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Submillimeter, Millimeter, and Microwave Spectral Line Catalogue

H. M. Pickett
R. L. Poynter
E. A. Cohen

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National Aeronautics and
Space Administration

Jet Propulsion Laboratory
California Institute of Technology
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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 206 atomic and molecular species and includes a total of 630,924 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 as a magnetic data tape recorded in card images, with one card image per spectral line, from the National Space Science Data Center, located at Goddard Space Flight Center.

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. 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				

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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-vl
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-vl
34001	O-18-O	41005	CH3CCD	44001	CS
44002	SiO	45001	C-13-S	46001	CS-34
48004	O3	48005	O3-v2	48006	O3-vl,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-vl,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-vl	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

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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 as a magnetic data tape recorded in card images, with one card image per spectral line, from the National Space Science Data Center at the Goddard Space Flight Center.

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 File

The catalog data tape is composed of 80-character card images, with one card image per spectral line. The format of each card image 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 $nm^2 \cdot MHz$ 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 ground 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 data tape also contains a second file with a species directory. Each element of this directory is an 80-character record with the following format:

TAG,	NAME,	NLINE,	QLOG,	VERSION
(I6,X,	A14,	I5,	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 logorithm 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.

3 INTENSITY UNITS AND CONVERSIONS

The units of intensity given in the catalog, nm^2·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 cm^{-1}/(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

$$I_{ba}(T) = (8\pi^3/3\mathrm{hc})\nu_{ba}\ {}^xS_{ba}\ \mu_x^2[e^{-E''/kT} - e^{-E'/kT}]/Q_{rs} \tag{1}$$

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$''$). **Care must be taken to assure that ${}^xS_{ba}$ and Q_{rs} are determined with the same state degeneracies.** 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 below. For the catalog, Eq. (1) 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 T$^{3/2}$ in the same limit. Explicitly, I_{ba}(T) is

$$\begin{aligned} I_{ba}(T) &= I_{ba}(T_\circ)[Q_{rs}(T_\circ)/Q_{rs}(T)]\frac{e^{-E''/kT} - e^{-E'/kT}}{e^{-E''/kT_\circ} - e^{-E'/kT_\circ}} && (2) \\ &\cong I_{ba}(T_\circ)\cdot(T_\circ/T)^{n+1}e^{-(1/T-1/T_\circ)E''/k} && (3) \end{aligned}$$

where n = 1 for a linear molecule and 3/2 for a nonlinear molecule. Eq. (3) requires that the energy spacings be small compared with kT.

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

$$\alpha_{\max} = \frac{I_{ba}(T)}{\Delta\nu}(T_\circ/T) \times 102.458\ \mathrm{cm}^{-1} \tag{4}$$

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 nm^2·MHz, and $\alpha_{\max}$ is in units of cm^{-1}. The corresponding value of $\alpha_{\max}$ in the thermal Doppler limit is

$$\alpha_{\max} = \frac{I_{ba}(T)p}{\Delta\nu_d}(T_\circ/T) \times 151.193\ \mathrm{cm}^{-1} \tag{5}$$

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

$$\Delta\nu_d = 1.17230 \times 10^{-6} \times \nu_{ba}\sqrt{(T/T_\circ)(28/m)} \tag{6}$$

in which m is the mass of the absorber (in atomic mass units). In Eqs. (6) - (9), 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

$$\sigma_{ba} = \frac{I_{ba}}{\nu_{ba}} \times 2.99792 \times 10^{-9}\ \mathrm{cm}^2. \tag{7}$$

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

$$\begin{aligned} A_{ba} &= I_{ba}(T)\ \nu_{ba}^2[Q_{rs}/g'][e^{-E''/kT} - e^{-E'/kT}]^{-1} \times 2.7964 \times 10^{-16}\ \mathrm{sec}^{-1} && (8) \\ &\cong I_{ba}(T_o)\ \nu_{ba}[Q_{rs}(T_o)/g']e^{E'/kT_o} \times 1.748 \times 10^{-9}\ \mathrm{sec}^{-1} && (9) \end{aligned}$$

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 below and on the directory portion of the tape.

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:

$$\varepsilon_n^2 = \sum_{kj} \frac{\partial \nu_n}{\partial p_k} \frac{\partial \nu_n}{\partial p_j}\ V_{kj} \tag{10}$$

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

$$(V^{-1})_{kj} = \sum_m \frac{\partial \nu_m}{\partial p_k} \frac{\partial \nu_m}{\partial p_j}\ \varepsilon_m^{-2} \tag{11}$$

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 ${}^{x}S_{ba}$, 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

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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:

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

For even-spin multiplicity:

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

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

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+	12001	C-atom	13001	C-13-atom
13002	CH	14001	N-atom	14002	N-atom-D-state
16001	O-atom	17001	OH	17002	NH3
17003	CH3D	17004	NH3-v2	18001	OD
18002	N-15-H3	18003	H2O	18004	NH2D
18005	H2O-v2	19001	HO-18	19002	HDO
19003	H2O-17	20001	D2O	20002	HF
20003	H2O-18	21001	HDO-18	21002	DF
25001	CCH	26001	CN	26002	CN-v1
27001	HCN	27002	HNC	27003	HCN-v2
28001	CO	28002	HC-13-N	28003	HCN-15
28004	DCN	28005	HNC-13	28006	HN-15-C
28007	DNC	29001	C-13-O	29002	HCO+
29003	CH2NH	29004	HCO	29005	NNH+
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+
31001	HCO-18+	31002	H2C-13-O	32001	O2
32002	O2-v1	32003	CH3OH	32004	H2CO-18
32005	O2 snglt dlta	33001	HO2	33002	O-17-O
34001	O-18-O	34002	H2S	34003	PH3
34004	H2O2	35001	HDS	36001	HCl
37001	DCl	38001	HCl-37	38002	C3H2
39001	C-13-3H2a	39002	C-13-3H2s	39003	C3HD
39004	DCl-37	40001	CH3CCH	40002	NaOH
41001	CH3CN	41002	CH3CC-13-H	41003	CH3C-13-CH
41004	C-13-H3CCH	41005	CH3CCD	41006	CH2DCCH
42001	CH3CN-15	42002	CH2CO	42003	NH2CN
43001	CHDCO	43002	HNCO	43003	AlO
44001	CS	44002	SiO	44003	CH3CHO-a
44004	N2O	44005	CH3CHO-e	44006	DNCO

TABLE 3. (continued)

Tag	Name	Tag	Name	Tag	Name
44007	HN-15-CO	44008	HNC-13-O	44009	N2O-v2
45001	C-13-S	45002	Si-29-O	45003	NH2CHO
45005	HCS+	45006	HNCO-18	45007	NN-15-O
45008	N-15-NO	46001	CS-34	46002	Si-30-O
46003	H2CS	46004	C2H5OH	46005	HCOOH
46006	NO2	46007	N2O-18	47001	H2C-13-s
47002	HC-13-OOH	47003	DCOOH	47004	HCOOD
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	49001	O3-sym-O-17
49002	O3-asym-O-17	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	50007	CH3Cl-35	51001	HCCCN
51002	ClO	51003	ClO-v1	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	53001	C2H3CN	53002	Cl-37-O
53003	C-13-CCO	53004	CC-13-CO	53005	CCC-13-O
53006	Cl-37-O-v1	54001	CH2CHC-13-N	54002	CH2C-13-HCN
54003	C-13-H2CHCN	54004	CH2CDCN	54005	HOCl-37
54006	CCCO-18	55001	C2H5CN	56001	CH3CH2C-13-N
56002	CH3C-13-H2CN	56003	C-13-H3CH2CN	56004	C2H5CN-15
56005	CH2DCH2CN-s	56006	CH2DCH2CN-a	60001	OCS
60002	SiS	61001	OC-13-S	61002	Si-29-S
62001	OC-34-S	62002	O-18-CS	62003	Si-30-S
62004	SiS-34	63001	HNO3	63002	HNO3 v7
63003	HNO3 v9	63004	HNO3 v6	63005	HNO3 v8
63006	HNO3 v5	64001	S2	64002	SO2
66001	COF2	67001	OCl-35-O	68001	CCCS
69001	OCl-37-O	70001	CCCS-34	75001	HCCCCCN
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	79001	HOONO2	80001	HBr-79
82001	HBr-81	95001	Br-79-O	97001	Br-81-O
97002	Cl-35-NO3	98001	H2SO4	99001	Cl-37-NO3
102001	ClOOCl	104001	Cl-37-OOCl		

Species Tag:	1001	Species Name:	H-atom
Version:	1		$^2S_{1/2}$ 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	Species 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	Species 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 =		A=	
μ_b =	0.000585	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	Species 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:	12001	Species 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	Species Name:	C-13-atom ^{13}C isotope
Version:	2		
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	Species Name:	CH
Version:	1		$^2\Pi$ states
Date:	Feb. 1984		
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:	14001	Species Name:	N-atom
Version:	1		$^4S_{3/2}$ 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	Species 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 $^2D_{5/2}$ state is 19,223 cm^{-1} above the ground $^4S_{3/2}$ state (C. E. Moore, 1949, Atomic Energy Levels I, National Bureau of Standards). The $^2D_{3/2}$ - $^2D_{5/2}$ 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 ^2D states to the ^4S states is 1.06×10^{-6} sec^{-1}. In contrast, the spontaneous emission rate from $^2D_{3/2}$ F = 5/2 to $^2D_{5/2}$ F = 7/2 is 3.15×10^{-9} sec^{-1}.

Species Tag:	16001	Species Name:	O-atom
Version:	2		^{3}P ground state
Date:	Mar. 1984		
Contributor:	H. M. Pickett		
Lines Listed:	2	Q(300.0)=	6.741
Freq. (GHz) <	3000	Q(225.0)=	6.324
Max. J:	1	Q(150.0)=	5.770
LOGSTR0=	-3.5	Q(75.00)=	5.156
LOGSTR1=	-5.2	Q(37.50)=	5.007
Isotope Corr.:	0.0	Q(18.75)=	5.000
Egy. (cm^{-1}) >	0.0	Q(9.375)=	5.000
μ_a =		A=	
μ_b =		B=	
μ_c =		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	Species Name:	OH
Version:	3		
Date:	Oct. 1990		
Contributor:	H. M. Pickett		
Lines Listed:	670	Q(300.0)=	81.489
Freq. (GHz) <	20937	Q(225.0)=	60.298
Max. J:	50	Q(150.0)=	40.142
LOGSTR0=	-15.0	Q(75.00)=	22.751
LOGSTR1=	-20.0	Q(37.50)=	17.033
Isotope Corr.:	0.0	Q(18.75)=	16.003
Egy. (cm^{-1}) >	0.0	Q(9.375)=	15.929
μ_a =	1.667	A=	
μ_b =		B=	556141.
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. 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.

Species Tag:	17002	Species 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 $J = 1 \rightarrow 0$, $K = 0$ 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	Species Name:	CH3D Mono-deutero methane
Version:	1		
Date:	Feb. 1980		
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	Species 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:	18001	Species Name:	OD
Version:	1		Hydroxyl radical,
Date:	May 1983		deuterium isotope
Contributor:	H. M. Pickett		
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	Species 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	Species Name:	H2O
Version:	4		Water
Date:	Oct. 1990		
Contributor:	R. L. Poynter H. M. Pickett		
Lines Listed:	783	Q(300.0)=	178.115
Freq. (GHz) <	29988	Q(225.0)=	116.011
Max. J:	12	Q(150.0)=	63.680
LOGSTR0=	-8.7	Q(75.00)=	23.169
LOGSTR1=	-11.8	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=	835840.29
μ_b =	1.855	B=	435351.72
μ_c =		C=	278138.70

The data set used in this new fit is based upon both the microwave and submillimeter lines reported by J. K. Messer, F. C. De Lucia, and P. Helminger, 1984, J. Mol. Spect. **105**, 139, and upon 720 ground state combination differences derived from the ν_2 data of G. Guelachvili, 1983, J. Opt. Soc. Am. **73**, 137. All of the submillimeter/microwave lines fit to within a 0.05-MHz RMS deviation, while the combination differences fit to within an RMS deviation of 0.00015 cm^{-1} (4 MHz). Because of the importance of this molecule in many applications, the upper frequency limit of the predicted lines has been extended to 10 THz (300 cm^{-1}). The dipole moment is from T. R. Dyke and J. S. Muenter, 1973, J. Chem. Phys. **59**, 3125. Other references are given in F. C. De Lucia, P. Helminger, and W. H. Kirchhoff, 1974, J. Phys. Chem. Ref. Data **3**, 211. 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 function includes contributions from the ν_2 state.

Species Tag:	18004	Species 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. De Lucia 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	Species Name:	H2O-v2
Version:	2		Water,
Date:	Mar. 1984		(010) bending state
Contributor:	H. M. Pickett		
Lines Listed:	292	Q(300.0)=	178.115
Freq. (GHz) <	9993	Q(225.0)=	116.011
Max. J:	10	Q(150.0)=	63.680
LOGSTR0=	-11.6	Q(75.00)=	23.169
LOGSTR1=	-12.2	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 =	1594.75	A=	993052
μ_b =	1.855	B=	440318.
μ_c =		C=	273710.

The rotational lines were determined by M. Herman, J. W. C. Johns, and A. R. W. McKellar, 1979, Can. J. Phys. **57**, 397, and H. Kuze, 1980, Astrophys. J. **239**, 1131. Additional combination differences were obtained from the data of G. Guelachvili, 1983, J. Opt. Soc. Am. **73**, 137. The partition function is the same as that used for the ground state.

Species Tag:	19001	Species Name:	HO-18
Version:	2		Hydroxyl radical,
Date:	May 1983		^{18}O isotope
Contributor:	H. M. Pickett		
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	Species 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	Species 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
μ_a =		A=	830283.294
μ_b =	1.8546	B=	435350.957
μ_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:	20001	Species Name:	D2O
Version:	2		
Date:	Dec. 1989		
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	Species 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
μ_a =	1.826526	A=	
μ_b =		B=	616365.
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 J. S. Muenter and W. Klemperer, 1970, J. Chem. Phys. **52**, 6033.

Species Tag:	20003	Species 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	Species Name:	HDO-18
Version:	1		Water HD^{18}O
Date:	Jan. 1991		
Contributor:	E. A. Cohen		

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	Species 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	Species Name:	CCH
Version:	1		CCH, $X^2\ \Sigma$ state
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:	26001	Species Name:	CN
Version:	1		Cyanide radical
Date:	Apr. 1983		
Contributor:	H. M. Pickett		

Lines Listed:	385	Q(300.0)=	663.896
Freq. (GHz) <	3493	Q(225.0)=	498.425
Max. J:	31	Q(150.0)=	332.889
LOGSTR0=	-5.0	Q(75.00)=	167.417
LOGSTR1=	-7.0	Q(37.50)=	84.723
Isotope Corr.:	0.	Q(18.75)=	43.411
Egy. (cm^{-1}) >	0.0	Q(9.375)=	22.798
μ_a =	3.0	A=	
μ_b =		B=	56693.46
μ_c =		C=	

The data and calculational method are from D. D. Skatrud *et al.*, 1983, J. Mol. Spect. **99**, 35.

Species Tag:	26002	Species Name:	CN-v1 Cyanide radical, v = 1 state
Version:	1		
Date:	Apr. 1983		
Contributor:	H. M. Pickett		

Lines Listed:	437	Q(300.0)=	663.896
Freq. (GHz) <	3460	Q(225.0)=	498.425
Max. J:	31	Q(150.0)=	332.889
LOGSTR0=	-9.3	Q(75.00)=	167.417
LOGSTR1=	-11.4	Q(37.50)=	84.723
Isotope Corr.:	0.	Q(18.75)=	43.411
Egy. (cm^{-1}) >	2068.7	Q(9.375)=	22.798
μ_a =	3.0	A=	
μ_b =		B=	56693.46
μ_c =		C=	

The data and calculational method are from D. D. Skatrud *et al.*, 1983, J. Mol. Spect. **99**, 35.

Species Tag:	27001	Species 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	Species Name:	HNC
Version:	1		Hydrogen isocyanide
Date:	Dec. 1977		
Contributor:	R. L. Poynter		
Lines Listed:	33	Q(300.0)=	138.229
Freq. (GHz) <	2978	Q(225.0)=	103.801
Max. J:	33	Q(150.0)=	69.295
LOGSTR0=	-2.5	Q(75.00)=	34.818
LOGSTR1=	-3.4	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 =	2.699	A=	
μ_b =		B=	45332.
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:	27003	Species 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:	28001	Species Name:	CO
Version:	2		Carbon monoxide
Date:	Jan. 1989		
Contributor:	H. M. Pickett		

Lines Listed:	91	Q(300.0)=	108.868
Freq. (GHz) <	9944	Q(225.0)=	81.715
Max. J:	91	Q(150.0)=	54.576
LOGSTR0=	-31.4	Q(75.00)=	27.454
LOGSTR1=	-34.5	Q(37.50)=	13.896
Isotope Corr.:	0.0	Q(18.75)=	7.122
Egy. (cm^{-1}) >	0.0	Q(9.375)=	3.744
μ_a =	0.1098	A=	
μ_b =		B=	57636.
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 J. S. Muenter, 1975, J. Mol. Spect. **55**, 490.

Species Tag:	28002	Species 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	Species Name:	HCN-15 Hydrogen cyanide, ^{15}N isotope
Version:	1		
Date:	Dec. 1979		
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	Species Name:	DCN Hydrogen cyanide, deuterium isotope
Version:	1		
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	Species Name:	HNC-13
Version:	1		Hydrogen isocyanide,
Date:	Dec. 1979		^{13}C isotope
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
μ_a =	2.699	A=	
μ_b =		B=	43545.61
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:	28006	Species 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	Species Name:	DNC
Version:	1		Hydrogen isocyanide,
Date:	Dec. 1979		deuterium isotope
Contributor:	R. L. Poynter		

Lines Listed:	39	Q(300.0)=	164.172
Freq. (GHz) <	2960	Q(225.0)=	123.254
Max. J:	39	Q(150.0)=	82.281
LOGSTR0=	-2.8	Q(75.00)=	41.305
LOGSTR1=	-4.0	Q(37.50)=	20.816
Isotope Corr.:	-3.824	Q(18.75)=	10.580
Egy. (cm^{-1}) >	0.0	Q(9.375)=	5.466
μ_a =	2.699	A=	
μ_b =		B=	38152.995
μ_c =		C=	

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

Species Tag:	29001	Species Name:	C-13-O
Version:	1		Carbon monoxide,
Date:	Dec. 1979		^{13}C isotope
Contributor:	R. L. Poynter		

Lines Listed:	27	Q(300.0)=	113.763
Freq. (GHz) <	2963	Q(225.0)=	85.448
Max. J:	27	Q(150.0)=	57.082
LOGSTR0=	-5.1	Q(75.00)=	28.701
LOGSTR1=	-5.5	Q(37.50)=	14.494
Isotope Corr.:	-1.955	Q(18.75)=	7.434
Egy. (cm^{-1}) >	0.0	Q(9.375)=	3.899
μ_a =	0.11	A=	
μ_b =		B=	55101.02
μ_c =		C=	

The experimental measurement was reported by B. Rosenblum, A. H. Nethercot, Jr., and C. H. Townes, 1958, Phys. Rev. **109**, 400. The dipole moment was measured by W. L. Meerts, F. H. De Leeuw, and A. Dymanus, 1977, Chem. Phys. **22**, 319.

Species Tag:	29002	Species Name:	HCO+
Version:	2		Formyl radical cation
Date:	Jan. 1984		
Contributor:	R. L. Poynter		

Lines Listed:	33	Q(300.0)=	140.508
Freq. (GHz) <	2931	Q(225.0)=	105.512
Max. J:	33	Q(150.0)=	70.437
LOGSTR0=	-2.4	Q(75.00)=	35.383
LOGSTR1=	-3.2	Q(37.50)=	17.861
Isotope Corr.:	0.	Q(18.75)=	9.101
Egy. (cm^{-1}) >	0.0	Q(9.375)=	4.729
μ_a =	3.30	A=	
μ_b =		B=	44594.419
μ_c =		C=	

The observed 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**, 219. The dipole moment was estimated theoretically by Woods *et al.*, above.

Species Tag:	29003	Species 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
$\mu_a =$	1.325	A=	196211.045
$\mu_b =$	1.530	B=	34532.395
$\mu_c =$		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	Species Name:	HCO
Version:	1		Formyl radical
Date:	June 1983		
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
$\mu_a =$	1.3626	A=	7829365.
$\mu_b =$	0.700	B=	44788.
$\mu_c =$	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	Species Name:	NNH+
Version:	1		
Date:	Jan. 1984		
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:	30001	Species Name:	CO-18
Version:	1		Carbon monoxide,
Date:	Dec. 1979		^{18}O isotope
Contributor:	R. L. Poynter		

Lines Listed:	27	Q(300.0)=	114.209
Freq. (GHz) <	2952	Q(225.0)=	85.783
Max. J:	27	Q(150.0)=	57.293
LOGSTR0=	-5.1	Q(75.00)=	28.807
LOGSTR1=	-5.5	Q(37.50)=	14.575
Isotope Corr.:	-2.690	Q(18.75)=	7.461
Egy. (cm^{-1}) >	0.0	Q(9.375)=	3.912
μ_a =	0.11	A=	
μ_b =		B=	54891.425
μ_c =		C=	

The experimental measurement was reported by B. Rosenblum, A. H., Nethercot, Jr., and C. H. Townes, 1958, Phys. Rev. **109**, 400. The dipole moment was reported by W. L. Meerts, F. H. De Leeuw, and A. Dymanus, 1977, Chem. Phys. **22**, 319.

Species Tag:	30002	Species Name:	HC-13-O+ Formyl radical cation, ^{13}C isotope
Version:	2		
Date:	Dec. 1983		
Contributor:	R. L. Poynter		
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	Species Name:	DCO+ Formyl radical cation, deuterium isotope
Version:	2		
Date:	Dec. 1983		
Contributor:	R. L. Poynter		

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	Species Name:	H2CO
Version:	1		Formaldehyde
Date:	Jan. 1980		
Contributor:	R. L. Poynter		

Lines Listed:	611	Q(300.0)=	2876.736
Freq. (GHz) <	2980	Q(225.0)=	1868.099
Max. J:	37	Q(150.0)=	1019.765
LOGSTR0=	-19.6	Q(75.00)=	361.743
LOGSTR1=	-7.2	Q(37.50)=	128.647
Isotope Corr.:	0.	Q(18.75)=	44.679
Egy. (cm^{-1}) >	0.0	Q(9.375)=	13.801
μ_a =	2.331	A=	281925.97
μ_b =		B=	38836.582
μ_c =		C=	34001.673

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

J. K. Bragg and A. H. Sharbaugh, 1949, Phys. Rev. **75**, 1774.

J. S. Chardon and D. Guichon, 1977, J. Phys. Paris **38**, 113, and 1975, J. Phys. Paris **34**, 791.

F. Y. Chu, S. M. Freund, J. W. C. Johns, and T. Oka, 1973, J. Mol. Spect. **48**, 328.

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.

A. F. Krupnov, L. I. Gershtein, V. G. Shustrov, and V. V. Polyakov, 1970, Opt. Spectrosc. (USSR) **28**, 257.

R. B. Lawrence and M. W. P. Strandberg, 1949, Phys. Rev. **75**, 1774.

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.

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

Species Tag:	30005	Species 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	Species 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	Species Name:	CH2ND Methylenimine, deuterium isotope on nitrogen atom
Version:	1		
Date:	Feb. 1981		
Contributor:	R. L. Poynter		
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	Species Name:	NO
Version:	1		Nitric oxide,
Date:	Feb. 1980		$^2\Pi$ ground 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	Species Name:	NND+
Version:	1		
Date:	Jan. 1984		
Contributor:	R. L. Poynter		

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:	31001	Species Name:	HCO-18+
Version:	2		Formyl radical cation,
Date:	Dec. 1983		^{18}O isotope
Contributor:	R. L. Poynter		

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	Species Name:	H2C-13-O Formaldehyde, ^{13}C isotope
Version:	1		
Date:	Jan. 1980		
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:	32001	Species Name:	O2 Molecular oxygen, $^{16}O_2$ v=0 state of the ground $^3\Sigma_g^-$ electronic state
Version:	3		
Date:	June 1989		
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	Species Name:	O2-v1
Version:	4		O_2 v=1 state
Date:	Dec. 1983		$^3\Sigma_g^-$
Contributor:	H. M. Pickett		electronic state

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	Species 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	Species 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. $(\text{cm}^{-1}) >$	0.0	Q(9.375)=	14.441
$\mu_a =$	-2.331	A=	281993.0
$\mu_b =$		B=	36903.6
$\mu_c =$		C=	32514.7

The experimental measurement 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	Species Name:	O2-snglt-dlta Oxygen molecule, metastable $a\ ^1\Delta_g$ state
Version:	1		
Date:	Sept. 1985		
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. Spect. **109**, 205.

Species Tag:	33001	Species Name:	HO2
Version:	2		Hydroperoxyl radical
Date:	May 1983		
Contributor:	H. M. Pickett		
Lines Listed:	19447	Q(300.0)=	4345.103
Freq. (GHz) <	9997	Q(225.0)=	2837.919
Max. J:	41	Q(150.0)=	1547.035
LOGSTR0=	-8.0	Q(75.00)=	548.403
LOGSTR1=	-8.0	Q(37.50)=	195.164
Isotope Corr.:	0	Q(18.75)=	70.210
Egy. (cm^{-1}) >	0.0	Q(9.375)=	27.593
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; and S. Saito, 1977, J. Mol. Spect. **65**, 229. The spectrum was computed using a full diagonalization of the spin-rotation Hamiltonian.

Species Tag:	33002	Species 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:	34001	Species Name:	O-18-O Molecular oxygen, single substituted ^{18}O isotope
Version:	2		
Date:	Oct. 1980		
Contributor:	H. M. Pickett		

Lines Listed:	383	Q(300.0)=	462.275
Freq. (GHz) <	2951	Q(225.0)=	346.976
Max. J:	61	Q(150.0)=	231.686
LOGSTR0=	-31.3	Q(75.00)=	116.439
LOGSTR1=	-17.6	Q(37.50)=	58.911
Isotope Corr.:	-2.389	Q(18.75)=	30.255
Egy. (cm^{-1}) >	-0.6	Q(9.375)=	16.121
μ_a =	magnetic	A=	
μ_b =		B=	40708.
μ_c =		C=	

The measurements and calculational method are from T. Amano and E. Hirota, 1974, J. Mol. Spect. **53**, 346. 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. The measured line at 233 GHz from W. Steinbach and W. Gordy, 1975, Phys. Rev. **A11**, 729, has been included in the catalog.

Species Tag:	34002	Species Name:	H2S
Version:	2		Hydrogen sulfide
Date:	July 1980		
Contributor:	R. L. Poynter		

Lines Listed:	311	Q(300.0)=	514.162
Freq. (GHz) <	2993	Q(225.0)=	333.964
Max. J:	15	Q(150.0)=	182.180
LOGSTR0=	-7.8	Q(75.00)=	65.524
LOGSTR1=	-9.2	Q(37.50)=	23.867
Isotope Corr.:	-0.022	Q(18.75)=	8.700
Egy. (cm^{-1}) >	0.0	Q(9.375)=	2.911
μ_a =		A=	310182.24
μ_b =	0.974	B=	270884.05
μ_c =		C=	141705.88

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. **41**, 333. The measurements were taken 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. The dipole moment was reported by C. Huiszoon and A. Dymanus, 1965, Physica **31**, 1049.

Species Tag:	34003	Species 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	Species Name:	H2O2
Version:	3		Hydrogen peroxide,
Date:	June 1989		first 3 torsinal states
Contributor:	H. M. Pickett		

Lines Listed:	8831	Q(300.0)=	9803.926
Freq. (GHz) <	9999	Q(225.0)=	5775.639
Max. J:	40	Q(150.0)=	2814.491
LOGSTR0=	-7.9	Q(75.00)=	895.159
LOGSTR1=	-8.0	Q(37.50)=	288.935
Isotope Corr.:	0.0	Q(18.75)=	88.859
Egy. (cm^{-1}) >	0.0	Q(9.375)=	26.681
μ_a =		A=	301878.
μ_b =		B=	26211.9
μ_c =	1.5728	C=	25099.14

The spectral lines and method of calculation are from P. Helminger, W. C. Bowman and F. C. De Lucia, 1981, J. Mol. Spect. **85**, 120, and W. Bowman, private communication. Additional lines and the dipole moment were measured by E. A. Cohen and H. M. Pickett, 1981, J. Mol. Spect. **87**, 582. Infrared combination differences from W. B. Olsen *et al.*, 1988, J. Mol. Spect. **127**, 12, were also used in the fit. The quantum number designation is v = 0 for τ = 1, 2 (n = 0), v = 1 for τ = 3, 4 (n = 0), and v = 2 for τ = 1, 2 (n = 1).

Species Tag: 35001
Version: 1
Date: Jan. 1980
Contributor: R. L. Poynter

Species Name: HDS
Hydrogen sulfide,
deuterium isotope

Lines Listed: 1138
Freq. (GHz) < 2998
Max. J: 20
LOGSTR0= -11.3
LOGSTR1= -9.3
Isotope Corr.: -3.523
Egy. (cm^{-1}) > 0.0
μ_a = 0.470
μ_b = 0.974
μ_c =

Q(300.0)= 430.923
Q(225.0)= 280.931
Q(150.0)= 153.426
Q(75.00)= 54.752
Q(37.50)= 19.756
Q(18.75)= 7.291
Q(9.375)= 2.829
A= 292351.302
B= 147861.801
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	Species 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	Species Name:	DCl
Version:	1		
Date:	Dec. 1990		
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
$\mu_a =$		A=	
$\mu_b =$	1.9044	B=	163356.2
$\mu_c =$		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:	38001	Species Name:	HCl-37
Version:	2		Hydrochloric acid
Date:	Jan. 1989		
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	Species Name:	C3H2
Version:	1		Cyclopropenylidene
Date:	Aug. 1987		
Contributor:	R. L. Poynter		

Lines Listed:	8916	Q(300.0)=	12240.524
Freq. (GHz) <	7630	Q(225.0)=	8152.671
Max. J:	35	Q(150.0)=	4498.834
LOGSTR0=	-10.0	Q(75.00)=	1597.718
LOGSTR1=	-10.0	Q(37.50)=	566.892
Isotope Corr.:	0.0	Q(18.75)=	201.837
Egy. (cm^{-1}) >	0.0	Q(9.375)=	72.410
μ_a =		A=	35092.8092(13)
μ_b =	3.4	B=	32212.5939(13)
μ_c =		C=	16749.0904(12)

The measured lines were taken from M. Bogey *et al.*, 1986, Chem. Phys. Lett. **125**, 383, and P. Thaddeus *et al.*, 1985, Astrophys. J. Lett. Ed. **299**, L63. The dipole moment was taken from T. J. Lee *et al.*, 1985, J. Am. Chem. Soc. **107**, 137.

Species Tag:	39001	Species Name:	C-13-3H2a Cyclopropenylidene, ^{13}C isotope off axis
Version:	1		
Date:	Aug. 1987		
Contributor:	R. L. Poynter		

Lines Listed:	2088	Q(300.0)=	5472.679
Freq. (GHz) <	2327	Q(225.0)=	3889.556
Max. J:	25	Q(150.0)=	2258.396
LOGSTR0=	-5.6	Q(75.00)=	819.974
LOGSTR1=	-5.0	Q(37.50)=	291.206
Isotope Corr.:	0.0	Q(18.75)=	103.681
Egy. (cm^{-1}) >	0.0	Q(9.375)=	37.179
μ_a =		A=	34857.3785(38)
μ_b =	3.4	B=	31288.2404(38)
μ_c =		C=	16443.0847(50)

The measured lines were taken from M. Bogey *et al.*, 1987, J. Mol. Spect. **122**, 313. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	39002	Species Name:	C-13-3H2s
Version:	1		Cyclopropenylidene,
Date:	Aug. 1987		^{13}C isotope on axis
Contributor:	R. L. Poynter		
Lines Listed:	1781	Q(300.0)=	10013.822
Freq. (GHz) <	2171	Q(225.0)=	7242.692
Max. J:	25	Q(150.0)=	4337.107
LOGSTR0=	-5.3	Q(75.00)=	1642.480
LOGSTR1=	-5.0	Q(37.50)=	588.979
Isotope Corr.:	0.0	Q(18.75)=	209.749
Egy. (cm^{-1}) >	0.0	Q(9.375)=	75.197
μ_a =		A=	33311.2856(76)
μ_b =	3.4	B=	32211.7753(76)
μ_c =		C=	16331.3254(53)

The measured lines were taken from M. Bogey *et al.*, 1987, J. Mol. Spect. **122**, 313. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	39003	Species Name:	C3HD
Version:	1		Mono-deutero
Date:	Aug. 1987		cyclopropenylidene
Contributor:	R. L. Poynter		
Lines Listed:	2178	Q(300.0)=	5791.619
Freq. (GHz) <	3191	Q(225.0)=	4190.829
Max. J:	25	Q(150.0)=	2489.431
LOGSTR0=	-7.0	Q(75.00)=	922.996
LOGSTR1=	-5.0	Q(37.50)=	328.700
Isotope Corr.:	-3.523	Q(18.75)=	116.977
Egy. (cm^{-1}) >	0.0	Q(9.375)=	41.899
μ_a =		A=	34517.5806(16)
μ_b =	3.4	B=	26965.7824(15)
μ_c =		C=	15098.7146(13)

The measured lines were taken from M. Bogey *et al.*, 1987, J. Mol. Spect. **122,** 313. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	39004	Species Name:	DCl-37
Version:	1		
Date:	Dec. 1990		
Contributor:	H. M. Pickett		

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 =		A=	
μ_b =	1.91003	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	Species 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
$\mu_a =$	0.75	A=	158590.
$\mu_b =$		B=	8545.86
$\mu_c =$		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 moment 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	Species Name:	NaOH
Version:	1		
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 =		A=	
μ_b =	1.0	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. Molect. Struc. **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:	41001	Species Name:	CH3CN
Version:	1		Acetonitrile
Date:	Dec. 1979		
Contributor:	R. L. Poynter		

Lines Listed:	1441	Q(300.0)=	15146.080
Freq. (GHz) <	1500	Q(225.0)=	9842.375
Max. J:	82	Q(150.0)=	5360.433
LOGSTR0=	-6.7	Q(75.00)=	1896.269
LOGSTR1=	-5.9	Q(37.50)=	673.132
Isotope Corr.:	0.	Q(18.75)=	246.320
Egy. (cm^{-1}) >	0.0	Q(9.375)=	96.095
μ_a =	3.919	A=	158290.
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.

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

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

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	Species Name:	CH3C-13-CH
Version:	1		Propyne,
Date:	Dec. 1979		^{13}C isotope
Contributor:	R. L. Poynter		on atom 2
	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	Species 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
$\mu_a =$	0.750	A=	158590.
$\mu_b =$		B=	8313.24
$\mu_c =$		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	Species Name:	CH3CCD Propyne, D isotope on on atom 1
Version:	2		
Date:	Jan. 1984		
Contributor:	R. L. Poynter		

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	Species 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:	42001	Species Name:	CH3CN-15
Version:	1		Acetonitrile,
Date:	Dec. 1979		^{15}N isotope
Contributor:	R. L. Poynter		

Lines Listed:	2755	Q(300.0)=	5226.368
Freq. (GHz) <	1753	Q(225.0)=	3394.690
Max. J:	99	Q(150.0)=	1847.566
LOGSTR0=	-26.4	Q(75.00)=	653.732
LOGSTR1=	-27.3	Q(37.50)=	232.060
Isotope Corr.:	-2.432	Q(18.75)=	84.859
Egy. (cm^{-1}) >	0.0	Q(9.375)=	33.083
μ_a =		A=	158290.
μ_b =	3.919	B=	9198.8993
μ_c =		C=	

The experimental measurements were obtained from A. Bauer and S. Maes, 1969, J. Phys. (Paris) **30**, 169, and J. Demaison, A. Dubrulle, D. Boucher, and J. Burie, 1969, J. Mol. Spect. **76**, 1. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	42002	Species 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	Species 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-Universität 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:	43001	Species Name:	CHDCO
Version:	1		Ketene,
Date:	Jan. 1980		mono deuterium isotope
Contributor:	R. L. Poynter		

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	Species 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	Species Name:	AlO
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:	44001	Species 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
μ_a =		A=	
μ_b =	1.957	B=	24495.562
μ_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	Species 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. Torring, 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	Species Name:	CH3CHO-a Acetaldehyde ground vibrational state, A species
Version:	1		
Date:	Jan. 1980		
Contributor:	R. L. Poynter		
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	Species 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	Species Name:	CH3CHO-e
Version:	1		Acetaldehyde
Date:	Dec. 1980		ground vibrational 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	Species 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	Species 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
μ_a =	1.602	A=	903185.4(14.6)
μ_b =	1.350	B=	10737.8252(58)
μ_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	Species 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	Species 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:	45001	Species Name:	C-13-S
Version:	2		Carbon monosulfide, ^{13}C isotope
Date:	Jan. 1984		
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	Species 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. Torring, 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	Species Name:	NH2CHO
Version:	2		NH_2CHO, 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	Species Name:	HCS+ Thioformyl radical cation
Version:	1		
Date:	Jan. 1990		
Contributor:	R. L. Poynter		
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	Species Name:	HNCO-18 Isocyanic acid, ^{18}O isotope
Version:	1		
Date:	Sept. 1988		
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	Species 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	Species 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:	46001	Species Name:	CS-34 Monosulfide, ^{34}S isotope
Version:	2		
Date:	Jan. 1984		
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	Species Name:	Si-30-O Silicon monoxide, ^{30}Si isotope
Version:	1		
Date:	Dec. 1979		
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. Torring, 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	Species 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
μ_a =	1.649	A=	291291.641
μ_b =		B=	17699.628
μ_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	Species Name:	C2H5OH
Version:	1		Ethyl alcohol,
Date:	Jan. 1980		ground *trans* state
Contributor:	R. L. Poynter		

Lines Listed:	1236	Q(300.0)=	17009.832
Freq. (GHz) <	1837	Q(225.0)=	11048.419
Max. J:	20	Q(150.0)=	6013.121
LOGSTR0=	-9.4	Q(75.00)=	2020.226
LOGSTR1=	-7.5	Q(37.50)=	747.653
Isotope Corr.:	0.	Q(18.75)=	267.547
Egy. (cm^{-1}) >	0.0	Q(9.375)=	95.236
μ_a =	0.046	A=	34891.75
μ_b =	1.438	B=	9350.635
μ_c =		C=	8135.236

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.

Additional measurements were made by E. A. Cohen, 1979, private communication. The dipole moment was reported by Takano *et al.*, above.

Species Tag:	46005	Species Name:	HCOOH Formic acid, ground *trans* state
Version:	1		
Date:	Jan. 1980		
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 [μ_a = 1.4214(21)D and μ_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	Species Name:	NO2
Version:	2		NO_2,
Date:	Jan. 1991		Nitrogen dioxide
Contributor:	H. M. Pickett		

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	Species 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:	47001	Species Name:	H2C-13-s Thioformaldehyde, ^{13}C isotope
Version:	1		
Date:	Jan. 1980		
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	Species 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	Species Name:	DCOOH
Version:	1		Formic acid,
Date:	Jan. 1980		deuterium isotope
Contributor:	R. L. Poynter		on C atom

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	Species 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:	48001	Species Name:	SO
Version:	1		$^3\Sigma$ ground state
Date:	Dec. 1979		
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	Species Name:	SO-v1
Version:	1		$^3\Sigma$ ground state,
Date:	Dec. 1979		v=1 vibrational state
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 v=0 (G. Herzberg, 1950, Spectra of Diatomic Molecules, Van Nostrands, New York).

Species Tag:	48003	Species 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	Species Name:	O3 Ozone, ground vibrational state
Version:	3		
Date:	May 1990		
Contributor:	H. M. Pickett		

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	Species 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	Species 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	Species 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	Species Name:	O3-v1,3+v2 Coriolis coupled states $\nu_1 + \nu_2$ and $\nu_2 + \nu_3$ or (110) and (011)
Version:	1		
Date:	Nov. 1990		
Contributor:	E. A. Cohen		
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:	49001	Species Name:	O3-sym-O-17
Version:	1		Ozone,
Date:	Mar. 1984		symmetric ^{17}O substitution
Contributor:	H. M. Pickett		

Lines Listed:	13267	Q(300.0)=	19116.141
Freq. (GHz) <	4168	Q(225.0)=	13037.672
Max. J:	42	Q(150.0)=	7299.617
LOGSTR0=	-7.8	Q(75.00)=	2597.168
LOGSTR1=	-7.2	Q(37.50)=	920.450
Isotope Corr.:	-3.432	Q(18.75)=	326.964
Egy. (cm^{-1}) >	0.0	Q(9.375)=	116.762
μ_a =		A=	102351.
μ_b =	0.5324	B=	13350.8
μ_c =		C=	11781.9

The spectra and calculation are from E. A. Cohen and H. M. Pickett, 1983, J. Mol. Struc. **97**, 97–100. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	49002	Species Name:	O3-asym-O-17 Ozone, asymmetric ^{17}O substitution
Version:	1		
Date:	Mar. 1984		
Contributor:	H. M. Pickett		
Lines Listed:	24138	Q(300.0)=	40541.531
Freq. (GHz) <	9971	Q(225.0)=	27327.520
Max. J:	37	Q(150.0)=	14832.003
LOGSTR0=	-9.7	Q(75.00)=	5256.541
LOGSTR1=	-9.4	Q(37.50)=	1862.516
Isotope Corr.:	-3.131	Q(18.75)=	661.607
Egy. (cm^{-1}) >	0.0	Q(9.375)=	236.211
μ_a =	0.0034	A=	105491.
μ_b =	0.5324	B=	12951.
μ_c =		C=	1508.

The spectra and calculation are from E. A. Cohen and H. M. Pickett, 1983, J. Mol. Struc. **97**, 97–100. Additional lines have been measured by E. A. Cohen and K. Hillig (unpublished data). The calculation includes quadrupole interactions of $\Delta N = 0, \pm 1, \pm 2$. The dipole moments are assumed values based on the structure and the value for the parent species.

Species Tag:	50001	Species Name:	S-34-O
Version:	1		$^3\Sigma$ ground state,
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	Species Name:	SO-18
Version:	1		$^3\Sigma$ ground state,
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	Species 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	Species 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	Species Name:	O3-s-O18-v2
Version:	1		ν_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)=	2445.119
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	Species 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)=	4994.591
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	Species Name:	CH3Cl-35
Version:	1		
Date:	Mar. 1989		
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:	51001	Species Name:	HCCCN
Version:	2		Cyanoacetylene
Date:	Mar. 1984		
Contributor:	R. L. Poynter		

Lines Listed:	154	Q(300.0)=	4122.874
Freq. (GHz) <	899	Q(225.0)=	3093.144
Max. J:	99	Q(150.0)=	2062.529
LOGSTR0=	-6.6	Q(75.00)=	1031.573
LOGSTR1=	-4.2	Q(37.50)=	516.416
Isotope Corr.:	0.	Q(18.75)=	258.643
Egy. (cm^{-1}) >	0.0	Q(9.375)=	129.837
μ_a =	3.724	A=	
μ_b =		B=	4549.059
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.

Species Tag:	51002	Species Name:	ClO
Version:	3		Chlorine monoxide,
Date:	Jan. 1991		$^2\Pi$ 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	Species Name:	ClO-v1
Version:	1		Chlorine monoxide,
Date:	Jan. 1991		$^2\Pi$ 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:	52001	Species Name:	HCCC-13-N Cyanoacetylene, ^{13}C isotope on atom 1
Version:	1		
Date:	Dec. 1979		
Contributor:	R. L. Poynter		

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=	
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	Species 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	Species Name:	HC-13-CCN Cyanoacetylene, ^{13}C isotope on atom 3
Version:	1		
Date:	Dec. 1979		
Contributor:	R. L. Poynter		
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	Species 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	Species Name:	DCCCN Cyanoacetylene, deuterium isotope
Version:	1		
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	Species 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 in the calculation is 20.

Species Tag:	52007	Species Name:	SiCC
Version:	1		Silicon dicarbide
Date:	Jan. 1990		
Contributor:	R. L. Poynter		
Lines Listed:	224	Q(300.0)=	2638.761
Freq. (GHz) <	477	Q(225.0)=	2120.801
Max. J:	20	Q(150.0)=	1454.789
LOGSTR0=	-9.6	Q(75.00)=	633.286
LOGSTR1=	-3.6	Q(37.50)=	234.423
Isotope Corr.:	0.0	Q(18.75)=	83.426
Egy. (cm^{-1}) >	0.0	Q(9.375)=	29.771
μ_a =	3.2	A=	52409.(182)
μ_b =		B=	13156.5(3)
μ_c =		C=	10447.0(3)

The line measurements were taken from P. Thaddeus *et al.*, 1984, Astrophys. J. Lett. Ed. **283**, L45, and L. E. Snyder *et al.*, 1985, Astrophys. J. Lett. Ed. **290**, L29. The dipole moment was estimated by S. Green, as quoted by Thaddeus *et al.* from an *ab initio* calculation.

Species Tag:	52008	Species Name:	CCCO
Version:	1		Tricarbon monoxide
Date:	Jan. 1990		
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	Species Name:	CH3Cl-37
Version:	1		
Date:	Mar. 1989		
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=	

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	Species 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 make 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	Species 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 make 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:	53001	Species Name:	C2H3CN
Version:	1		Acrylonitrile
Date:	Jan. 1980		
Contributor:	R. L. Poynter		

Lines Listed:	3697	Q(300.0)=	26199.932
Freq. (GHz) <	2616	Q(225.0)=	17017.658
Max. J:	35	Q(150.0)=	9261.899
LOGSTR0=	-8.8	Q(75.00)=	3243.396
LOGSTR1=	-8.0	Q(37.50)=	1159.845
Isotope Corr.:	0	Q(18.75)=	410.960
Egy. (cm^{-1}) >	0.0	Q(9.375)=	145.814
μ_a =	3.68	A=	49850.712
μ_b =	1.25	B=	4971.0849
μ_c =		C=	4513.8005

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**, 777.

M. C. L. Gerry and G. Winnewisser, 1973, J. Mol. Spect. **48**, 1.

M. C. L. Gerry, K. Yamada, and G. Winnewisser, 1979, J. Phys. Chem. Ref. Data **8**, 107.

The dipole moment was measured by W. W. Wilcox, J. H. Goldstein, and J. W. Simmons, 1954, J. Chem. Phys. **22**, 516.

Species Tag:	53002	Species Name:	Cl-37-O
Version:	3		Chlorine monoxide,
Date:	Jan. 1991		$^2\Pi$ 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	Species Name:	C-13-CCO
Version:	1		Tricarbon monoxide,
Date:	Jan. 1990		^{13}C isotope
Contributor:	R. L. Poynter		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 =		A=	
μ_b =	2.391	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	Species Name:	CC-13-CO
Version:	1		Tricarbon monoxide,
Date:	Jan. 1990		^{13}C isotope
Contributor:	R. L. Poynter		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 =		A=	
μ_b =	2.391	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	Species Name:	CCC-13-O
Version:	1		Tricarbon monoxide,
Date:	Jan. 1990		^{13}C isotope
Contributor:	R. L. Poynter		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 =		A=	
μ_b =	2.391	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	Species Name:	Cl-37-O-v1
Version:	1		Chlorine monoxide,
Date:	Jan. 1991		$^2\Pi$ 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:	54001	Species 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 methods used on this species were the same as for the parent species, given in tag no. 53001. 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	Species Name:	CH2C-13-HCN Acrylonitrile, ^{13}C iostope on atom 2
Version:	1		
Date:	Jan. 1980		
Contributor:	R. L. Poynter		

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 methods used on this species were the same as for the parent species, given in tag no. 53001. 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	Species 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 methods used on this species were the same as for the parent species, given in tag no. 53001. 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	Species Name:	CH2CDCN Acrylonitrile, deuterium isotope on atom 2
Version:	1		
Date:	Jan. 1980		
Contributor:	R. L. Poynter		
Lines Listed:	322	Q(300.0)=	29696.148
Freq. (GHz) <	769	Q(225.0)=	19288.559
Max. J:	10	Q(150.0)=	10500.263
LOGSTR0=	-9.1	Q(75.00)=	3711.933
LOGSTR1=	-6.5	Q(37.50)=	1312.502
Isotope Corr.:	-3.824	Q(18.75)=	402.161
Egy. (cm^{-1}) >	0.0	Q(9.375)=	155.453
μ_a =	3.68	A=	40198.6
μ_b =	1.25	B=	4934.35
μ_c =		C=	4388.41

The methods used on this species were the same as for the parent species, given in tag no. 53001. 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:	54005	Species 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	Species Name:	CCCO-18 Tricarbon monoxide, ^{18}O atom
Version:	1		
Date:	Jan. 1990		
Contributor:	R. L. Poynter		
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 =		A=	
μ_b =	2.391	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:	55001	Species Name:	C2H5CN
Version:	2		Ethyl cyanide
Date:	Jan. 1981		
Contributor:	R. L. Poynter		
Lines Listed:	3684	Q(300.0)=	111840.781
Freq. (GHz) <	1122	Q(225.0)=	70892.414
Max. J:	21	Q(150.0)=	39554.867
LOGSTR0=	-9.0	Q(75.00)=	12589.251
LOGSTR1=	-8.2	Q(37.50)=	4595.154
Isotope Corr.:	0	Q(18.75)=	1406.371
Egy. (cm^{-1}) >	0.0	Q(9.375)=	650.878
μ_a =	3.85	A=	27663.66
μ_b =	1.23	B=	4714.144
μ_c =		C=	4235.041

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.

H. Mader, H. M. Heise, and H. Dreizler, 1973, Z. Naturforsch. **29a**, 164.

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

Species Tag:	56001	Species 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 moment was assumed to be the same as for the parent species.

Species Tag:	56002	Species Name:	CH3C-13-H2CN ^{13}C isotope on atom 2
Version:	2		
Date:	Jan. 1981		
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 was assumed to be the same as for the parent species, tag no. 55001.

Species Tag:	56003	Species 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
μ_a =	3.84	A=	27342.174
μ_b =	1.37	B=	4597.939
μ_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 moment was assumed to be the same as for the parent species, tag no. 55001.

Species Tag:	56004	Species 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
μ_a =	3.84	A=	27541.953
μ_b =	1.37	B=	4574.771
μ_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. Mader, and H. Dreizler, 1976, Z. Naturforsch. **31a**, 1228. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	56005	Species Name:	CH2DCH2CN-s Ethyl cyanide, deuterium isotope on methyl carbon *trans* to CN group
Version:	2		
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. Mader, H. M. Heise, and H. Dreizler, 1973, Z. Naturforsch. **29a**, 164. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	56006	Species Name:	CH2DCH2CN-a Ethyl cyanide, deuterium isotope on methyl carbon *gauche* to the CN group
Version:	2		
Date:	Jan. 1981		
Contributor:	R. L. Poynter		
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. Mader, N. M. Heise, and H. Dreizler, 1973, Z. Naturforsch. **29a**, 164. The dipole moment was assumed to be the same as for the parent species.

Species Tag:	60001	Species 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	Species 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
μ_a =	1.730	A=	
μ_b =		B=	9077.45
μ_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. Torring, 1969, Z. Naturforsch. **24a**, 1422.

Species Tag:	61001	Species 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	Species 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:	62001	Species 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	Species 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	Species 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
μ_a =	1.730	A=	
μ_b =		B=	8755.33
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:	62004	Species 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:	63001	Species 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
μ_a =	1.986	A=	13010.9867
μ_b =	0.882	B=	12099.9025
μ_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	Species 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. (cm^{-1}) >	579.0	Q(9.375)=	155.812
μ_a =	1.986	A=	13028.93
μ_b =	0.882	B=	12098.63
μ_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	Species 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
$\mu_a =$	1.986	A=	12999.00
$\mu_b =$	0.882	B=	12015.11
$\mu_c =$		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	Species 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. (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	Species Name:	HNO3-v8 Nitric acid, $\nu_8 = 1$ state
Version:	1		
Date:	Aug. 1990		
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. (cm^{-1}) >	763.2	Q(9.375)=	155.812
μ_a =	1.986	A=	12998.04
μ_b =	0.882	B=	12005.51
μ_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	Species 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:	64001	Species 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	Species Name:	SO2
Version:	3		Sulfur dioxide
Date:	Jan. 1987		
Contributor:	E. A. Cohen		

Lines Listed:	10654	Q(300.0)=	5916.978
Freq. (GHz) <	7682	Q(225.0)=	3841.493
Max. J:	75	Q(150.0)=	2090.258
LOGSTR0=	-9.5	Q(75.00)=	738.924
LOGSTR1=	-10.0	Q(37.50)=	261.638
Isotope Corr.:	-0.022	Q(18.75)=	92.832
Egy. (cm^{-1}) >	0.0	Q(9.375)=	33.067
μ_a =		A=	60778.55
μ_b =	1.633	B=	10318.073
μ_c =		C=	8799.703

These measurements are based on fits to the data of P. A. Helminger and F. C. De Lucia, 1985, J. Mol. Spect. **111**, 66; the data of M. Carlotti *et al.*, 1984, J. Mol. Spect. **106**, 235; and the compilation of F. J. Lovas, 1985, J. Phys. Chem. Ref. Data **14**, 395. In addition, unpublished far-infrared laser sideband measurements made at JPL have been included for transitions with $K_a \leq 28$. The dipole moment is from D. Patel *et al.*, 1979, J. Chem. Phys. **70**, 1979.

Species Tag:	66001	Species 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:	67001	Species Name:	OCl-35-O
Version:	1		Chlorine dioxide,
Date:	Sept. 1988		^{35}Cl isotope
Contributor:	H. M. Pickett		
Lines Listed:	20815	Q(300.0)=	51689.211
Freq. (GHz) <	2730	Q(225.0)=	34395.371
Max. J:	52	Q(150.0)=	18888.602
LOGSTR0=	-7.9	Q(75.00)=	6683.440
LOGSTR1=	-6.0	Q(37.50)=	2365.375
Isotope Corr.:	-0.122	Q(18.75)=	839.073
Egy. (cm^{-1}) >	0.6	Q(9.375)=	298.813
μ_a =		A=	52081.26
μ_b =	1.784	B=	9952.67
μ_c =		C=	8334.16

The lines were obtained from M. Tandoura *et al.*, 1982, J. Mol. Spect. **95**, 157. The dipole moment is from W. M. Tolles *et al.*, 1962, J. Chem. Phys. **37**, 927. The Hamiltonian used included electronic and nuclear spin coupling terms with full diagonalization of the energy matrix.

Species Tag:	68001	Species Name:	CCCS
Version:	1		Tricarbon monosulfide
Date:	Aug. 1987		
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	Species Name:	OCl-37-O
Version:	1		Chlorine dioxide
Date:	Sept. 1989		
Contributor:	H. M. Pickett		

Lines Listed:	20799	Q(300.0)=	52420.
Freq. (GHz) <	2695	Q(225.0)=	34906.
Max. J:	52	Q(150.0)=	19173.
LOGSTR0=	-8.0	Q(75.00)=	6784.2
LOGSTR1=	-6.0	Q(37.50)=	2401.6
Isotope Corr.:	-0.611	Q(18.75)=	851.92
Egy. (cm^{-1}) >	0.6	Q(9.375)=	303.32
μ_a =		A=	50736.83
μ_b =	1.784	B=	9953.17
μ_c =		C=	8299.07

The lines were obtained from M. Tandoura *et al.*, 1982, J. Mol. Spect. **95**, 157. The dipole moment is from W. M. Tolles *et al.*, 1962, J. Chem. Phys. **37**, 927. The Hamiltonian used included electronic and nuclear spin coupling terms with full diagonalization of the energy matrix.

Species Tag:	70001	Species Name:	CCCS-34
Version:	1		Tricarbon monosulfide,
Date:	Aug. 1987		^{34}S atom
Contributor:	R. L. Poynter		
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:	75001	Species 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:	76001	Species 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	Species 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	Species 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	Species 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	Species 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	Species Name:	HCCCCCN-15 Cyanodiacetylene, ^{15}N isotope
Version:	1		
Date:	Dec. 1979		
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	Species 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
μ_a =	4.329	A=	
μ_b =		B=	1271.056
μ_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:	79001	Species 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
μ_a =	1.185	A=	11994.5
μ_b =	0.94	B=	4665.2
μ_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	Species Name:	HBr-79
Version:	1		Hydrogen bromide,
Date:	Feb. 1980		^{79}Br isotope
Contributor:	R. L. Poynter		
	H. M. Pickett		

Lines Listed:	19	Q(300.0)=	101.205
Freq. (GHz) <	2996	Q(225.0)=	73.350
Max. J:	6	Q(150.0)=	50.373
LOGSTR0=	-2.1	Q(75.00)=	26.351
LOGSTR1=	-2.9	Q(37.50)=	13.912
Isotope Corr.:	-2.96	Q(18.75)=	7.773
Egy. (cm^{-1}) >	0.0	Q(9.375)=	4.934
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. The dipole moment was also reported by these same authors in a later publication, and updated in F. A. Van Dijk and A. Dymanus, 1971, 26th Symposium on Molecular Structure and Spectroscopy, Columbus, Ohio, R12, p. 80.

Species Tag:	82001	Species Name:	HBr-81
Version:	1		Hydrogen bromide,
Date:	Feb. 1980		^{81}Br isotope
Contributor:	R. L. Poynter		
	H. M. Pickett		

Lines Listed:	19	Q(300.0)=	101.251
Freq. (GHz) <	2995	Q(225.0)=	73.367
Max. J:	6	Q(150.0)=	50.385
LOGSTR0=	-2.1	Q(75.00)=	26.357
LOGSTR1=	-2.9	Q(37.50)=	13.916
Isotope Corr.:	-0.306	Q(18.75)=	7.775
Egy. (cm^{-1}) >	0.0	Q(9.375)=	4.935
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. The dipole moment was also reported by these same authors in a later publication, and updated in F. A. Van Dijk and A. Dymanus, 1971, 26th Symposium on Molecular Structure and Spectroscopy, Columbus, Ohio, R12, p. 80.

Species Tag:	95001	Species Name:	Br-79-O
Version:	1		Bromine monoxide,
Date:	Feb. 1980		^{79}Br isotope,
Contributor:	H. M. Pickett		$^{2}\Pi_{3/2}$ state
Lines Listed:	850	Q(300.0)=	3897.625
Freq. (GHz) <	1287	Q(225.0)=	2938.327
Max. J:	51	Q(150.0)=	1965.170
LOGSTR0=	-9.0	Q(75.00)=	989.464
LOGSTR1=	-10.2	Q(37.50)=	501.996
Isotope Corr.:	-0.296	Q(18.75)=	259.537
Egy. (cm^{-1}) >	0.0	Q(9.375)=	136.804
μ_a =	1.765	A=	
μ_b =		B=	12830.4
μ_c =		C=	

Several measurements near 63 GHz are from F. X. Powell and D. R. Johnson, 1969, J. Chem. Phys. **50,** 4596. The remainder of the data are given by E. A. Cohen, H. M. Pickett, and M. Geller, 1981, J. Mol. Spect. **87,** 459.

Species Tag:	97001	Species Name:	Br-81-O
Version:	1		Bromine monoxide,
Date:	Feb. 1980		^{81}Br isotope,
Contributor:	H. M. Pickett		$^{2}\Pi_{3/2}$ state

Lines Listed:	850	Q(300.0)=	3913.813
Freq. (GHz) <	1281	Q(225.0)=	2950.529
Max. J:	51	Q(150.0)=	1973.332
LOGSTR0=	-9.0	Q(75.00)=	993.574
LOGSTR1=	-10.1	Q(37.50)=	503.965
Isotope Corr.:	-0.306	Q(18.75)=	259.298
Egy. (cm^{-1}) >	0.0	Q(9.375)=	137.246
μ_a =	1.794	A=	
μ_b =		B=	12777.08
μ_c =		C=	

Several measurements near 63 GHz are from F. X. Powell and D. R. Johnson, 1969, J. Chem. Phys. **50,** 4596. The remainder of the data are given by E. A. Cohen, H. M. Pickett, and M. Geller, 1981, J. Mol. Spect. **87**, 459.

Species Tag:	97002	Species Name:	Cl-35-NO3 Chlorine nitrate
Version:	1		
Date:	Mar. 1984		
Contributor:	H. M. Pickett		
Lines Listed:	4198	Q(300.0)=	100530.953
Freq. (GHz) <	829	Q(225.0)=	65298.008
Max. J:	60	Q(150.0)=	35546.746
LOGSTR0=	-7.4	Q(75.00)=	12566.078
LOGSTR1=	-5.9	Q(37.50)=	4447.335
Isotope Corr.:	-0.122	Q(18.75)=	1573.983
Egy. (cm^{-1}) >	3.0	Q(9.375)=	557.057
μ_a =	0.72	A=	12105.8
μ_b =	0.28	B=	2777.0
μ_c =		C=	2258.1

The frequency data and dipole moments are taken from R. D. Suenram and F. J. Lovas, 1977, J. Mol. Spect. **65**, 239. The chlorine hyperfine structure is omitted in this version of the catalog since the splittings are generally smaller than the width of stratospheric lines.

Species Tag:	98001	Species Name:	H2SO4
Version:	1		Sulfuric acid
Date:	Feb. 1991		
Contributor:	R. L. Poynter		

Lines Listed:	2359	Q(300.0)=	54980.468
Freq. (GHz) <	415	Q(225.0)=	41344.750
Max. J:	30	Q(150.0)=	27068.792
LOGSTR0=	-7.0	Q(75.00)=	12672.200
LOGSTR1=	-6.7	Q(37.50)=	5613.645
Isotope Corr.:	-0.022	Q(18.75)=	2292.303
Egy. (cm^{-1}) >	0.0	Q(9.375)=	859.007
μ_a =		A=	5160.581
μ_b =		B=	5024.599
μ_c =	2.725	C=	4881.080

The experimental frequency measurements and dipole moment were taken from R. L. Kuczkowski, R. D. Suenram, and F. J. Lovas, 1981, J. Am. Chem. Soc. **103**, 2561. The maximum J value was extended well beyond what would be taken as the usual cutoff from the available data. This extrapolation was employed to sketch out what lines might exist at the higher frequencies and absorb radiation in the Venus atmosphere. These lines show huge predicted errors and their frequencies will be grossly wrong. However, they will give an idea of the absorption that might be expected at these frequencies. Measurements are planned in the future to reduce these errors.

Species Tag:	99001	Species Name:	Cl-37-NO3
Version:	1		Chlorine nitrate
Date:	Mar. 1984		
Contributor:	H. M. Pickett		

Lines Listed:	4182	Q(300.0)=	103109.797
Freq. (GHz) <	810	Q(225.0)=	66973.047
Max. J:	60	Q(150.0)=	36450.195
LOGSTR0=	-7.5	Q(75.00)=	12888.428
LOGSTR1=	-5.9	Q(37.50)=	4560.368
Isotope Corr.:	-0.611	Q(18.75)=	1614.358
Egy. (cm^{-1}) >	2.4	Q(9.375)=	571.742
μ_a =	0.72	A=	12105.4
μ_b =	0.28	B=	2707.6
μ_c =		C=	2207.6

The frequency data and dipole moments are taken from R. D. Suenram and F. J. Lovas, 1977, J. Mol. Spect. **65**, 239. The chlorine hyperfine structure is omitted in this version of the catalog since the splittings are generally smaller than the width of stratospheric lines.

Species Tag:	102001	Species 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	Species 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.