitions as reported in the reference. Note that N is not a good quantum number and that in this calculation the naming of the $N_J = 2_1$ and 0_1 is the reverse of that in the reference. Yamamoto *et al.*, report 9 individual hyperfine components due to the ^{13}C splitting and 17 unresolved doublets. As a result the measured frequencies have not been merged. Only calculated frequencies are listed.

Species Tag:	57002	Name:	CC-13S
Version:	1		Dicarbon monosulfide
Date:	Nov. 1993		$C^{13}CS$, X $^3\Sigma^-$
Contributor:	E. A. Cohen		
Lines Listed:	1015	Q(300.0)=	5715.285
Freq. (GHz) <	1283	Q(225.0)=	4260.324
Max. J:	99	Q(150.0)=	2806.041
LOGSTR0=	-8.0	Q(75.00)=	1354.115
LOGSTR1=	-6.0	Q(37.50)=	632.479
Isotope Corr.:	-1.955	Q(18.75)=	278.997
Egy. (cm^{-1}) >	0.0	Q(9.375)=	113.410
μ_a =	2.9	A=	
μ_b =		B=	6446.96588(80)
μ_c =		C=	

The measurements were taken from S. Yamamoto *et al.*, 1990, Astrophys. J. 361, 318. The dipole moment was quoted in this paper from an *ab initio* calculation by A. Murakami. Uniform weighting of the reported measurements reproduces the molecular parameters given in the referenced paper. An assigned uncertainty of 35 kHz for each measured line produces approximately the same 1σ uncertainties for calculated transitions as reported in the reference. Note that N is not a good quantum number and that in this calculation the naming of the $N_J = 2_1$ and 0_1 is the reverse of that in the reference. Yamamoto *et al.*, report 4 individual hyperfine components due to the ^{13}C splitting and 15 unresolved doublets. As a result the measured frequencies have not been merged. Only calculated frequencies are listed.

Species Tag:	58001	Name:	CCS-34
Version:	1		Dicarbon monosulfide
Date:	Nov. 1993		CC^{34}S, X $^{3}\Sigma^{-}$
Contributor:	E. A. Cohen		
Lines Listed:	565	Q(300.0)=	2907.635
Freq. (GHz) $<$	1988	Q(225.0)=	2167.408
Max. J:	99	Q(150.0)=	1427.520
LOGSTR0=	-8.0	Q(75.00)=	688.832
LOGSTR1=	-8.0	Q(37.50)=	321.694
Isotope Corr.:	-1.376	Q(18.75)=	141.864
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	57.635
μ_a =	2.9	A=	
μ_b =		B=	6335.88385(35)
μ_c =		C=	

The measurements were taken from S. Yamamoto *et al.*, 1990, Astrophys. J. 361, 318. The dipole moment was quoted in this paper from an *ab initio* calculation by A. Murakami. The relative weights of the reported measurements have been chosen to reproduce the molecular parameters in the referenced paper. An assigned uncertainty of 20 kHz for a line given unit weight in the paper produces approximately the same 1σ uncertainties for calculated transitions as reported in the reference. Note that N is not a good quantum number and that in this calculation the naming of the $N_J = 2_1$ and 0_1 is the reverse of that in the reference.

Species Tag:	**58002**	**Name:**	**NaCl**
Version:	**1**		**Sodium chloride,**
Date:	**Feb. 1995**		**^{35}Cl isotope**
Contributor:	**M. L. Delitsky**		
	H. M. Pickett		
Lines Listed:	**99**	**Q(300.0)=**	**962.7255**
Freq. (GHz) <	**1229.9**	**Q(225.0)=**	**721.6494**
Max. J:	**98**	**Q(150.0)=**	**480.8774**
LOGSTR0=	**-10.0**	**Q(75.00)=**	**240.4394**
LOGSTR1=	**-100.0**	**Q(37.50)=**	**120.3454**
Isotope Corr.:	**-0.122**	**Q(18.75)=**	**60.3298**
Egy. (cm^{-1}) >	**0**	**Q(9.375)=**	**30.3307**
μ_a =	**9.000**	**A=**	
μ_b =		**B=**	**6513.050**
μ_c =		**C=**	

The observed laboratory frequency measurements were taken from P. L. Clouser and W. Gordy, 1964, Phys. Rev. 134, A863.

The dipole moment is taken from K. H. Hellwege, Ed., 1974, Landolt-Börnstein, Numerical Data and Functional Relationships in Science and Technology, Group II., Vol. 6, Molecular Constants, Springer-Verlag, Heidelberg.

This calculation does not include the hyperfine splittings for the chlorine and sodium atoms.

Species Tag:	60001	Name:	OCS
Version:	2		Carbonyl sulfide
Date:	Jan. 1981		
Contributor:	R. L. Poynter		
Lines Listed:	99	Q(300.0)=	1028.253
Freq. (GHz) <	1200	Q(225.0)=	771.614
Max. J:	99	Q(150.0)=	514.399
LOGSTR0=	-6.3	Q(75.00)=	257.276
LOGSTR1=	-5.7	Q(37.50)=	128.825
Isotope Corr.:	-0.022	Q(18.75)=	64.580
Egy. (cm^{-1}) >	0.0	Q(9.375)=	32.456
μ_a =	0.715	A=	
μ_b =		B=	6081.4921
μ_c =		C=	

The measurements were taken from the data sets given in A. Dubrulle, J. Demaison, J. Burie, and D. Boucher, 1980, Z. Naturforsch. 35a, 471, and F. J. Lovas, 1978, J. Phys. Chem. Ref. Data 7, 1445. The dipole moment has been remeasured by J. M. L. J. Reinartz and A. Dymanus, 1974, Chem. Phys. Lett. 24, 346.

Species Tag:	60002	Name:	SiS
Version:	1		Silicon monosulfide
Date:	Dec. 1979		
Contributor:	R. L. Poynter		

Lines Listed:	97	Q(300.0)=	688.970
Freq. (GHz) <	1740	Q(225.0)=	517.130
Max. J:	97	Q(150.0)=	344.826
LOGSTR0=	-5.0	Q(75.00)=	172.544
LOGSTR1=	-6.5	Q(37.50)=	86.417
Isotope Corr.:	-0.057	Q(18.75)=	43.371
Egy. (cm^{-1}) >	0.0	Q(9.375)=	21.857
$\mu_a =$	1.730	A=	
$\mu_b =$		B=	9077.45
$\mu_c =$		C=	

The experimental measurements are summarized in E. Tiemann, 1976, J. Phys. Chem. Ref. Data 5, 1147. The dipole moment was measured by J. Hoeft, F. J. Lovas, E. Tiemann, and T. Törring, 1969, Z. Naturforsch. 24a, 1422.

Species Tag:	**60003**	**Name:**	**CH3OCHO-a**
Version:	**1**		**Methyl Formate,**
Date:	**Oct. 1992**		**ground vibrational state,**
Contributor:	**H. M. Pickett**		**A state**

Lines Listed:	**16153**	**Q(300.0)=**	**64850.87**
Freq. (GHz) <	**9999**	**Q(225.0)=**	**42120.19**
Max. J:	**60**	**Q(150.0)=**	**22918.47**
LOGSTR0=	**-9.0**	**Q(75.00)=**	**8102.16**
LOGSTR1=	**-7.0**	**Q(37.50)=**	**2866.56**
Isotope Corr.:	**0.0**	**Q(18.75)=**	**1015.36**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**360.40**
μ_a =	**1.63**	**A=**	**19985.71**
μ_b =	**0.68**	**B=**	**6914.75**
μ_c =		**C=**	**5304.48**

The data set used is referenced by G. M. Plummer, G. A. Blake, E. Herbst, and F. C. De Lucia, 1984, Astrophys. J. Suppl. 55, 633. The dipole moments are from R. F. Curl, Jr., 1959, J. Chem. Phys. 30, 1529. The spectrum has been fit to a rigid rotor with distortion.

Species Tag:	60004	Name:	CH3OCHO-e
Version:	1		Methyl Formate,
Date:	Oct. 1992		ground vibrational state,
Contributor:	H. M. Pickett		E state

Lines Listed:	17260	Q(300.0)=	64850.87
Freq. (GHz) <	9999	Q(225.0)=	42120.19
Max. J:	60	Q(150.0)=	22918.47
LOGSTR0=	-9.0	Q(75.00)=	8102.16
LOGSTR1=	-7.0	Q(37.50)=	2866.56
Isotope Corr.:	0.0	Q(18.75)=	1015.36
Egy. (cm^{-1}) >	0.0139	Q(9.375)=	360.40
μ_a =	1.63	A=	19982.26
μ_b =	0.68	B=	6913.81
μ_c =		C=	5304.74

The data set used is referenced by G. M. Plummer, E. Herbst, F. C. De Lucia, and G. A. Blake, 1986, Astrophys. J. Suppl. 60, 949. The lines were fit to a Hamiltonian that included Fourier series in the energy and in $P_b^2 - P_c^2$. No D_{ab} was used. The dipole moments are from R. F. Curl, Jr., 1959, J. Chem. Phys. 30, 1529.

Species Tag:	60005	Name:	NaCl-37
Version:	1		Sodium chloride,
Date:	Feb. 1995		^{37}Cl isotope
Contributor:	M. L. Delitsky H. M. Pickett		
Lines Listed:	99	Q(300.0)=	983.7530
Freq. (GHz) $<$	1227.19	Q(225.0)=	737.4152
Max. J:	98	Q(150.0)=	491.3806
LOGSTR0=	-10.0	Q(75.00)=	245.6872
LOGSTR1=	-100.0	Q(37.50)=	122.9683
Isotope Corr.:	-0.611	Q(18.75)=	61.6411
Egy. (cm^{-1}) $>$	0	Q(9.375)=	30.9862
μ_a =	9.000	A=	
μ_b =		B=	6373.748
μ_c =		C=	

The observed laboratory frequency measurements were taken from P. L. Clouser and W. Gordy, 1964, Phys. Rev. 134, A863.

The dipole moment is taken from K. H. Hellwege, Ed., 1974, Landolt-Börnstein, Numerical Data and Functional Relationships in Science and Technology, Group II., Vol. 6, Molecular Constants, Springer-Verlag, Heidelberg.

This calculation does not include the hyperfine splittings for the chlorine and sodium atoms.

Species Tag:	61001	Name:	OC-13-S
Version:	2		Carbonyl sulfide,
Date:	Jan. 1981		^{13}C isotope
Contributor:	R. L. Poynter		

Lines Listed:	99	Q(300.0)=	1031.573
Freq. (GHz) $<$	1196	Q(225.0)=	773.927
Max. J:	99	Q(150.0)=	515.941
LOGSTR0=	-6.3	Q(75.00)=	258.167
LOGSTR1=	-5.7	Q(37.50)=	129.241
Isotope Corr.:	-1.977	Q(18.75)=	64.789
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	32.561
μ_a =	0.715	A=	
μ_b =		B=	6061.924
μ_c =		C=	

The measurements were taken from the data sets given in A. Dubrulle, J. Demaison, J. Burie, and D. Boucher, 1980, Z. Naturforsch. 35a, 471, and F. J. Lovas, 1978, J. Phys. Chem. Ref. Data 7, 1445. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	61002	Name:	Si-29-S
Version:	1		Silicon monoxide,
Date:	Dec. 1979		^{29}Si isotope
Contributor:	R. L. Poynter		

Lines Listed:	98	Q(300.0)=	701.778
Freq. (GHz) <	1725	Q(225.0)=	526.866
Max. J:	98	Q(150.0)=	351.237
LOGSTR0=	-5.0	Q(75.00)=	175.752
LOGSTR1=	-6.5	Q(37.50)=	88.024
Isotope Corr.:	-1.349	Q(18.75)=	44.177
Egy. (cm^{-1}) >	0.0	Q(9.375)=	22.259
μ_a =	1.730	A=	
μ_b =		B=	8910.66
μ_c =		C=	

The measurements were taken from the data set given in F. J. Lovas, 1978, J. Phys. Chem. Ref. Data 7, 1445. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	61003	Name:	C5H
Version:	1		2,4-Pentadiynylidyne
Date:	Jan. 1996		X $^2\Pi$ states
Contributor:	J. C. Pearson		

Lines Listed:	2594	Q(300.0)=	19320.9749
Freq. (GHz) $<$	1343	Q(225.0)=	14461.6754
Max. J:	99	Q(150.0)=	9365.1357
LOGSTR0=	-10.0	Q(75.00)=	4259.8111
LOGSTR1=	-10.0	Q(37.50)=	1828.1797
Isotope Corr.:		Q(18.75)=	760.1560
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	338.6917
μ_a =	4.881	A=	
μ_b =		B=	2395.1
μ_c =		C=	

The observed lines are from: C. A. Gottlieb, E. W. Gottlieb and P. Thaddeus, 1986, Astron. Astrophys. 164, L5. J. Cernicharo, M. Guelin and C. M. Walmsley, 1987, Astron. Astrophys. 172, L5. C. A. Gottlieb, J. C. Pearson, D. R. Woodward and P. Thaddeus, 1988, Private Communication.

The dipole was calculated by D. E. Woon, 1995, Private Communication.

Species Tag:	**62001**	**Name:**	**OCS-34**
Version:	**2**		**Carbonyl sulfide,**
Date:	**Jan. 1981**		**^{34}S isotope**
Contributor:	**R. L. Poynter**		

Lines Listed:	**99**	**Q(300.0)=**	**1053.901**
Freq. (GHz) $<$	**1170**	**Q(225.0)=**	**777.678**
Max. J:	**99**	**Q(150.0)=**	**527.230**
LOGSTR0=	**-6.3**	**Q(75.00)=**	**263.755**
LOGSTR1=	**-5.6**	**Q(37.50)=**	**132.038**
Isotope Corr.:	**-1.376**	**Q(18.75)=**	**66.191**
Egy. (cm^{-1}) $>$	**0.0**	**Q(9.375)=**	**33.258**
μ_a =	**0.715**	**A=**	
μ_b =		**B=**	**5932.8338**
μ_c =		**C=**	

The measurements were taken from the data sets given in A. Dubrulle, J. Demaison, J. Burie, and D. Boucher, 1980, Z. Naturforsch. 35a, 471, and F. J. Lovas, 1978, J. Phys. Chem. Ref. Data 7, 1445. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	**62002**	**Name:**	**O-18-CS**
Version:	**2**		**Carbonyl sulfide,**
Date:	**Jan. 1981**		**^{18}O isotope**
Contributor:	**R. L. Poynter**		

Lines Listed:	**99**	**Q(300.0)=**	**1095.973**
Freq. (GHz) <	**1126**	**Q(225.0)=**	**822.432**
Max. J:	**99**	**Q(150.0)=**	**548.151**
LOGSTR0=	**-6.4**	**Q(75.00)=**	**274.284**
LOGSTR1=	**-5.4**	**Q(37.50)=**	**137.309**
Isotope Corr.:	**-2.712**	**Q(18.75)=**	**68.818**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**34.578**
μ_a =	**0.715**	**A=**	
μ_b =		**B=**	**5704.8574**
μ_c =		**C=**	

The measurements were taken from the data sets given in A. Dubrulle, J. Demaison, J. Burie, and D. Boucher, 1980, Z. Naturforsch. 35a, 471, and F. J. Lovas, 1978, J. Phys. Chem. Ref. Data 7, 1445. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	62003	Name:	Si-30-S
Version:	1		Silicon monosulfide,
Date:	Dec. 1979		^{30}Si isotope
Contributor:	R. L. Poynter		

Lines Listed:	99	Q(300.0)=	714.332
Freq. (GHz) $<$	1713	Q(225.0)=	536.167
Max. J:	99	Q(150.0)=	357.437
LOGSTR0=	-5.1	Q(75.00)=	178.855
LOGSTR1=	-6.5	Q(37.50)=	89.598
Isotope Corr.:	-1.528	Q(18.75)=	44.957
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	22.646
$\mu_a =$	1.730	A=	
$\mu_b =$		B=	8755.33
$\mu_c =$		C=	

The measurements were taken from the data set given in F. J. Lovas, 1978, J. Phys. Chem. Ref. Data 7, 1445. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	62004	Name:	SiS-34
Version:	1		Silicon monosulfide,
Date:	Dec. 1979		^{34}S isotope
Contributor:	R. L. Poynter		

Lines Listed:	99	Q(300.0)=	708.272
Freq. (GHz) $<$	1726	Q(225.0)=	531.741
Max. J:	99	Q(150.0)=	354.487
LOGSTR0=	-5.1	Q(75.00)=	177.378
LOGSTR1=	-6.6	Q(37.50)=	88.838
Isotope Corr.:	1.411	Q(18.75)=	44.586
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	22.465
μ_a =	1.730	A=	
μ_b =		B=	8828.86
μ_c =		C=	

The measurements were taken from the data set given in F. J. Lovas, 1978, J. Phys. Chem. Ref. Data 7, 1445. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	62005	Name:	AlCl
Version:	1		Aluminum monochloride,
Date:	Feb. 1995		^{35}Cl isotope
Contributor:	M. L. Delitsky		
	H. M. Pickett		
Lines Listed:	11525	Q(300.0)=	20627.2202
Freq. (GHz) $<$	1290.1	Q(225.0)=	15465.7093
Max. J:	90	Q(150.0)=	10308.5745
LOGSTR0=	-10.0	Q(75.00)=	5156.0145
LOGSTR1=	-100.0	Q(37.50)=	2581.4501
Isotope Corr.:	-0.122	Q(18.75)=	1294.6056
Egy. (cm^{-1}) $>$	0	Q(9.375)=	651.3125
μ_a =	1.000	A=	
μ_b =		B=	7288.724
μ_c =		C=	

The only observed laboratory frequency measurements are of the the J = 1 - 0 transition reported in K. D. Hensel *et al.*, 1993, J. Chem. Phys. 99, 3320. The D, H, and L parameters were fixed from Dunham $\mathbf{Y}_{ij}$ coefficients given in H. G. Hedderich *et al.*, 1993, J. Chem. Phys. 99, 8363.

The dipole moment is an assumed value.

Species Tag:	62006	Name:	C5D
Version:	1		2,4-Pentadiynylidyne
Date:	Jan. 1996		deuterium isotope,
Contributor:	J. C. Pearson		X $^2\Pi$ states
Lines Listed:	4436	Q(300.0)=	30492.8367
Freq. (GHz) $<$	1303	Q(225.0)=	22913.4567
Max. J:	99	Q(150.0)=	14870.1208
LOGSTR0=	-10.0	Q(75.00)=	6766.2080
LOGSTR1=	-10.0	Q(37.50)=	2903.8713
Isotope Corr.:	-3.824	Q(18.75)=	1207.1955
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	537.6068
μ_a =	4.881	A=	
μ_b =		B=	2262.1
μ_c =		C=	

The observed lines are from: T. Hirota, H. Ozawa, Y. Sekimoto and S. Yamamoto, 1995, J. Mol. Spect. 174, 196. C. A. Gottlieb, J. C. Pearson, D. R. Woodward and P. Thaddeus, 1988, Private Communication.

The dipole was calculated by D. E. Woon, 1995, Private Communication.

Species Tag:	**63001**	**Name:**	**HNO3**
Version:	**3**		**Nitric acid**
Date:	**Jan. 1991**		
Contributor:	**E. A. Cohen**		
Lines Listed:	**36551**	**Q(300.0)=**	**27938.295**
Freq. (GHz) <	**2114**	**Q(225.0)=**	**18150.984**
Max. J:	**90**	**Q(150.0)=**	**9878.703**
LOGSTR0=	**-9.0**	**Q(75.00)=**	**3493.815**
LOGSTR1=	**-7.3**	**Q(37.50)=**	**1236.801**
Isotope Corr.:	**0**	**Q(18.75)=**	**438.329**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**155.812**
$\mu_a =$	**1.986**	**A=**	**13010.9867**
$\mu_b =$	**0.882**	**B=**	**12099.9025**
$\mu_c =$		**C=**	**6260.6680**

The data set used in this fit is that of R. L. Crownover *et al.*, 1988, J. Quant. Spectrosc. Radiat. Transfer 40, 39, and references cited therein, and infrared lines measured by K. M. Evenson, 1983, private communication. Unpublished data from Evenson have not been merged into the catalog. There are many unresolved asymmetry multiplets in the data set. For the purpose of fitting, these were usually assigned to a single component. The merged file reflects this. The dipole moment was taken from the remeasurements report by A. P. Cox and J. M. Riveros, 1965, J. Chem. Phys. 42, 3106. Very small quadrupole splittings were resolvable for only the J = 0 transitions at dry-ice temperatures. Because of the extremely large number of lines for this molecule, these splittings were not included in our predictions. Information on these quadrupole splittings can be found in D. J. Millen and J. R. Morton, 1960, J. Chem. Soc. 1523.

Species Tag:	**63002**	**Name:**	**HNO3-v7**
Version:	**1**		**Nitric acid,**
Date:	**Aug. 1990**		$\nu_7 = 1$ **state**
Contributor:	**E. A. Cohen**		

Lines Listed:	**16478**	**Q(300.0)=**	**27938.295**
Freq. (GHz) <	**1000**	**Q(225.0)=**	**18150.984**
Max. J:	**80**	**Q(150.0)=**	**9878.703**
LOGSTR0=	**-8.9**	**Q(75.00)=**	**3493.815**
LOGSTR1=	**-7.3**	**Q(37.50)=**	**1236.801**
Isotope Corr.:	**0.0**	**Q(18.75)=**	**438.329**
Egy. $(\mathrm{cm}^{-1}) >$	**579.0**	**Q(9.375)=**	**155.812**
$\mu_a =$	**1.986**	**A=**	**13028.93**
$\mu_b =$	**0.882**	**B=**	**12098.63**
$\mu_c =$		**C=**	**6201.609**

The data were taken from R. A. Booker ***et al.*****, 1988, J. Mol. Spect. 128, 62. The dipole moment was assumed to be the same as for the ground state.**

Species Tag:	63003	Name:	HNO3-v9
Version:	1		Nitric acid,
Date:	Aug. 1990		$\nu_9 = 1$ state
Contributor:	E. A. Cohen		
Lines Listed:	32404	Q(300.0)=	55872.746
Freq. (GHz) <	1000	Q(225.0)=	45698.316
Max. J:	79	Q(150.0)=	19756.049
LOGSTR0=	-9.0	Q(75.00)=	6987.149
LOGSTR1=	-7.3	Q(37.50)=	2473.432
Isotope Corr.:	0.0	Q(18.75)=	876.597
Egy. (cm^{-1}) >	458.2	Q(9.375)=	311.602
μ_a =	1.986	A=	12999.00
μ_b =	0.882	B=	12015.11
μ_c =		C=	6255.243

These measurements have been fitted to data from F. C. De Lucia, private communication. The data are unpublished and have not been merged with the predicted spectrum. Because torsional splitting is observable for this state but is negligible for the other HNO_3 states included in the catalog, the partition function that is used to calculate intensities has been doubled. The dipole moment was assumed to be the same as for the ground state. The b dipole allows transitions between torsional states.

Species Tag:	**63004**	**Name:**	**HNO3-v6**
Version:	**1**		**Nitric acid,**
Date:	**Aug. 1990**		$\nu_6 = 1$ **state**
Contributor:	**E. A. Cohen**		

Lines Listed:	**15704**	**Q(300.0)=**	**27938.295**
Freq. (GHz) $<$	**1000**	**Q(225.0)=**	**18150.984**
Max. J:	**79**	**Q(150.0)=**	**9878.703**
LOGSTR0=	**-9.0**	**Q(75.00)=**	**3493.815**
LOGSTR1=	**-7.3**	**Q(37.50)=**	**1236.801**
Isotope Corr.:	**0.0**	**Q(18.75)=**	**438.329**
Egy. $(\text{cm}^{-1}) >$	**646.8**	**Q(9.375)=**	**155.812**
μ_a =	**1.986**	**A=**	**13006.32**
μ_b =	**0.882**	**B=**	**12057.46**
μ_c =		**C=**	**6282.345**

The data were taken from R. A. Booker *et al.*, **1988, J. Mol. Spect. 128, 306. The dipole moment was assumed to be the same as for the ground state.**

Species Tag:	**63005**	**Name:**	**HNO3-v8**
Version:	**1**		**Nitric acid,**
Date:	**Aug. 1990**		$\nu_8 = 1$ **state**
Contributor:	**E. A. Cohen**		

Lines Listed:	**14537**	**Q(300.0)=**	**27938.295**
Freq. (GHz) <	**1000**	**Q(225.0)=**	**18150.984**
Max. J:	**79**	**Q(150.0)=**	**9878.703**
LOGSTR0=	**-9.0**	**Q(75.00)=**	**3493.815**
LOGSTR1=	**-7.3**	**Q(37.50)=**	**1236.801**
Isotope Corr.:	**0.0**	**Q(18.75)=**	**438.329**
Egy. $(\mathrm{cm}^{-1}) >$	**763.2**	**Q(9.375)=**	**155.812**
$\mu_a =$	**1.986**	**A=**	**12998.04**
$\mu_b =$	**0.882**	**B=**	**12005.51**
$\mu_c =$		**C=**	**6260.814**

These measurements are based on the data of R. L. Crownover *et al.*, **1988, J. Quant. Spectrosc. Radiat. Transfer 40, 39. The dipole moment was assumed to be the same as for the ground state.**

Species Tag:	63006	Name:	HNO3-v5
Version:	1		Nitric acid,
Date:	Aug. 1990		$\nu_5 = 1$ state
Contributor:	E. A. Cohen		

Lines Listed:	13269	Q(300.0)=	27938.295
Freq. (GHz) <	999	Q(225.0)=	18150.984
Max. J:	79	Q(150.0)=	9878.703
LOGSTR0=	-8.9	Q(75.00)=	3493.815
LOGSTR1=	-7.3	Q(37.50)=	1236.801
Isotope Corr.:	0.0	Q(18.75)=	438.329
Egy. (cm^{-1}) >	878.6	Q(9.375)=	155.812
μ_a =	1.986	A=	13003.61
μ_b =	0.882	B=	12044.39
μ_c =		C=	6242.055

These measurements have been fitted to data from F. C. De Lucia, private communication. The data are unpublished and have not been merged with the predicted spectrum. There is apparently some perturbation due to the proximity of $2\nu_9$. This is not taken into account in this calculation, and the user is cautioned that some transitions may be in error by more than the calculated uncertainties indicate. The dipole moment was assumed to be the same as for the ground state.

Species Tag:	**63007**	**Name:**	**PS**
Version:	**1**		*nu*=**0,1**
Date:	**Jan. 1997**		$^2\Pi_r$ **States**
Contributor:	**J. C. Pearson**		
Lines Listed:	**2340**	**Q(300.0)=**	**3522.0557**
Freq. (GHz) <	**1733**	**Q(225.0)=**	**2406.1374**
Max. J:	**99**	**Q(150.0)=**	**1476.0583**
LOGSTR0=	**-10.0**	**Q(75.00)=**	**708.1562**
LOGSTR1=	**-10.0**	**Q(37.50)=**	**354.8808**
Isotope Corr.:	**-0.022**	**Q(18.75)=**	**179.0140**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**91.1080**
μ_a =	**2.0**	**A=**	
μ_b =		**B=**	**8895.8**
μ_c =		**C=**	

The data were taken from: M. Ohishi, S. Yamamoto, S. Saito, K. Kawaguchi, H. Suzuki, N. Kaifu, S-I Ishikawa, S. Takano, T. Tsujo and W. Unno, 1988, Astrophys. J. 329, 511 and K. Kawaguchi, E. Hirota, M. Ohishi, H. Suzuki, S. Takano, S. Yamamoto and S. Saito, 1988, J. Mol. Spectrosc. 130, 81. The ground state A value was fixed to the electronic emmission value of N. A. Narasimham and T. K. Balasbramanian, 1971, J. Mol. Spectrosc. 37, 371.

The dipole is unknown so the 2.0 Debye estimate of Ohishi *et al.* dipole was used in the calculations.

Species Tag:	63008	Name:	PO2
Version:	1		Phosphorus dioxide
Date:	Jan. 1997		X $^2A_1$
Contributor:	H. S. P. Müller		

Lines Listed:	7323	Q(300.0)=	20857.700
Freq. (GHz) $<$	1999	Q(225.0)=	13586.589
Max. J:	60	Q(150.0)=	7385.832
LOGSTR0=	-7.8	Q(75.00)=	2605.404
LOGSTR1=	-6.7	Q(37.50)=	920.677
Isotope Corr.:		Q(18.75)=	325.861
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	115.585
μ_a =		A=	104506.98
μ_b =	0.5	B=	8598.190
μ_c =		C=	7921.508

The lines are from K. Kawaguchi, S. Saito, E. Hirota, and N. Ohashi, 1985, J. Chem. Phys. 82, 4893. The dipole moment is an assumed value.

Species Tag:	64001	Name:	S2
Version:	2		Diatomic sulfur
Date:	Oct. 1989		
Contributor:	H. M. Pickett		

Lines Listed:	174	Q(300.0)=	989.464
Freq. (GHz) <	2823	Q(225.0)=	725.604
Max. J:	71	Q(150.0)=	462.488
LOGSTR0=	-8.4	Q(75.00)=	203.751
LOGSTR1=	-9.3	Q(37.50)=	82.130
Isotope Corr.:	-0.044	Q(18.75)=	30.733
Egy. (cm^{-1}) >	0.0	Q(9.375)=	12.437
μ_a =		A=	
μ_b =		B=	8831.2
μ_c =		C=	

The experimentally measured lines are given in H. M. Pickett and T. L. Boyd, 1979, J. Mol. Spect. 75, 53. Additional combination differences were taken from E. H. Fink, H. Kruse, and D. A. Ramsay, 1986, J. Mol. Spect. 119, 377. The intensities of the magnetic dipole allowed transitions were calculated using the g values given in Pickett and Boyd. Hund's case (b) nomenclature is used even though the states are closer to Hund's case (a) for low J. The J = N + 1 states correlate with $\Sigma = 0$, and the J = N − 1 and J = N states correlate with $\Sigma = \pm 1$ states of p = $\pm (-1)^J$ inversion parity, respectively. The value of Q is determined from a sum over states to J = 80.

Species Tag:	64002	Name:	SO2
Version:	4		Sulfur dioxide
Date:	Nov. 1996		
Contributor:	H. S. P. Müller E. A. Cohen		
Lines Listed:	13573	Q(300.0)=	5918.720
Freq. (GHz) $<$	7682	Q(225.0)=	3841.714
Max. J:	99	Q(150.0)=	2090.601
LOGSTR0=	-10.0	Q(75.00)=	739.016
LOGSTR1=	-10.0	Q(37.50)=	261.662
Isotope Corr.:	-0.022	Q(18.75)=	92.841
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	33.070
μ_a =		A=	60778.550
μ_b =	1.6331	B=	10318.074
μ_c =		C=	8799.703

These measurements are based on fits to the data of (1) P. A. Helminger and F. C. De Lucia, 1985, J. Mol. Spect. 111, 66; (2) the compilation of F. J. Lovas, 1985, J. Phys. Chem. Ref. Data 14, 395; (3) E. A. Alekseev, S. F. Dyubko, V. V. Ilyushin, and S. V. Podnos, 1996, J. Mol. Spect. 176, 316; and from (4) E. Klisch, S. P. Belov, and G. Winnewisser, private communication (1996). In addition, unpublished far-infrared laser sideband measurements made at JPL have been included for transitions with $K_a \leq 28$. Most of these transitions have been measured relative to well predicted lines; these lines and lines with large uncertainties (5 MHz) have not been merged.

The dipole moment is from (5) D. Patel D. Margolese, and T. R. Dyke, 1979, J. Chem. Phys. 70, 2740.

Species Tag:	**64003**	**Name:**	**AlCl-37**
Version:	**1**		**Aluminum monochloride,**
Date:	**Feb. 1995**		**^{37}Cl isotope**
Contributor:	**M. L. Delitsky** **H. M. Pickett**		
Lines Listed:	**11326**	**Q(300.0)=**	**21123.1371**
Freq. (GHz) <	**1260.2**	**Q(225.0)=**	**15837.5364**
Max. J:	**90**	**Q(150.0)=**	**10556.3508**
LOGSTR0=	**-10.0**	**Q(75.00)=**	**5279.8481**
LOGSTR1=	**-100.0**	**Q(37.50)=**	**2643.3531**
Isotope Corr.:	**-0.611**	**Q(18.75)=**	**1325.5532**
Egy. (cm^{-1}) >	**0**	**Q(9.375)=**	**666.7844**
μ_a =	**1.000**	**A=**	
μ_b =		**B=**	**7117.51219**
μ_c =		**C=**	

The only observed laboratory frequency measurements are of the the J = 1 - 0 transition reported in K. D. Hensel *et al.*, 1993, J. Chem. Phys. 99, 3320. The D, H, and L parameters were fixed from Dunham $\mathbf{Y}_{ij}$ coefficients given in H. G. Hedderich *et al.*, 1993, J. Chem. Phys. 99, 8363.

The dipole moment is an assumed value.

Species Tag:	64004	Name:	C4O
Version:	1		Tetracarbon monoxide
Date:	April 1996		X $^3\Sigma^-$
Contributor:	H. S. P. Müller		

Lines Listed:	535	Q(300.0)=	7965.1375
Freq. (GHz) $<$	478	Q(225.0)=	5970.2221
Max. J:	99	Q(150.0)=	3975.5997
LOGSTR0=	-9.5	Q(75.00)=	1981.2949
LOGSTR1=	-7.5	Q(37.50)=	984.3175
Isotope Corr.:		Q(18.75)=	485.9881
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	237.0869
μ_a =	2.577	A=	
μ_b =		B=	2351.262
μ_c =		C=	

The data were taken from Y. Ohshima, Y. Endo, and T. Ogata, 1995, J. Chem. Phys. 102 1493.

The dipole moment is from an *ab initio* calculation: N. Moazzen-Ahmadi and F. Zerbetto, 1995, J. Chem. Phys. 103, 6343.

The partition function has been calculated up to $J = 199$ because of the low rotational constant.

Species Tag:	64005	Name:	SO2-v2
Version:	1		Sulfur dioxide
Date:	Nov. 1996		$v_2 = 1$
Contributor:	H. S. P. Müller		
Lines Listed:	9225	Q(300.0)=	5868.004
Freq. (GHz) $<$	5900	Q(225.0)=	3808.619
Max. J:	99	Q(150.0)=	2071.956
LOGSTR0=	-10.0	Q(75.00)=	732.578
LOGSTR1=	-9.5	Q(37.50)=	259.376
Isotope Corr.:	-0.022	Q(18.75)=	92.028
Egy. (cm^{-1}) $>$	517.75	Q(9.375)=	32.780
μ_a =		A=	61954.816
μ_b =	1.6261	B=	10320.397
μ_c =		C=	8783.856

These measurements are based on fits to the data of (1) P. A. Helminger and F. C. De Lucia, 1985, J. Mol. Spect. 111, 66; (2) the compilation of F. J. Lovas, 1985, J. Phys. Chem. Ref. Data 14, 395; and (3) E. A. Alekseev, S. F. Dyubko, V. V. Ilyushin, and S. V. Podnos, 1996, J. Mol. Spect. 176, 316. Some higher distortion constants have been fixed to values of the $^{32}SO_2$ isotopomer.

The dipole moment is from (4) D. Patel D. Margolese, and T. R. Dyke, 1979, J. Chem. Phys. 70, 2740.

Species Tag:	65001	Name:	S-33-O2
Version:	1		Sulfur dioxide
Date:	Nov. 1996		^{33}S isotope
Contributor:	H. S. P. Müller		
Lines Listed:	19048	Q(300.0)=	23881.212
Freq. (GHz) $<$	3451	Q(225.0)=	15501.797
Max. J:	78	Q(150.0)=	8433.669
LOGSTR0=	-8.0	Q(75.00)=	2982.020
LOGSTR1=	-6.5	Q(37.50)=	1055.834
Isotope Corr.:	-2.125	Q(18.75)=	374.621
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	133.439
μ_a =		A=	59856.482
μ_b =	1.6331	B=	10318.296
μ_c =		C=	8780.138

These measurements are based on fits to the data from (1) the compilations of F. J. Lovas, 1978, J. Phys. Chem. Ref. Data 7, 1445, and 1985, J. Phys. Chem. Ref. Data 14, 395; and from (2) E. Klisch, P. Schilke, S. P. Belov, and G. Winnewisser, 1996, J. Mol. Spect. 186, 314. Some higher distortion constants have been fixed to values of the ^{32}SO$_2$ isotopomer or an average of the ^{32}SO$_2$ and ^{34}SO$_2$ isotopomers. Predictions for high J ($>$ *ca.* 60) or K_a ($>$ *ca.* 15) quantum numbers should be taken with care.

Because sizable ^{33}S quadrupole splittings have been observed for moderately high values of J and K_a the predictions contain these hyperfine splittings for all transitions.

The dipole moment is assumed to be the same as for the ^{32}S isotope.

Species Tag:	66001	Name:	COF2
Version:	1		Carbonyl fluoride
Date:	Mar. 1988		
Contributor:	E. A. Cohen		

Lines Listed:	23090	Q(300.0)=	61418.617
Freq. (GHz) $<$	2982	Q(225.0)=	39884.121
Max. J:	90	Q(150.0)=	21707.002
LOGSTR0=	-9.0	Q(75.00)=	7677.150
LOGSTR1=	-9.0	Q(37.50)=	2717.064
Isotope Corr.:	0.0	Q(18.75)=	962.941
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	342.137
μ_a =	0.951	A=	11813.553
μ_b =		B=	11753.047
μ_c =		C=	5880.897

The data below 200 GHz and μ are from J. H. Carpenter, 1974, J. Mol. Spect. 50, 82. The data above 200 GHz were reported by E. A. Cohen and W. Lewis-Bevin, 1991, J. Mol. Spect. 148, 378. The dipole moment was measured by V. W. Laurie *et al.*, 1962, J. Chem. Phys. 37, 2995.

Species Tag:	66002	Name:	S-34-O2
Version:	2		Sulfur dioxide
Date:	Nov. 1996		^{34}S isotope
Contributor:	H. S. P. Müller		
Lines Listed:	11894	Q(300.0)=	6020.754
Freq. (GHz) <	6830	Q(225.0)=	3907.935
Max. J:	99	Q(150.0)=	2126.082
LOGSTR0=	-9.5	Q(75.00)=	751.749
LOGSTR1=	-9.3	Q(37.50)=	266.168
Isotope Corr.:	-1.376	Q(18.75)=	94.439
Egy. (cm^{-1}) >	0.0	Q(9.375)=	33.638
μ_a =		A=	58991.183
μ_b =	1.6331	B=	10318.510
μ_c =		C=	8761.303

These measurements are based on fits to the data of (1) P. A. Helminger and F. C. De Lucia, 1985,J. Mol. Spect. 111, 66; (2) the compilation of F. J. Lovas, 1985, J. Phys. Chem. Ref. Data 14, 395; (3) E. A. Alekseev, S. F. Dyubko, V. V. Ilyushin, and S. V. Podnos, 1996, J. Mol. Spect. 176, 316; and from (4) E. Klisch, S. P. Belov, and G. Winnewisser, private communication (1996). Some higher distortion constants have been fixed to values of the $^{32}SO_2$ isotopomer.

The dipole moment is assumed to be the same as for the ^{32}S isotope.

Species Tag:	**66003**	**Name:**	**CaNC**
Version:	**1**		**Calcium monoisocyanide,**
Date:	**Sept. 1995**		**X $^2\Sigma$**
Contributor:	**J. C. Pearson**		

Lines Listed:	**259**	**Q(300.0)=**	**3092.1611**
Freq. (GHz) $<$	**710**	**Q(225.0)=**	**2321.4848**
Max. J:	**88**	**Q(150.0)=**	**1547.1452**
LOGSTR0=	**-8.0**	**Q(75.00)=**	**773.3097**
LOGSTR1=	**-8.0**	**Q(37.50)=**	**386.8252**
Isotope Corr.:		**Q(18.75)=**	**193.7040**
Egy. (cm^{-1}) $>$	**0.0**	**Q(9.375)=**	**97.1764**
μ_a =	**1.000**	**A=**	
μ_b =		**B=**	**4048.74**
μ_c =		**C=**	

The observed lines were measured by T. C. Steimle, S. Saito and S. Takano, 1993, Astrophys. J. 410, L49. The dipole moment is unknown and has been assumend to be unity. The molecule is in a $^2\Sigma$ electronic ground state.

Species Tag:	**66004**	**Name:**	**SOO-18**
Version:	**1**		**Sulfur dioxide**
Date:	**Nov. 1996**		**$^{16}O^{18}O$ isotope**
Contributor:	**H. S. P. Müller**		

Lines Listed:	**9758**	**Q(300.0)=**	**12706.042**
Freq. (GHz) <	**3550**	**Q(225.0)=**	**8247.949**
Max. J:	**80**	**Q(150.0)=**	**4487.201**
LOGSTR0=	**-7.5**	**Q(75.00)=**	**1586.536**
LOGSTR1=	**-6.5**	**Q(37.50)=**	**561.686**
Isotope Corr.:	**-2.690**	**Q(18.75)=**	**199.254**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**70.946**
μ_a =	**0.0328**	**A=**	**59101.185**
μ_b =	**1.6327**	**B=**	**9724.645**
μ_c =		**C=**	**8331.562**

These measurements are based on fits to the data from (1) the compilation of F. J. Lovas, 1978, J. Phys. Chem. Ref. Data 7, 1445; and from (2) E. Klisch, S. P. Belov, and G. Winnewisser, private communication (1996). Some higher distortion constants have been fixed to values of the $^{32}SO_2$ isotopomer.

The dipole moment is assumed to be the same as for the ^{32}S isotope; the rotation of the axis system has been taken into account.

Species Tag:	**67001**	**Name:**	**OCl-35-O**
Version:	**2**		**Chlorine dioxide, X $^2B_1$**
Date:	**June 1997**		**^{35}Cl isotope**
Contributor:	**H. S. P. Müller**		
Lines Listed:	**57232**	**Q(300.0)=**	**53692.691**
Freq. (GHz) <	**3430**	**Q(225.0)=**	**34883.128**
Max. J:	**80**	**Q(150.0)=**	**19012.112**
LOGSTR0=	**-8.3**	**Q(75.00)=**	**6760.418**
LOGSTR1=	**-7.3**	**Q(37.50)=**	**2421.250**
Isotope Corr.:	**-0.122**	**Q(18.75)=**	**879.102**
Egy. (cm^{-1}) >		**Q(9.375)=**	**327.910**
μ_a =		**A=**	**52081.249**
μ_b =	**1.79195**	**B=**	**9952.605**
μ_c =		**C=**	**8334.219**

The lines were taken from (1) M. Tanoura, K. Chiba, K. Tanaka, and T. Tanaka, 1982, J. Mol. Spect. 95, 157 and (2) H. S. P. Müller, G. O. Sørensen, M. Birk, and R. R. Friedl, 1997, J. Mol. Spect. 186, 177. The Hamiltonian is the same as used in (2). The fit is a combined one for both isotopomers. The archived files are consequently for both isotopomers; a parameter file from a fit using Watson's A reduction is archived as ocloA.par. The dipole moment is from (3) K. Tanaka and T. Tanaka, 1983, J. Mol. Spect. 98, 425.

Species Tag:	68001	Name:	CCCS
Version:	1		Tricarbon monosulfide
Date:	Aug. 1987		X $^1\Sigma^+$
Contributor:	R. L. Poynter		
Lines Listed:	99	Q(300.0)=	2142.397
Freq. (GHz) <	572	Q(225.0)=	1619.198
Max. J:	99	Q(150.0)=	1081.683
LOGSTR0=	-5.9	Q(75.00)=	541.003
LOGSTR1=	-2.4	Q(37.50)=	270.707
Isotope Corr.:	0.0	Q(18.75)=	135.519
Egy. (cm^{-1}) >	0.0	Q(9.375)=	67.920
μ_a =		A=	
μ_b =	3.6	B=	2890.38010(23)
μ_c =		C=	

The measurements were taken from S. Yammoto *et al.*, 1987, Astrophys. J. Lett. Ed. 317, L119. The dipole moment was quoted in this paper from an *ab initio* calculation by A. Murakami. There is a typographical error in the $J^{'} = 41$ line reported in this paper.

Species Tag:	**69001**	**Name:**	**OCl-37-O**
Version:	**2**		**Chlorine dioxide, X** $^2B_1$
Date:	**Sept. 1989**		^{37}**Cl isotope**
Contributor:	**H. S. P. Müller**		

Lines Listed:	**49388**	**Q(300.0)=**	**52512.570**
Freq. (GHz) $<$	**3273**	**Q(225.0)=**	**35415.780**
Max. J:	**80**	**Q(150.0)=**	**19302.330**
LOGSTR0=	**-8.0**	**Q(75.00)=**	**6863.530**
LOGSTR1=	**-7.0**	**Q(37.50)=**	**2458.122**
Isotope Corr.:	**-0.611**	**Q(18.75)=**	**892.447**
Egy. (cm^{-1}**)** $>$		**Q(9.375)=**	**332.857**
μ_a =		**A=**	**50736.864**
μ_b =	**1.79210**	**B=**	**9953.123**
μ_c =		**C=**	**8299.136**

The lines were taken from (1) M. Tanoura, K. Chiba, K. Tanaka, and T. Tanaka, 1982, J. Mol. Spect. 95, 157 and (2) H. S. P. Müller, G. O. Sørensen, M. Birk, and R. R. Friedl, 1997, J. Mol. Spect. 186, 177. The Hamiltonian is the same as used in (2). The fit is a combined one for both isotopomers. The archived files are consequently for both isotopomers, see O^{35}**ClO, tag number 69001. The dipole moment is from (3) K. Tanaka and T. Tanaka, 1983, J. Mol. Spect. 98, 425.**

Species Tag:	**69002**	**Name:**	**C3H7CN**
Version:	**1**		**Butyronitrile or**
Date:	**Jan. 1996**		**n-Propyl cyanide,**
Contributor:	**J. C. Pearson**		**anti and gauche forms**
Lines Listed:	**60671**	**Q(300.0)=**	**120097.057**
Freq. (GHz) $<$	**2000**	**Q(225.0)=**	**79160.238**
Max. J:	**99**	**Q(150.0)=**	**41231.375**
LOGSTR0=	**-10.0**	**Q(75.00)=**	**12254.662**
LOGSTR1=	**-10.0**	**Q(37.50)=**	**3632.345**
Isotope Corr.:	**0.0**	**Q(18.75)=**	**1197.204**
Egy. (cm^{-1}) $>$	**0.0, 92**	**Q(9.375)=**	**421.579**
μ_a =	**3.597**	**A=**	**23667.8**
μ_b =	**0.984**	**B=**	**2268.1**
μ_c =		**C=**	**2153.0**

Butyronitrile is found in two conformers anti and gauche. The anti form is denoted by state 0 while the gauche form is state 1. The dipoles and rotational constants given are for the lower energy anti form which is about 92 cm^{-1} below the gauche form. There is no evidence of the two forms interacting in the ground state. Lines and dipoles were taken from:

E. Hirota, J. Chem. Phys. 37, 2918 (1962). J. Demaison and H. Dreizler, Z. Naturforsch. 37a, 199 (1982). G. Wlodarczak, L. Martinache, J. Demaison, K.-M. Marstokk and H. Mollendal, J. Mol. Spect. 127, 178 (1988). K. Vormann and H. Dreizler, Z. Naturforsch. 43a, 338 (1988).

The gauche form has the following dipole moments μ_a = 3.272D and μ_b = 2.139D. The quadrupole has been resolved and is presented in Vormann *et at.* and Demaison *et al.*, above. No quadrupole was used in this calculation.

Species Tag:	70001	Name:	CCCS-34
Version:	1		Tricarbon monosulfide,
Date:	Aug. 1987		X $^1\Sigma^+$
Contributor:	R. L. Poynter		^{34}S atom
Lines Listed:	99	Q(300.0)=	2192.805
Freq. (GHz) $<$	558	Q(225.0)=	1658.823
Max. J:	99	Q(150.0)=	1108.664
LOGSTR0=	-5.9	Q(75.00)=	554.498
LOGSTR1=	-2.5	Q(37.50)=	277.396
Isotope Corr.:	-1.376	Q(18.75)=	138.867
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	69.599
μ_a =		A=	
μ_b =	3.6	B=	2820.36892(131)
μ_c =		C=	

The measurements were taken from S. Yammoto *et al.*, 1987, Astrophys. J. Lett. Ed. 317, L119. The dipole moment was assumed to be the same as for the parent molecule.

Species Tag:	**71001**	**Name:**	**MnO**
Version:	**1**		**$^6\Sigma^+$ ground state**
Date:	**Sept. 2000**		
Contributor:	**H. M. Pickett**		
Lines Listed:	**12510**	**Q(300.0)=**	**14853.4**
Freq. (GHz) <	**9999**	**Q(225.0)=**	**11133.7**
Max. J:	**50**	**Q(150.0)=**	**7388.8**
LOGSTR0=	**-8.0**	**Q(75.00)=**	**3644.8**
LOGSTR1=	**-10**	**Q(37.50)=**	**1778.4**
Isotope Corr.:	**0.0**	**Q(18.75)=**	**853.7**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**404.4**
μ_a =	**3.22**	**A=**	
μ_b =		**B=**	**15025.815**
μ_c =		**C=**	

The data and Hamiltonian are from K. Namiki and S. Saito, 1997, J. Chem. Phys. 107, 8848.

Species Tag:	73001	Name:	C6H
Version:	1		Linear C_6H radical,
Date:	Dec. 1994		X $^2\Pi$ states
Contributor:	H. M. Pickett		

Lines Listed:	3031	Q(300.0)=	30789.8127
Freq. (GHz) $<$	825	Q(225.0)=	24332.8802
Max. J:	98	Q(150.0)=	16565.6319
LOGSTR0=	-10.0	Q(75.00)=	7871.6218
LOGSTR1=		Q(37.50)=	3519.7042
Isotope Corr.:	0.0	Q(18.75)=	1487.9395
Egy. (cm^{-1}) $>$	0.0479	Q(9.375)=	626.7718
μ_a =	5.9	A=	
μ_b =		B=	1391.18
μ_c =		C=	

The laboratory measurements of the frequency are described in J. C. Pearson, C. A. Gottlieb, D. R. Woodward, and P. Thaddeus, 1988, Astron. Astrophys. 189, L13-L15, and a list of the measured lines from this work was supplied by C. A. Gottlieb. These lines above 140 GHz were supplemented with interstelllar measurents in TMC-1 at lower frequency from J. Cernicharo, M. Guelin, K. M. Menten, and C. M. Walmsley, 1987, Astron. Astrophys. 181, L1-L4 and H. Suzuki, M. Ohishi, N. Kaifu, S. Ishikawa, T. Kasuga, S. Saito, and K. Kawaguchi, 1986, Publ. Astron. Soc. Japan 38, 911-917. The spectra were fit using a Hunds case (b) Hamiltonian, but the quantum numbers were converted to case (a) quanta.

The dipole moment is from a quantum calculation of F. Pauzat and Y. Ellinger, 1989, Astron. Astrophys. 216, 305-309.

Species Tag:	74001	Name:	KCl
Version:	1		Potassium chloride,
Date:	Feb. 1995		^{35}Cl isotope
Contributor:	M. L. Delitsky H. M. Pickett		
Lines Listed:	99	Q(300.0)=	1627.0645
Freq. (GHz) <	748.53	Q(225.0)=	1221.9565
Max. J:	99	Q(150.0)=	814.4216
LOGSTR0=	-10.0	Q(75.00)=	407.0976
LOGSTR1=	-100.0	Q(37.50)=	203.6454
Isotope Corr.:	-0.122	Q(18.75)=	101.9723
Egy. (cm^{-1}) >	0	Q(9.375)=	51.1494
μ_a =	10.30	A=	
μ_b =		B=	3844.544
μ_c =		C=	

The observed laboratory frequency measurements were taken from P. L. Clouser and W. Gordy, 1964, Phys. Rev. 134, A863.

The dipole moment is taken from K. H. Hellwege, Ed., 1974, Landolt-Börnstein, Numerical Data and Functional Relationships in Science and Technology, Group II., Vol. 6, Molecular Constants, Springer-Verlag, Heidelberg.

This calculation does not include the hyperfine splittings for the chlorine and potassium atoms.

Species Tag:	**74002**	**Name:**	**C2H5OOCH** **Ethyl formate,** **trans and gauche**
Version:	**1**		
Date:	**Jan. 1996**		
Contributor:	**J. C. Pearson**		
Lines Listed:	**60671**	**Q(300.0)=**	**120097.057**
Freq. (GHz) <	**2000**	**Q(225.0)=**	**79160.238**
Max. J:	**70**	**Q(150.0)=**	**41231.375**
LOGSTR0=	**-8.0**	**Q(75.00)=**	**12254.662**
LOGSTR1=	**-8.0**	**Q(37.50)=**	**3632.345**
Isotope Corr.:	**0.0**	**Q(18.75)=**	**1197.204**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**421.579**
μ_a =	**1.85**	**A=**	**17746.7**
μ_b =	**0.69**	**B=**	**2904.7**
μ_c =	**0.0**	**C=**	**2579.1**

Ethyl formate is found in two conformers, trans and gauche. The trans form is denoted by state 0 while the gauche form is state 1. The dipoles and rotational constants given are for the lower energy trans form which is about 60 ± 20 cm^{-1} below the gauche form. There is no evidence that the two forms interact in the ground state. Lines and dipoles were taken from: J. M. Riveros and E. B. Wilson, 1967, J. Chem. Phys. 46, 4605. R. Meyer and E. B. Wilson, 1970, J. Chem. Phys. 53, 3969. J. Demaison, D. Boucher, J. Burie, and A. Dubrulle, 1984, Z. Naturforsch. 39a, 560.

The gauche form has the following dipole moments $\mu_a = 1.44$ D, $\mu_b = 1.05$ D, $\mu_c = 0.25$ D.

Species Tag:	**75001**	**Name:**	**HCCCCCN**
Version:	**1**		**Cyanodiacetylene**
Date:	**Dec. 1979**		
Contributor:	**R. L. Poynter**		
Lines Listed:	**99**	**Q(300.0)=**	**4695.696**
Freq. (GHz) <	**264**	**Q(225.0)=**	**3315.890**
Max. J:	**99**	**Q(150.0)=**	**2314.729**
LOGSTR0=	**-6.7**	**Q(75.00)=**	**1174.086**
LOGSTR1=	**-2.6**	**Q(37.50)=**	**587.219**
Isotope Corr.:	**0**	**Q(18.75)=**	**293.765**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**147.062**
μ_a =		**A=**	
μ_b =	**4.330**	**B=**	**1331.33**
μ_c =		**C=**	

The experimental measurements were taken from A. J. Alexander, H. W. Kroto, and D. R. M. Walton, 1976, J. Mol. Spect. 62, 175. The dipole moment was measured by these same authors.

Species Tag:	75002	Name:	H2NCH2COOH I
Version:	1		Glycine, Conformer I
Date:	Jan. 1996		ground and first
Contributor:	H. S. P. Müller		excited torsional states

Lines Listed:	27217	Q(300.0)=	124879.8881
Freq. (GHz) <	1000	Q(225.0)=	100530.4504
Max. J:	40	Q(150.0)=	68673.2239
LOGSTR0=	-11.0	Q(75.00)=	29376.5224
LOGSTR1=	-8.0	Q(37.50)=	10752.5529
Isotope Corr.:		Q(18.75)=	3810.1565
Egy. (cm^{-1}) >	0.0	Q(9.375)=	1350.3826
μ_a =	0.911	A=	10341.530
μ_b =	0.607	B=	3876.1798
μ_c =		C=	2912.3525

This is the lowest energy conformer of glycine. The data were taken from (1) R. D. Suenram and F. J. Lovas, 1980, J. Am. Chem. Soc. 102, 7180 (millimeter wave region), and (2) F. J. Lovas, Y. Kawashima, J.-U. Grabow, R. D. Suenram, G. T. Fraser, and E. Hirota, 1995, Astrophys. J. Lett. 455, 201; (microwave region, dipole moment, and ^{14}N quadrupole coupling).

The ground and first excited states have been fit simultaneously, using only changes in the vibrational constants for the excited state. The reported hyperfine splittings have been used in the fit, but because they were well below 1 MHz for the strongest lines, they have not been included in the catalog file. The estimated torsional energy of 72 cm^{-1} has been taken from an *ab initio* calculation (SCF/DZP, scaled by 0.9; (3) C. H. Hu, M. Shen, and H. F. Schaefer, III, 1993, J. Am. Chem. Soc. 115, 2923).

In (1) lines were also reported for the second and third excited torsional state.

For the relative intensities between ground and first excited torsional states the approximate position of the torsional state was taken into account. Because there are several low lying vibrational modes that have not been investgated, the partition function was calculated for the ground state alone, including the nitrogen spin degeneracy. The partition function was calculated up to $J = 150$ because of the small rotational constants.

Species Tag:	75003	Name:	H2NCH2COOH II
Version:	1		Glycine, Conformer II
Date:	Jan. 1996		ground and first
Contributor:	H. S. P. Müller		excited torsional states
Lines Listed:	26544	Q(300.0)=	124879.8881
Freq. (GHz) <	1000	Q(225.0)=	100530.4504
Max. J:	40	Q(150.0)=	68673.2239
LOGSTR0=	-11.0	Q(75.00)=	29376.5224
LOGSTR1=	-8.0	Q(37.50)=	10752.5529
Isotope Corr.:		Q(18.75)=	3810.1565
Egy. (cm^{-1}) >	700.0	Q(9.375)=	1350.3826
μ_a =	5.372	A=	10130.152
μ_b =	0.930	B=	4071.5075
μ_c =		C=	3007.4892

This conformer of glycine is ≈700 cm^{-1} higher in energy than conformer I (2, 3). The data were taken from (1) R. D. Suenram and F. J. Lovas, 1978, J. Mol. Spectrosc. 72, 372 (millimeterwave region), and (2) F. J. Lovas, Y. Kawashima, J.-U. Grabow, R. D. Suenram, G. T. Fraser, and E. Hirota, 1995, Astrophys. J. Lett. 455, 201; (microwave region, dipole moment, and ^{14}N quadrupole coupling).

The ground and first excited states have been fit simultaneously, using only changes in the vibrational constants and D_{JK} for the excited state. The estimated torsional energy of 87 cm^{-1} has been taken from an *ab initio* calculation (SCF/DZP, scaled by 0.9; (3) C. H. Hu, M. Shen, and H. F. Schaefer, III, 1993, J. Am. Chem. Soc. 115, 2923).

For low J (< 10) hyperfine splittings are included in the catalog.

For the relative intensities between ground and first excited torsional states the approximate position of the torsional state was taken into account. Because there are several low lying vibrational modes that have not been investgated, the partition function was calculated for the ground state of the lower energy conformation including the nitrogen spin degeneracy. The partition function was calculated up to $J = 150$ because of the small rotational constants.

Species Tag:	76001	Name:	HCCCCC-13-N Cyanodiacetylene, ^{13}C isotope on atom 1
Version:	1		
Date:	Dec. 1979		
Contributor:	R. L. Poynter		

Lines Listed:	99	Q(300.0)=	4742.421
Freq. (GHz) <	261	Q(225.0)=	3448.260
Max. J:	99	Q(150.0)=	2336.684
LOGSTR0=	-6.7	Q(75.00)=	1185.768
LOGSTR1=	-2.6	Q(37.50)=	593.062
Isotope Corr.:	-1.933	Q(18.75)=	296.688
Egy. (cm^{-1}) >	0.0	Q(9.375)=	148.525
μ_a =	4.330	A=	
μ_b =		B=	1318.18
μ_c =		C=	

The experimental measurements were taken from A. J. Alexander, H. W. Kroto, and D. R. M. Walton, 1976, J. Mol. Spect. 62, 175. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	**76002**	**Name:**	**HCCCC-13-CN**
Version:	**1**		**Cyanodiacetylene,**
Date:	**Dec. 1979**		**^{13}C isotope**
Contributor:	**R. L. Poynter**		**on atom 2**
Lines Listed:	**99**	**Q(300.0)=**	**4700.024**
Freq. (GHz) <	**264**	**Q(225.0)=**	**3417.433**
Max. J:	**99**	**Q(150.0)=**	**2316.862**
LOGSTR0=	**-6.7**	**Q(75.00)=**	**1174.897**
LOGSTR1=	**-2.6**	**Q(37.50)=**	**587.760**
Isotope Corr.:	**-1.955**	**Q(18.75)=**	**294.036**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**147.197**
μ_a =	**4.329**	**A=**	
μ_b =		**B=**	**1330.11**
μ_c =		**C=**	

The experimental measurements were taken from A. J. Alexander, H. W. Kroto, and D. R. M. Walton, 1976, J. Mol. Spect. 62, 175. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	**76003**	**Name:**	**HCCC-13-CCN**
Version:	**1**		**Cyanodiacetylene,**
Date:	**Dec. 1979**		**^{13}C isotope**
Contributor:	**R. L. Poynter**		**on atom 3**

Lines Listed:	**99**	**Q(300.0)=**	**4700.024**
Freq. (GHz) $<$	**264**	**Q(225.0)=**	**3417.433**
Max. J:	**99**	**Q(150.0)=**	**2317.395**
LOGSTR0=	**-6.7**	**Q(75.00)=**	**1175.168**
LOGSTR1=	**-2.6**	**Q(37.50)=**	**587.895**
Isotope Corr.:	**-1.955**	**Q(18.75)=**	**294.103**
Egy. (cm^{-1}) $>$	**0.0**	**Q(9.375)=**	**147.231**
μ_a =	**4.329**	**A=**	
μ_b =		**B=**	**1329.95**
μ_c =		**C=**	

The experimental measurements were taken from A. J. Alexander, H. W. Kroto, and D. R. M. Walton, 1976, J. Mol. Spect. 62, 175. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	**76004**	**Name:**	**HCC-13-CCCN**
Version:	**1**		**Cyanodiacetylene,**
Date:	**Dec. 1979**		**^{13}C isotope**
Contributor:	**R. L. Poynter**		**on atom 4**
Lines Listed:	**99**	**Q(300.0)=**	**4744.604**
Freq. (GHz) <	**261**	**Q(225.0)=**	**3449.849**
Max. J:	**99**	**Q(150.0)=**	**2337.222**
LOGSTR0=	**-6.7**	**Q(75.00)=**	**1186.042**
LOGSTR1=	**-2.6**	**Q(37.50)=**	**593.335**
Isotope Corr.:	**-1.955**	**Q(18.75)=**	**296.825**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**148.594**
μ_a =	**4.329**	**A=**	
μ_b =		**B=**	**1317.689**
μ_c =		**C=**	

The experimental measurements were taken from A. J. Alexander, H. W. Kroto, and D. R. M. Walton, 1976, J. Mol. Spect. 62, 175. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	**76005**	**Name:**	**HC-13-CCCCN**
Version:	**1**		**Cyanodiacetylene,**
Date:	**Dec. 1979**		**^{13}C isotope**
Contributor:	**R. L. Poynter**		**on atom 5**
Lines Listed:	**99**	**Q(300.0)=**	**4820.588**
Freq. (GHz) $<$	**257**	**Q(225.0)=**	**3500.258**
Max. J:	**99**	**Q(150.0)=**	**2372.466**
LOGSTR0=	**-6.8**	**Q(75.00)=**	**1205.313**
LOGSTR1=	**-2.6**	**Q(37.50)=**	**602.976**
Isotope Corr.:	**-1.955**	**Q(18.75)=**	**301.648**
Egy. (cm^{-1}) $>$	**0.0**	**Q(9.375)=**	**150.973**
μ_a =	**4.329**	**A=**	
μ_b =		**B=**	**1296.88**
μ_c =		**C=**	

The experimental measurements were taken from A. J. Alexander, H. W. Kroto, and D. R. M. Walton, 1976, J. Mol. Spect. 62, 175. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	**76006**	**Name:**	**HCCCCCN-15**
Version:	**1**		**Cyanodiacetylene,**
Date:	**Dec. 1979**		**^{15}N isotope**
Contributor:	**R. L. Poynter**		

Lines Listed:	**99**	**Q(300.0)=**	**4813.931**
Freq. (GHz) <	**258**	**Q(225.0)=**	**3495.425**
Max. J:	**99**	**Q(150.0)=**	**2369.737**
LOGSTR0=	**-6.8**	**Q(75.00)=**	**1203.372**
LOGSTR1=	**-2.6**	**Q(37.50)=**	**602.005**
Isotope Corr.:	**-2.432**	**Q(18.75)=**	**301.162**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**150.765**
μ_a =	**4.329**	**A=**	
μ_b =		**B=**	**1298.639**
μ_c =		**C=**	

The experimental measurements were taken from A. J. Alexander, H. W. Kroto, and D. R. M. Walton, 1976, J. Mol. Spect. 62, 175. The dipole moment was measured by the same authors.

Species Tag:	**76007**	**Name:**	**DCCCCCN**
Version:	**1**		**Cyanodiacetylene,**
Date:	**Dec. 1979**		**deuterium isotope**
Contributor:	**R. L. Poynter**		
Lines Listed:	**99**	**Q(300.0)=**	**4918.131**
Freq. (GHz) <	**252**	**Q(225.0)=**	**3564.512**
Max. J:	**99**	**Q(150.0)=**	**2417.130**
LOGSTR0=	**-6.8**	**Q(75.00)=**	**1229.419**
LOGSTR1=	**-2.6**	**Q(37.50)=**	**615.035**
Isotope Corr.:	**-3.824**	**Q(18.75)=**	**307.681**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**153.993**
$\mu_a =$	**4.329**	**A=**	
$\mu_b =$		**B=**	**1271.056**
$\mu_c =$		**C=**	

The experimental measurements were taken from A. J. Alexander, H. W. Kroto, and D. R. N. Walton, 1976, J. Mol. Spect. 62, 175. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	**76008**	**Name:**	**KCl-37**
Version:	**1**		**Potassium chloride,**
Date:	**Feb. 1995**		**^{37}Cl isotope**
Contributor:	**M. L. Delitsky** **H. M. Pickett**		
Lines Listed:	**99**	**Q(300.0)=**	**1673.9444**
Freq. (GHz) <	**727.608**	**Q(225.0)=**	**1257.6038**
Max. J:	**99**	**Q(150.0)=**	**838.2397**
LOGSTR0=	**-10.0**	**Q(75.00)=**	**418.9994**
LOGSTR1=	**-100.0**	**Q(37.50)=**	**209.5943**
Isotope Corr.:	**-0.611**	**Q(18.75)=**	**104.9462**
Egy. (cm^{-1}) >	**0**	**Q(9.375)=**	**52.6362**
μ_a =	**10.30**	**A=**	
μ_b =		**B=**	**3735.251**
μ_c =		**C=**	

The observed laboratory frequency measurements were taken from P. L. Clouser and W. Gordy, 1964, Phys. Rev. 134, A863.

The dipole moment is taken from K. H. Hellwege, Ed., 1974, Landolt-Börnstein, Numerical Data and Functional Relationships in Science and Technology, Group II., Vol. 6, Molecular Constants, Springer-Verlag, Heidelberg.

This calculation does not include the hyperfine splittings for the chlorine and potassium atoms.

Species Tag:	76009	Name:	C4Si
Version:	1		^{28}Si isotope
Date:	Feb. 1996		
Contributor:	H. S. P. Müller		

Lines Listed:	229	Q(300.0)=	4077.1428
Freq. (GHz) $<$	700	Q(225.0)=	3057.7099
Max. J:	229	Q(150.0)=	2038.4265
LOGSTR0=	-7.0	Q(75.00)=	1019.3010
LOGSTR1=	-7.0	Q(37.50)=	509.7975
Isotope Corr.:	-0.055	Q(18.75)=	255.0607
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	127.6962
μ_a =	6.3	A=	
μ_b =		B=	1533.772
μ_c =		C=	

The transitions and dipole were taken from M. Ohishi, N. Kaifu, K. Kawaguchi, A. Murakami, S. Saito, S. Yamamoto, S.-I. Ishikawa, Y. Fujita, Y. Shiratori, and W. M. Irvine, 1989, Astrophys. J. 345, L83. The dipole moment is an *ab initio* value.

Species Tag:	76010	Name:	C5O
Version:	1		Pentacarbon monoxide
Date:	May 1996		X $^1\Sigma^+$
Contributor:	H. S. P. Müller		

Lines Listed:	99	Q(300.0)=	4574.6813
Freq. (GHz) <	271	Q(225.0)=	3430.8963
Max. J:	99	Q(150.0)=	2287.2410
LOGSTR0=	-8.0	Q(75.00)=	1143.7201
LOGSTR1=	-3.0	Q(37.50)=	572.0100
Isotope Corr.:		Q(18.75)=	286.1677
Egy. (cm^{-1}) >	0.0	Q(9.375)=	143.2498
μ_a =	4.057	A=	
μ_b =		B=	1366.8471
μ_c =		C=	

The data were taken from T. Ogata, Y. Ohshima, and Y. Endo, 1995, J. Am. Chem. Soc. 117 3593.

The dipole moment is from an *ab initio* calculation: P. Botschwina, J. Flügge, and P. Sebald, 1995, J. Phys. Chem. 99 9755. N. Moazzen-Ahmadi and F. Zerbetto, 1995, J. Chem. Phys. 103, 6343, obtained 3.376. The former calculation is expected to be more reliable.

The partition function has been calculated up to $J = 250$ because of the low rotational constant.

Species Tag:	**79001**	**Name:**	**HOONO2**
Version:	**1**		**Peroxynitric acid**
Date:	**Jan. 1987**		
Contributor:	**H. M. Pickett**		
Lines Listed:	**50775**	**Q(300.0)=**	**120032.797**
Freq. (GHz) $<$	**2078**	**Q(225.0)=**	**86596.430**
Max. J:	**50**	**Q(150.0)=**	**49796.613**
LOGSTR0=	**-7.0**	**Q(75.00)=**	**16657.125**
LOGSTR1=	**-7.0**	**Q(37.50)=**	**5638.972**
Isotope Corr.:	**0.0**	**Q(18.75)=**	**1987.009**
Egy. (cm^{-1}) $>$	**0.3**	**Q(9.375)=**	**702.910**
$\mu_a =$	**1.185**	**A=**	**11994.5**
$\mu_b =$	**0.94**	**B=**	**4665.2**
$\mu_c =$	**1.288**	**C=**	**3997.2**

The experimental measurements and calculation are described in R. D. Suenram, F. J. Lovas, and H. M. Pickett, 1986, J. Mol. Spect. 116, 406.

Species Tag:	**80001**	**Name:**	**HBr-79**
Version:	**2**		**Hydrogen bromide,**
Date:	**Apr. 1993**		**^{79}Br isotope**
Contributor:	**H. M. Pickett**		

Lines Listed:	**143**	**Q(300.0)=**	**103.423**
Freq. (GHz) <	**9999**	**Q(225.0)=**	**78.368**
Max. J:	**20**	**Q(150.0)=**	**53.343**
LOGSTR0=	**-8.0**	**Q(75.00)=**	**28.358**
LOGSTR1=	**-8.0**	**Q(37.50)=**	**15.912**
Isotope Corr.:	**-0.296**	**Q(18.75)=**	**9.773**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**6.934**
μ_a =	**0.828**	**A=**	
μ_b =		**B=**	**250357.6**
μ_c =		**C=**	

The experimental data were taken from F. A. Van Dijk and A. Dymanus, 1969, Chem. Phys. Lett. 4, 170 and G. Di Lonardo, L. Fusina, P. De Natale, M. Inguscio, and M. Prevedelli, 1991, J. Mol. Spect. 148, 86. The dipole moment was reported in F. A. Van Dijk and A. Dymanus, 1971, 26th Symposium on Molecular Structure and Spectroscopy, Columbus, Ohio, R12, p. 80.

Species Tag:	81001	Name:	Cl-35-NO2
Version:	1		Nitryl chloride,
Date:	May 1996		^{35}Cl isotope
Contributor:	H. S. P. Müller		

Lines Listed:	3520	Q(300.0)=	87532.1324
Freq. (GHz) <	600	Q(225.0)=	55251.5340
Max. J:	80	Q(150.0)=	29375.3141
LOGSTR0=	-10.6	Q(75.00)=	10285.6424
LOGSTR1=	-7.3	Q(37.50)=	3637.3396
Isotope Corr.:	-0.122	Q(18.75)=	1287.8512
Egy. (cm^{-1}) >	0.0	Q(9.375)=	456.7436
μ_a =	0.53 ± 0.01	A=	13290.137
μ_b =		B=	5175.4968
μ_c =		C=	3719.5377

The ground state microwave and millimeter wave data were taken from (1) T. Oka and Y. Morino, 1963, J. Mol. Spectrosc. 11, 349; and (2) R. R. Filgueira, P. Forti, and G. Corbelli, 1975, J. Mol. Spectrosc. 57, 97. Hyperfine splittings were not taken into account.

Also included in the fit are several infrared transitions: (3) ν_4 at 1684 cm^{-1}, J. Orphal, M. Morillion-Chapey, and G. Guelachvili, 1994, J. Mol. Spectrosc. 165 315; (4) ν_1 at 1282 and $2\nu_6$ at 1305 cm^{-1} (Fermi resonance), J. Orphal, G. Guelachvili, and M. Morillion-Chapey, 1994, J. Mol. Spectrosc. 166 280; (5) ν_3 at 370 cm^{-1} and ν_2 at 793 cm^{-1}, J. Orphal *et al.*, to be published.

The dipole moment is from D. F. Eagle, T. L. Weatherly, and Q. Williams, 1966, J. Chem. Phys. 44, 847. It should be noted that a dipole moment of 0.42 ± 0.01 D was reported by D. J. Millen and K. M. Sinnot, 1958, J. Chem. Soc., 350. This value is based on a much smaller data set and seems to be less reliable.

The partition function has been calculated up to $J = 99$ because of the low rotational constant. The vibrational states used in the fit were also used in the calculation of the partition function. It should be noted that these are not all (low-lying) modes that occur.

Species Tag:	**82001**	**Name:**	**HBr-81**
Version:	**2**		**Hydrogen bromide,**
Date:	**Apr. 1993**		**^{81}Br isotope**
Contributor:	**H. M. Pickett**		

Lines Listed:	**143**	**Q(300.0)=**	**103.454**
Freq. (GHz) <	**9999**	**Q(225.0)=**	**78.392**
Max. J:	**20**	**Q(150.0)=**	**53.358**
LOGSTR0=	**-8.0**	**Q(75.00)=**	**28.366**
LOGSTR1=	**-8.0**	**Q(37.50)=**	**15.916**
Isotope Corr.:	**-0.306**	**Q(18.75)=**	**9.774**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**6.935**
μ_a =	**0.828**	**A=**	
μ_b =		**B=**	**250250.2**
μ_c =		**C=**	

The experimental data were taken from F. A. Van Dijk and A. Dymanus, 1969, Chem. Phys. Lett. 4, 170 and G. Di Lonardo, L. Fusina, P. De Natale, M. Inguscio, and M. Prevedelli, 1991, J. Mol. Spect. 148, 86. The dipole moment was reported in F. A. Van Dijk and A. Dymanus, 1971, 26th Symposium on Molecular Structure and Spectroscopy, Columbus, Ohio, R12, p. 80.

Species Tag:	**88001**	**Name:**	**C6O**
Version:	**1**		**Hexacarbon monoxide**
Date:	**April 1996**		**X $^3\Sigma^-$**
Contributor:	**H. S. P. Müller**		
Lines Listed:	**567**	**Q(300.0)=**	**21997.6444**
Freq. (GHz) <	**208**	**Q(225.0)=**	**16479.0126**
Max. J:	**99**	**Q(150.0)=**	**10960.8936**
LOGSTR0=	**-9.5**	**Q(75.00)=**	**5443.4866**
LOGSTR1=	**-7.0**	**Q(37.50)=**	**2685.5413**
Isotope Corr.:		**Q(18.75)=**	**1307.7628**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**621.0766**
μ_a =	**3.630**	**A=**	
μ_b =		**B=**	**849.7571**
μ_c =		**C=**	

The data were taken from Y. Ohshima, Y. Endo, and T. Ogata, 1995, J. Chem. Phys. 102 1493.

The dipole moment is from an *ab initio* calculation: N. Moazzen-Ahmadi and F. Zerbetto, 1995, J. Chem. Phys. 103, 6343.

The partition function has been calculated up to $J = 360$ because of the low rotational constant.

Species Tag:	89001	Name:	Sr-88-H
Version:	1		X $^{2}\Sigma^{+}$,
Date:	Mar. 1995		^{88}SrH
Contributor:	H. M. Pickett		

Lines Listed:	391	Q(300.0)=	232.702
Freq. (GHz) $<$	6115	Q(225.0)=	174.141
Max. J:	30	Q(150.0)=	116.359
LOGSTR0=	-7.0	Q(75.00)=	58.803
LOGSTR1=	-7.9	Q(37.50)=	30.075
Isotope Corr.:	-0.0825	Q(18.75)=	15.758
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	8.672
μ_a =	1.0	A=	
μ_b =		B=	108927.85
μ_c =		C=	

The observed data are from C. I. Frum, J. J. Oh, E. A. Cohen, and H. M. Pickett, 1994, J. Mol. Spect. 163, 339-348. The dipole moment is arbitrary.

Species Tag:	90001	Name:	Sr-88-D
Version:	1		X $^2\Sigma^+$,
Date:	Mar. 1995		^{88}Sr^2H isotope
Contributor:	H. M. Pickett		
Lines Listed:	922	Q(300.0)=	694.865
Freq. (GHz) <	4352	Q(225.0)=	514.280
Max. J:	42	Q(150.0)=	341.665
LOGSTR0=	-7.2	Q(75.00)=	171.593
LOGSTR1=	-8.0	Q(37.50)=	86.776
Isotope Corr.:	-3.9064	Q(18.75)=	44.422
Egy. (cm^{-1}) >	0.0	Q(9.375)=	23.297
μ_a =	1.0	A=	
μ_b =		B=	55349.11
μ_c =		C=	

The observed data are from C. I. Frum, J. J. Oh, E. A. Cohen, and H. M. Pickett, 1994, J. Mol. Spect. 163, 339-348. The dipole moment is arbitrary.

Species Tag:	92001	Name:	C5S
Version:	1		
Date:	Jan. 1996		X $^1\Sigma^+$
Contributor:	J. C. Pearson		

Lines Listed:	99	Q(300.0)=	5227.015
Freq. (GHz) $<$	183	Q(225.0)=	4371.654
Max. J:	99	Q(150.0)=	3219.957
LOGSTR0=	-7.2	Q(75.00)=	1689.457
LOGSTR1=	-5.8	Q(37.50)=	847.178
Isotope Corr.:	-0.046	Q(18.75)=	423.753
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	212.042
μ_a =	1.0	A=	
μ_b =		B=	922.7
μ_c =		C=	

The experimental measurements are from: Y. Kasai, O. Kinichi, Y. Oshima, Y. Hirahara, Y. Endo, K. Kawaguchi and A. Murakami, 1993, Astrophys. J. 410, L45.

The dipole is not known so the calculation has been done with unit dipole. The dipole is believed to be at least 3 Debye.

Species Tag:	**94001**	**Name:**	**C5S-34**
Version:	**1**		
Date:	**Jan. 1996**		**X $^1\Sigma^+$,**
Contributor:	**J. C. Pearson**		**^{34}S isotope**
Lines Listed:	**99**	**Q(300.0)=**	**5301.102**
Freq. (GHz) <	**178**	**Q(225.0)=**	**4446.777**
Max. J:	**99**	**Q(150.0)=**	**3279.163**
LOGSTR0=	**-7.2**	**Q(75.00)=**	**1731.874**
LOGSTR1=	**-5.8**	**Q(37.50)=**	**868.816**
Isotope Corr.:	**-1.399**	**Q(18.75)=**	**434.572**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**217.451**
μ_a =	**1.0**	**A=**	
μ_b =		**B=**	**899.7**
μ_c =		**C=**	

The experimental measurements are from: Y. Kasai, O. Kinichi, Y. Oshima, Y. Hirahara, Y. Endo, K. Kawaguchi and A. Murakami, 1993, Astrophys. J. 410, L45.

The dipole is not known so the calculation has been done with unit dipole. The dipole is believed to be at least 3 Debye.

Species Tag:	**95001**	**Name:**	**Br-79-O**
Version:	**2**		**Bromine monoxide, $v = 0$**
Date:	**Aug. 2000**		**^{79}Br isotope,**
Contributor:	**E. A. Cohen**		**$X_1\,^2\Pi_{3/2}$ and $X_2\,^2\Pi_{1/2}$ states**
Lines Listed:	**1892**	**Q(300.0)=**	**3941.167**
Freq. (GHz) <	**2172**	**Q(225.0)=**	**2932.182**
Max. J:	**86.5**	**Q(150.0)=**	**1949.832**
LOGSTR0=	**-8.0**	**Q(75.00)=**	**973.813**
LOGSTR1=	**-8.0**	**Q(37.50)=**	**486.125**
Isotope Corr.:	**-0.296**	**Q(18.75)=**	**242.308**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**120.345**
μ_a =	**1.780**	**A=**	
μ_b =		**B=**	**12779.365**
μ_c =		**C=**	

The spectrum was calculated from a combined fit of rotational spectra of all four isotopic species ^{79,81}Br^{16,18}O as well as available infrared spectra. The fit is described by B. J. Drouin, *et al.* 2000, J. Mol. Spectrosc. (in press). The data and parameter files have been deposited with the journal. Note that the quantum number field has been changed. In this version it is N, Λ, v, $J + 1/2$, F. The parity is given by the sign of Λ.

Species Tag:	**95002**	**Name:**	**Br-79-O v=1**
Version:	**1**		**Bromine monoxide, $v = 1$**
Date:	**Aug. 2000**		**^{79}Br isotope,**
Contributor:	**E. A. Cohen**		**$X_1\,^2\Pi_{3/2}$ and $X_2\,^2\Pi_{1/2}$ states**

Lines Listed:	**1314**	**Q(300.0)=**	**3941.167**
Freq. (GHz) $<$	**1889**	**Q(225.0)=**	**2932.182**
Max. J:	**75.5**	**Q(150.0)=**	**1949.832**
LOGSTR0=	**-8.0**	**Q(75.00)=**	**973.813**
LOGSTR1=	**-8.0**	**Q(37.50)=**	**486.125**
Isotope Corr.:	**-0.296**	**Q(18.75)=**	**242.308**
Egy. (cm^{-1}) $>$	**0.0**	**Q(9.375)=**	**120.345**
μ_a =	**1.780**	**A=**	
μ_b =		**B=**	**12669.758**
μ_c =		**C=**	

The spectrum was calculated from a combined fit of rotational spectra of all four isotopic species ^{79,81}Br^{16,18}O as well as available infrared spectra. The fit is described by B. J. Drouin, *et al.* 2000, J. Mol. Spectrosc. (in press). The data and parameter files have been deposited with the journal. Note that the quantum number field has been changed. In this version it is $N,\ ,\Lambda,\ v,\ J+1/2,\ F.$ The parity is given by the sign of Λ.

Species Tag:	96001	Name:	HOBr-79
Version:	1		Hypobromous acid
Date:	Dec. 1994		
Contributor:	E. A. Cohen		

Lines Listed:	9898	Q(300.0)=	13552.774
Freq. (GHz) $<$	9471	Q(225.0)=	8796.667
Max. J:	70	Q(150.0)=	4785.832
LOGSTR0=	-8.0	Q(75.00)=	1692.421
LOGSTR1=	-6.0	Q(37.50)=	599.428
Isotope Corr.:	-0.2964	Q(18.75)=	213.623
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	82.475
μ_a =	0.000	A=	613679.92
μ_b =	1.384	B=	10576.608
μ_c =		C=	10383.061

The calculation is based on pure rotational data from Koga *et al.*, 1989, J. Mol. Spect. 138, 467 and on infrared data from the high resolution spectrum of the ν_1 band from Cohen *et al.*, 1995, J. Mol. Spectrosc. 173, 55. The maximum value of K_a observed in the infrared is 5. The reader is cautioned that transitions involving higher values K_a in the catalog are extrapolations which may be considerably less accurate than the calculated uncertainties indicate.

Species Tag:	**97001**	**Name:**	**Br-81-O**
Version:	**2**		**Bromine monoxide, $v = 0$**
Date:	**Aug. 2000**		**^{81}Br isotope,**
Contributor:	**E. A. Cohen**		**$X_1\,{}^2\Pi_{3/2}$ and $X_2\,{}^2\Pi_{1/2}$ states**

Lines Listed:	**1892**	**Q(300.0)=**	**3957.594**
Freq. (GHz) <	**2164**	**Q(225.0)=**	**2944.406**
Max. J:	**86.5**	**Q(150.0)=**	**1957.963**
LOGSTR0=	**-8.0**	**Q(75.00)=**	**977.877**
LOGSTR1=	**-8.0**	**Q(37.50)=**	**488.157**
Isotope Corr.:	**-0.306**	**Q(18.75)=**	**243.324**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**120.855**
μ_a =	**1.780**	**A=**	
μ_b =		**B=**	**12726.305**
μ_c =		**C=**	

The spectrum was calculated from a combined fit of rotational spectra of all four isotopic species ^{79,81}Br^{16,18}O as well as available infrared spectra. The fit is described by B. J. Drouin, *et al.* 2000, J. Mol. Spectrosc. (in press). The data and parameter files have been deposited with the journal. Note that the quantum number field has been changed. In this version it is N, Λ, v, $J + 1/2$, F.

Species Tag:	97002	Name:	Cl-35-ONO2
Version:	2		Chlorine nitrate
Date:	Oct. 1996		^{35}Cl isotope
Contributor:	H. S. P. Müller		
Lines Listed:	78323	Q(300.0)=	614310.627
Freq. (GHz) $<$	1000	Q(225.0)=	372267.704
Max. J:	99	Q(150.0)=	181443.199
LOGSTR0=	-10.0	Q(75.00)=	54099.169
LOGSTR1=	-7.3	Q(37.50)=	17894.505
Isotope Corr.:	-0.122	Q(18.75)=	6296.771
Egy. (cm^{-1}) $>$		Q(9.375)=	2230.345
μ_a =	0.72	A=	12105.78
μ_b =	0.28	B=	2777.001
μ_c =		C=	2258.151

The frequencies are taken from (1) R. D. Suenram and D. R. Johnson, 1977, J. Mol. Spectrosc. 65, 239; (2) R. D. Suenram and F. J. Lovas, 1984, J. Mol. Spectrosc. 105, 351; and (3) H. S. P. Müller, P. Helminger, and S. H. Young, 1997, J. Mol. Spectrosc. 181, 363.

The data for both isotopomers (^{35}Cl and ^{37}Cl) in the $v = 0$ and $v_9 = 1$ states has been fit simultaneously as described in (3). Lines outside four times the experimental uncertainties were omitted and have not been merged. A fit of similar qualtity is achieved when only lines of this species are used. While the data for this species is archived in the usual way, the combined fit is archived as clg.*.

Because ^{35}Cl hyperfine splittings were important in the fit, the catalog entry presented includes these splittings even though they are in general much smaller than the width of stratospheric lines.

The dipole moment is from (1). The partition function takes into account the torsional mode at *ca.* 120 cm^{-1}. Because of the small rotational constants the partition function has been calculated up to $J = 150$. Transitions with $J > 99$ are not included because at stratospheric temperatures their intensity is expected to be very small, even though some of them may be stronger than listed low J lines at room temperature.

Species Tag:	**97003**	**Name:**	**Br-81-O v=1**
Version:	**1**		**Bromine monoxide, $v = 1$**
Date:	**Aug. 2000**		**^{81}Br isotope,**
Contributor:	**E. A. Cohen**		**$X_1\,^2\Pi_{3/2}$ and $X_2\,^2\Pi_{1/2}$ states**

Lines Listed:	**1313**	**Q(300.0)=**	**3957.594**
Freq. (GHz) $<$	**1881**	**Q(225.0)=**	**2944.406**
Max. J:	**75.5**	**Q(150.0)=**	**1957.963**
LOGSTR0=	**-8.0**	**Q(75.00)=**	**977.877**
LOGSTR1=	**-8.0**	**Q(37.50)=**	**488.157**
Isotope Corr.:	**-0.306**	**Q(18.75)=**	**243.324**
Egy. (cm^{-1}) $>$	**0.0**	**Q(9.375)=**	**120.855**
$\mu_a =$	**1.780**	**A=**	
$\mu_b =$		**B=**	**12617.383**
$\mu_c =$		**C=**	

The spectrum was calculated from a combined fit of rotational spectra of all four isotopic species ^{79,81}Br^{16,18}O as well as available infrared spectra. The fit is described by B. J. Drouin, *et al.* 2000, J. Mol. Spectrosc. (in press). The data and parameter files have been deposited with the journal. Note that the quantum number field has been changed. In this version it is N, Λ, v, $J + 1/2$, F.

Species Tag:	**98001**	**Name:**	**H2SO4**
Version:	**3**		**Sulfuric acid**
Date:	**July 2, 2002**		
Contributor:	**E. A. Cohen**		

Lines Listed:	**20939**	**Q(300.0)=**	**155955.250**
Freq. (GHz) <	**1000**	**Q(225.0)=**	**101274.475**
Max. J:	**99**	**Q(150.0)=**	**55118.831**
LOGSTR0=	**-7.0**	**Q(75.00)=**	**19489.469**
LOGSTR1=	**-7.0**	**Q(37.50)=**	**6894.456**
Isotope Corr.:	**-0.022**	**Q(18.75)=**	**2441.181**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**865.964**
μ_a =		**A=**	**5160.581**
μ_b =		**B=**	**5024.549**
μ_c =	**2.725**	**C=**	**4881.023**

The present version contains calculated frequencies only. It is based on work in progress at this laboratory. The data set contains transitions near 120, 300, 400, and 650 GHz measured at JPL as well as the $1_{10} - 0_{00}$ transition measured at the University of Minnesota.

Species Tag:	98002	Name:	HOBr-81
Version:	1		Hypobromous acid
Date:	Dec. 1994		
Contributor:	E. A. Cohen		
Lines Listed:	9920	Q(300.0)=	13611.629
Freq. (GHz) <	9469	Q(225.0)=	8834.883
Max. J:	70	Q(150.0)=	4806.617
LOGSTR0=	-8.0	Q(75.00)=	1699.763
LOGSTR1=	-6.0	Q(37.50)=	602.023
Isotope Corr.:	-0.3057	Q(18.75)=	214.544
Egy. (cm^{-1}) >	0.0	Q(9.375)=	82.827
μ_a =	0.000	A=	613676.13
μ_b =	1.384	B=	10530.431
μ_c =		C=	10338.555

The calculation is based on pure rotational data from Koga *et al.*, 1989, J. Mol. Spect. 138, 467 and on infrared data from the high resolution spectrum of the ν_1 band from Cohen *et al.*, 1995, J. Mol. Spectrosc. 173, 55. The maximum value of K_a observed in the infrared is 5. The reader is cautioned that transitions involving higher values K_a in the catalog are extrapolations which may be considerably less accurate than the calculated uncertainties indicate.

Species Tag:	99001	Name:	Cl-37-ONO2
Version:	2		Chlorine nitrate
Date:	Oct. 1996		^{37}Cl isotope
Contributor:	H. S. P. Müller		
Lines Listed:	49505	Q(300.0)=	629987.497
Freq. (GHz) <	889	Q(225.0)=	381776.321
Max. J:	99	Q(150.0)=	186077.183
LOGSTR0=	-9.3	Q(75.00)=	55480.326
LOGSTR1=	-6.7	Q(37.50)=	18351.122
Isotope Corr.:	-0.611	Q(18.75)=	6457.304
Egy. (cm^{-1}) >		Q(9.375)=	2287.107
μ_a =	0.72	A=	12105.33
μ_b =	0.28	B=	2700.974
μ_c =		C=	2207.604

The frequencies are taken from (1) R. D. Suenram and D. R. Johnson, 1977, J. Mol. Spectrosc. 65, 239; (2) R. D. Suenram and F. J. Lovas, 1984, J. Mol. Spectrosc. 105, 351; and (3) H. S. P. Müller, P. Helminger, and S. H. Young, 1997, J. Mol. Spectrosc. 181, 363.

The data for both isotopomers (^{35}Cl and ^{37}Cl) in the $v = 0$ and $v_9 = 1$ states has been fit simultaneously as described in (3). Lines outside four times the experimental uncertainties were omitted and have not been merged. A fit of similar qualtity is achieved when only lines of this species are used and H_K is held fixed. While the data for this species is archived in the usual way, the combined fit is archived as clg.*.

Because ^{37}Cl hyperfine splittings were important in the fit, the catalog entry presented includes these splittings even though they are in general much smaller than the width of stratospheric lines.

The dipole moment, estimated to be the same as for the ^{35}Cl isotopomer, is from (1). The partition function takes into account the torsional mode at *ca.* 120 cm^{-1}. Because of the small rotational constants the partition function has been calculated up to $J = 150$. Transitions with $J > 99$ are not included because at stratospheric temperatures their intensity is expected to be very small, even though some of them may be stronger than listed low J lines at room temperature.

Species Tag:	99002	Name:	HC$_7$N
Version:	1		Cyanohexatriyne
Date:	Dec. 1994		
Contributor:	M. L. Delitsky H. M. Pickett		
Lines Listed:	518	Q(300.0)=	19760.7948
Freq. (GHz) <	112.7862	Q(225.0)=	17448.1553
Max. J:	99	Q(150.0)=	13889.0325
LOGSTR0=	-10.0	Q(75.00)=	8088.1668
LOGSTR1=	-100.0	Q(37.50)=	4154.2349
Isotope Corr.:	-0.0354	Q(18.75)=	2079.1318
Egy. (cm^{-1}) >	0.0	Q(9.375)=	1040.0620
μ_a =	5.0	A=	
μ_b =		B=	564.0007
μ_c =		C=	

The observed frequency measurements were taken from L.F Rodriguez and E.F Chaisson, 1980, Mon. Not. R. Astr. Soc. 192, 651. F. Tolle *et al.*, 1981, Astron. Astrophys. 95, 143. C. A. Olano *et al.*, 1988, Astron. Astrophys. 196, 194. Truong-Bach *et al.*, 1988, Astron. Astrophys. 199, 291. J. Cernicharo *et al.*, 1986, Astron. Astrophys. 1 60, 181.

The dipole moment was taken from the extrapolation by H. W. Kroto *et al.*, 1978, Astrophys. J. 219, L133.

Species Tag:	100001	Name:	C7O
Version:	1		Heptacarbon monoxide
Date:	May 1996		X $^1\Sigma^+$
Contributor:	H. S. P. Müller		

Lines Listed:	99	Q(300.0)=	10912.5313
Freq. (GHz) $<$	114	Q(225.0)=	8184.1697
Max. J:	99	Q(150.0)=	5455.9817
LOGSTR0=	-8.0	Q(75.00)=	2728.0359
LOGSTR1=	-3.5	Q(37.50)=	1364.1543
Isotope Corr.:		Q(18.75)=	682.2363
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	341.2831
μ_a =	4.417	A=	
μ_b =		B=	572.9410
μ_c =		C=	

The data were taken from T. Ogata, Y. Ohshima, and Y. Endo, 1995, J. Am. Chem. Soc. 117 3593.

The dipole moment is from an *ab initio* calculation: N. Moazzen-Ahmadi and F. Zerbetto, 1995, J. Chem. Phys. 103, 6343.

The partition function has been calculated up to $J = 360$ because of the low rotational constant.

Species Tag:	102001	Name:	ClOOCl
Version:	1		Chlorine peroxide
Date:	Aug. 1990		(ClO dimer)
Contributor:	E. A. Cohen		

Lines Listed:	17266	Q(300.0)=	426874.344
Freq. (GHz) $<$	1000	Q(225.0)=	277268.281
Max. J:	99	Q(150.0)=	151112.312
LOGSTR0=	-7.0	Q(75.00)=	53382.613
LOGSTR1=	-7.0	Q(37.50)=	18866.881
Isotope Corr.:	-0.244	Q(18.75)=	6674.211
Egy. (cm^{-1}) $>$	0.5	Q(9.375)=	2363.198
μ_a =		A=	13109.45
μ_b =	0.72	B=	2409.79
μ_c =		C=	2139.68

The data were reported by M. Birk *et al.*, 1989, J. Chem. Phys. 91, 6598. The dipole moment is based on unpublished measurements by M. Birk, R. R. Friedl, and E. A. Cohen.

Species Tag:	104001	Name:	Cl-37-OOCl
Version:	1		Chlorine peroxide
Date:	Aug. 1990		(ClO dimer)
Contributor:	E. A. Cohen		^{37}ClOO^{35}Cl
Lines Listed:	17482	Q(300.0)=	439238.281
Freq. (GHz) <	1000	Q(225.0)=	285233.281
Max. J:	99	Q(150.0)=	155417.594
LOGSTR0=	-7.0	Q(75.00)=	54928.781
LOGSTR1=	-7.0	Q(37.50)=	19408.863
Isotope Corr.:	-0.432	Q(18.75)=	6865.939
Egy. (cm^{-1}) >	0.8	Q(9.375)=	2431.083
μ_a =		A=	13013.07
μ_b =	0.72	B=	2349.01
μ_c =		C=	2089.29

The data were reported by M. Birk *et al.*, 1989, J. Chem. Phys. 91, 6598. The dipole moment is based on unpublished measurements by M. Birk, R. R. Friedl, and E. A. Cohen.

Species Tag:	111001	Name:	OBr-79-O
Version:	1		Bromine dioxide, X $^{2}B_{1}$
Date:	June 1997		^{79}Br isotope
Contributor:	H. S. P. Müller		

Lines Listed:	52631	Q(300.0)=	92147.140
Freq. (GHz) <	2000	Q(225.0)=	59881.060
Max. J:	80	Q(150.0)=	32618.198
LOGSTR0=	-8.5	Q(75.00)=	11579.660
LOGSTR1=	-6.3	Q(37.50)=	4134.614
Isotope Corr.:	-0.296	Q(18.75)=	1492.190
Egy. (cm^{-1}) >		Q(9.375)=	549.968
μ_a =		A=	28024.518
μ_b =	2.81	B=	8233.173
μ_c =		C=	6345.433

The lines, the Hamiltonian, and the fitting are described in H. S. P. Müller, C. E. Miller, and E. A. Cohen, 1997, J. Chem. Phys. 107, 8292. The dipole moment was assumed to be the same as for O^{81}BrO, tag no. 113001. The parameters used in the combined fit of both isotopomers and all observed vibrational states are archived under tag no. 111001.

Species Tag:	**112001**	**Name:**	**Se-80-O2**
Version:	**1**		**Selenium Dioxide,**
Date:	**Sept. 1995**		**^{80}Se isotope**
Contributor:	**H. S. P. Müller**		
Lines Listed:	**7484**	**Q(300.0)=**	**10779.685**
Freq. (GHz) <	**2510**	**Q(225.0)=**	**6996.362**
Max. J:	**99**	**Q(150.0)=**	**3805.880**
LOGSTR0=	**-8.0**	**Q(75.00)=**	**1345.345**
LOGSTR1=	**-7.0**	**Q(37.50)=**	**476.116**
Isotope Corr.:	**-0.303**	**Q(18.75)=**	**168.775**
Egy. (cm^{-1}) >	**0.0**	**Q(9.375)=**	**60.006**
μ_a =		**A=**	**28826.532**
μ_b =	**2.7**	**B=**	**8676.6837**
μ_c =		**C=**	**6651.8979**

The data were taken from (1) H. Takeo, E. Hirota, and Y. Morino, 1970, J. Mol. Spect. 34, 370 (microwave region, dipole moment), and (2) E. A. Alekseev, O. I. Bashkakov, S. F. Dyubko, and B. I. Polevoi, 1986, Opt. Spektrosk. 60 49; Opt. Spectrosc. (USSR) 60, 30 (submillimeter region).

The spectroscopic constants used in the fit were the same as in (2): Watson's A reduction with up to octic distortion constants.

Species Tag:	112002	Name:	C8O
Version:	1		Octacarbon monoxide
Date:	April 1996		X $^{3}\Sigma^{-}$
Contributor:	H. S. P. Müller		

Lines Listed:	644	Q(300.0)=	46470.4032
Freq. (GHz) $<$	207	Q(225.0)=	34777.1480
Max. J:	99	Q(150.0)=	23075.2173
LOGSTR0=	-9.9	Q(75.00)=	11375.8620
LOGSTR1=	-7.0	Q(37.50)=	5531.6130
Isotope Corr.:		Q(18.75)=	2619.3581
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	1180.9848
μ_a =	4.629	A=	
μ_b =		B=	400.6418
μ_c =		C=	

The data were taken from Y. Ohshima, Y. Endo, and T. Ogata, 1995, J. Chem. Phys. 102 1493.

The dipole moment is from an *ab initio* calculation: N. Moazzen-Ahmadi and F. Zerbetto, 1995, J. Chem. Phys. 103, 6343.

The partition function has been calculated up to $J = 360$ because of the low rotational constant.

Species Tag:	**113001**	**Name:**	**OBr-81-O**
Version:	**1**		**Bromine dioxide, X $^2B_1$**
Date:	**June 1997**		**^{81}Br isotope**
Contributor:	**H. S. P. Müller**		

Lines Listed:	**52631**	**Q(300.0)=**	**92550.906**
Freq. (GHz) <	**2000**	**Q(225.0)=**	**60143.825**
Max. J:	**80**	**Q(150.0)=**	**32761.294**
LOGSTR0=	**-8.5**	**Q(75.00)=**	**11630.398**
LOGSTR1=	**-6.3**	**Q(37.50)=**	**4152.689**
Isotope Corr.:	**-0.306**	**Q(18.75)=**	**1498.684**
Egy. (cm^{-1}) >		**Q(9.375)=**	**552.340**
μ_a =		**A=**	**27824.891**
μ_b =	**2.81**	**B=**	**8233.255**
μ_c =		**C=**	**6335.137**

The lines, the Hamiltonian, and the fitting are described in H. S. P. Müller, C. E. Miller, and E. A. Cohen, 1997, J. Chem. Phys. 107, 8292. The dipole moment was also from that study. The parameters used in the combined fit of both isotopomers and all observed vibrational states are archived under tag no. 111001.

Species Tag:	123001	Name:	HC_9N
Version:	1		Cyanooctatetrayne
Date:	Dec. 1994		
Contributor:	M. L. Delitsky		
	H. M. Pickett		
Lines Listed:	99	Q(300.0)=	7998.1962
Freq. (GHz) $<$	57.52	Q(225.0)=	7453.8407
Max. J:	99	Q(150.0)=	6511.8249
LOGSTR0=	-100.0	Q(75.00)=	4541.3320
LOGSTR1=	-100.0	Q(37.50)=	2624.6426
Isotope Corr.:	-0.0451	Q(18.75)=	1344.3403
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	672.7302
$\mu_a =$	5.6	A=	
$\mu_b =$		B=	290.5183
$\mu_c =$		C=	

The experimental frequency measurements were taken from M. Iida, Y. Ohshima, and Y. Endo, 1991, Astrophys. J. 371, L45. The dipole moment was taken from N. W. Broten *et al.*, 1978, Astrophys. J. 223, L105.

Species Tag:	124001	Name:	C9O
Version:	1		Nonacarbon monoxide
Date:	May 1996		X $^1\Sigma^+$
Contributor:	H. S. P. Müller		

Lines Listed:	100	Q(300.0)=	21237.3998
Freq. (GHz) $<$	59	Q(225.0)=	15958.1034
Max. J:	100	Q(150.0)=	10641.4691
LOGSTR0=	-8.0	Q(75.00)=	5320.7441
LOGSTR1=	-3.5	Q(37.50)=	2660.4931
Isotope Corr.:		Q(18.75)=	1330.4018
Egy. (cm^{-1}) $>$	0.0	Q(9.375)=	665.3648
μ_a =	5.421	A=	
μ_b =		B=	293.7361
μ_c =		C=	

The data were taken from T. Ogata, Y. Ohshima, and Y. Endo, 1995, J. Am. Chem. Soc. 117 3593.

The dipole moment is from an *ab initio* calculation: N. Moazzen-Ahmadi and F. Zerbetto, 1995, J. Chem. Phys. 103, 6343.

The partition function has been calculated up to $J = 360$ because of the low rotational constant.

Species Tag:	147001	Name:	$HC_{11}N$
Version:	2		Cyanodecapentayne
Date:	Oct. 1996		
Contributor:	H. S. P. Müller		
Lines Listed:	99	Q(300.0)=	35656.4133
Freq. (GHz) <	33.5	Q(225.0)=	27406.6011
Max. J:	99	Q(150.0)=	18464.7988
LOGSTR0=	-15.0	Q(75.00)=	9244.1190
LOGSTR1=	-4.0	Q(37.50)=	4622.1729
Isotope Corr.:	-0.0548	Q(18.75)=	2311.2379
Egy. (cm^{-1}) >	0.0	Q(9.375)=	1155.7819
μ_a =	6.2	A=	
μ_b =		B=	169.0629
μ_c =		C=	

The experimental lines are from M. J. Travers, M. C. McCarthy, P. Kalmus, C. A. Gottlieb, and P. Thaddeus, 1996, Astrophys. J. 469, L65. Because of the small rotational constant the partition function has been calculated up to $J = 350$.

Previously reported interstellar lines from M. B. Bell *et al.*, 1982, Nature 295, 389, and M. B. Bell and H. E. Matthews, 1985, Astrophys. J. 291, L63 are in error.

The dipole moment was estimated from an extrapolation in N. W. Broten, 1978, Astrophys. J. 223, L105. (i.e. continuing from the series HC_7N and HC_9N.)