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Submillimeter, Millimeter, and Microwave Spectral Line Catalogue

R.L. Poynter
H.M. Pickett

June 1, 1984

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National Aeronautics and
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ABSTRACT

This report describes a computer accessible catalogue of submillimeter, millimeter, and microwave spectral lines in the frequency range between 0 and 10000 GHz (i.e., wavelengths longer than 30 μm). The catalogue 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, lower state energy, and quantum number assignment.

The catalogue 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 catalogue will add more atoms and molecules and update the present listings (151 species) as new data appear.

The catalogue is available from the authors as a magnetic tape recorded in card images and as a set of microfiche records.

FOREWORD

This version of the Submillimeter Spectral Line Catalogue incorporates a number of changes: (1) quantum number format, (2) addition of a complete set of partition functions for each species, (3) a detailed description of the computer tape physical format, (4) a computer accessible directory of species, (5) a table of relative abundances of the isotopes under terrestrial conditions, (6) a table of the starting positions for each species on the tape, (7) a new format for the individual species descriptions, (8) eighteen new species, and (9) thirty revised species. The new and revised species are as follows:

New Species, Rev. 2 (18)

TAG	NAME
13002	CH
17004	NH3-V2
20001	D20
25001	CCH
26001	CN
26002	CN-V1
29004	HCO
29005	NNH+
30009	NND+
33001	H02
46006	N02
48007	03-2V2
49001	03-SYM-0-17
49002	03-ASYM-0-17
50005	03-S-018-V2
50006	03-A-018-V2
97002	CL-35-N03
99001	CL-37-N03

Revised Species, Rev. 2 (30)

TAG	NAME
16001	0-ATOM
17001	OH
17002	NH3
18001	OD
18003	H20
18005	H20-V2
19001	H0-18
19002	HD0
27001	HCN
29002	HCO+
30002	HC-13-0+
30003	DCO+
31001	HCO-18+
32001	02
32002	02-V1
34001	0-18-0
41005	CH3CCD
44001	CS
44002	SIO
45001	C-13-S
46001	CS-34
48004	03
48005	03-V2
48006	03-V1,3
50003	03-SYM-0-18
50004	03-ASYM-0-18
52006	HOCL
54005	HOCL-37
63001	HN03
64002	S02

For reference, the new and revised species listed in the previous version of this catalogue are given below:

New Species, Rev. 1 (9)

TAG	NAME
18004	NH2D
18005	H20-V2
34004	H202
44005	CH3CHO-E
48005	03-V2
48006	03-V1,3
52006	HOCL
54005	HOCL-37
63001	HN03

Revised Species, Rev. 1 (24)

TAG	NAME
17002	NH3
18002	N-15-H3
18003	H20
29003	CH2NH
30007	CH2ND
32001	02
32002	02-V1
32003	CH30H
34001	0-18-0
34002	H2S
34003	PH3
45003	NH2CHO
51002	CLO
53002	CL-37-0
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	0-18-CS

CONTENTS

I. Introduction

This report describes a computer accessible catalogue of submillimeter, millimeter, and microwave spectral lines in the frequency range between 0 and 10000 GHz (i.e. wavelengths longer than 30μm). The catalogue is intended to be used as a guide in the planning of spectral line observations and as a reference which can facilitate identification and analysis of observed spectral lines. The selection of lines for the catalogue is based on the projected needs of astronomers and atmospheric scientists.

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

The catalogue is available as a magnetic data tape recorded in card images, with one card image per spectral line. The authors will reproduce the catalogue onto a tape furnished by the user without charge on a limited basis. The format of the data is given in Section II. Section III 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 IV, while species specific comments are reserved for Section VI. Section V gives the format of quantum numbers as they appear in the catalogue. Documentation for each molecular or atomic species is listed in Section VI 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.

The catalogue is also available on microfiche in both a frequency and species ordered format. The fiche version is available without charge on a limited basis upon written request to the authors.

II. Format of Data Tape

The catalogue data tape is composed of 80 character card images, with one card image per spectral line. The format of each card image is given below:

```
FREQ  ,  ERR  ,  LGINT,  DR  ,  ELOW  ,  GUP,  TAG, QNFORM,  QN',  QN"

(F13.4,  F8.4 ,  F8.4 ,  I2  ,  F10.4 ,  I3 ,  I7 ,  I4   ,  6I2,  6I2,X)
```

FREQ: Frequency of the line in MHz.

ERR: Estimated or experimental error of FREQ in MHz.

LGINT: Base 10 logarithm of the integrated intensity in units of nm^2 MHz at 300 K. (See Section III for conversions to other units.)

DR: Degrees of freedom in the rotational partition function (0 for atoms, 2 for linear molecules, 3 for non-linear molecules).

ELOW: 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.

QNFORM: identifies the format of the quantum numbers given in the field QN. These quantum number formats are given in Section V. (They are different from previous editions.)

QN': Quantum numbers for the upper state coded according to QNFORM.

QN": Quantum numbers for the lower state.

The catalogue 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)

NAME: an ASCII name for the species

NLINE: number of lines in catalogue

QLOG: a seven element vector containing the base 10 logorithm of the partition function for temperatures of 300K, 225K, 150K, 75K, 37.5K, 18.25K, 9.375K respectively.

VERSION: version of the calculation for this species in the catalogue.

Physical Format of Tape

Density: 800 or 1600 bytes/inch on 9 tracks

Encoding: ASCII

Logical Record Size: 80 characters (i.e. 1 card image)

First file (catalogue):

Blocking: 3600 characters per block (i.e. 45 card images)

Length: 4778 blocks followed by end-of-file mark,
for a total of 214994 lines

Character Set Used: 1 2 3 4 5 6 7 8 9 0. -

Second file (directory):

Blocking: 80 characters per block

Length: 151 blocks followed by end of file mark

In the first file, each card image contains the information for a single spectral line. The lines are ordered by species tag and are ordered within a species by frequency. In the second file, each card image contains directory information for a single species. The species are ordered by the species tag.

III. Intensity Units and Conversions

The units of intensity given in the catalogue, nm^2 MHz, are based on the integral of the absorption cross section over the spectral lineshape. The value of the intensity is calculated for 300K and is directly comparable with the common infrared intensity unit of cm^{-1}/(molecule/cm^2). The latter is obtainable by dividing the catalogue intensity by 2.9979 x 10^{+18}.

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

$$I_{ba}(T) = (8\pi^3/3hc)\nu_{ba}\ {}^{x}S_{ba}\ \mu_x^2\ [\exp(-E''/kT) - \exp(-E'/kT)]/Q_{rs} \qquad (1)$$

where ν_{ba} is the line frequency, ${}^{x}S_{ba}$ 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 ${}^{x}S_{ba}$ and Q_{rs} are determined with 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 or vibrational Boltzmann factor is included. For the catalogue, Eq. (1) is evaluated for T=300K.

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 to kT. For non-linear molecules Q_{rs} is proportional to $T^{3/2}$ in the same limit. Explicitly, I_{ba} (T) is

$$I_{ba}(T) = I_{ba}(300K)\ [Q_{rs}(300)/Q_{rs}(T)]\ [\exp(-E''/kT)-\exp(-E'/kT)]/ \qquad (2)$$

$$[\exp(-E''/k\cdot 300K)-\exp(-E'/k\cdot 300K)]$$

$$\cong I_{ba}(300K)\cdot(300K/T)^{n+1}\ \exp[-(1/T - 1/300K)E''/k] \qquad (2a)$$

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

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

$$\alpha_{max} = [I_{ba}(T)/\Delta\nu](300K/T) \times 102.46 \tag{3}$$

in which $\Delta\nu$ is the half-width at half-height in MHz at 1 torr partial pressure of absorber at temperature T, I_{ba} is in units of nm^2 MHz, and α_{max} is in units of cm^{-1}. The corresponding value of α_{max} in the thermal Doppler limit is

$$\alpha_{max} = [I_{ba}(T)p/\nu_{ba}](300K/T)^{3/2}(m/28)^{1/2} \times 1.2898 \times 10^{8} \tag{4}$$

in which p is the partial pressure of absorber in torr, and m is the mass of the absorber (in atomic mass units). In Eq. (4) - (6), 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

$$\sigma_{ba} = [I_{ba}/\nu_{ba}] \times 2.9979 \times 10^{-9}\ cm^2. \tag{5}$$

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

$$A_{ba} = I_{ba}(T)\ \nu_{ba}{}^2[Q_{rs}/g'][\exp(-E''/kT)-\exp(-E'/kT)]^{-1} \times 2.7964 \times 10^{-16} \tag{6}$$

$$\cong I_{ba}\ (300K)\ \nu_{ba}\ [Q_{rs}(300K)/g']\ \exp\ [E'/k\cdot 300K] \times 1.748 \times 10^{-9}\ sec^{-1} \tag{6a}$$

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 catalogue. Values of Q_{rs} are listed in Section VI.

IV. General Comments on Precision

The expected errors of the frequency as listed in the catalogue 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:

$$\varepsilon_n^{\,2} = \sum_{kj} \frac{\partial \nu_n}{\partial p_k} \frac{\partial \nu_n}{\partial p_j} V_{kj} \qquad (7)$$

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

$$(V^{-1})_{kj} = \sum_{m} \frac{\partial \nu_m}{\partial p_k} \frac{\partial \nu_m}{\partial p_j} \varepsilon_m^{-2} \qquad (8)$$

in which the summation over m is over the experimental lines using experimental uncertainties, 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 more 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. (7) and (8). 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 input error estimates. Lines with an expected error greater than 1 GHz have been dropped from the catalogue.

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 which 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 function does not enter directly because the catalogue intensities are 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 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.

There are many molecular models that 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 becasue 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 set up, and provides a uniform output format for the final results. Most important, the basic treatment is the same for every molecule, regardless of the model used, so that a high degree of consistancy 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, which 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.

V. Format of Quantum Numbers

For this edition of the catalogue we have attempted to put the quantum number format conventions into a more rational and computer accessible form. First, the upper and lower quantum number sets have been separated into distinct fields. Second, the quantum format designations have been redefined to have more accessible information encoded in them. The quantum number format designation, QNFORM, is a 4 digit quantity in the catalogue. We will divide QNFORM into a series of digits so that

$$\mathrm{QNFORM} = Q*100 + H*10 + \mathrm{NQN}$$

in which Q determines the type of molecule (see table below), 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 catalogue all half integer quantum numbers are rounded up to the next integer.

TABLE I. QUANTUM NUMBER FORMATS

type	Q	ITD	quantum order
atom	0	0	(J),(F),....
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+1/2,Ω+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 rounded up
2. The sign of Λ and K refers to parity under inversion <u>not</u> sign of operator. NOTE: Wang symmetry is related to parity by $(-1)^{J+S+e}$ or $(-1)^{N+e}$ where e=0 for all states except Σ^- states
3. Quantum numbers in parentheses optional

VI. Documentation by Species

In this edition of the catalogue, several of the species have spectra which are extended to 10000 GHz, so the documentation below includes a maximum frequency cutoff. For almost all species a strength cutoff was also employed:

$$10^{LGINT} > 10^{LOGSTR0} + (\nu/300\ GHz)^2 * 10^{LOGST1}$$

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 are H_2O and O_3.) 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 catalogue. The spin statistics included are only a partial set but are consistent with the intensities in the catalogue.

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

TABLE II. Assumed Relative Abundances of Isotopes for Catalogue Description

	log (rel. abundance)		log (rel. abundance)
^{1}H	0.	^{29}Si	-1.327
^{2}H	-3.824	^{30}Si	-1.506
^{12}C	0.	^{32}S	-0.022
^{13}C	-1.955	^{33}S	-2.125
^{14}N	0.	^{34}S	-1.376
^{15}N	-2.432	^{35}Cl	-0.122
^{16}O	0.	^{37}Cl	-0.611
^{17}O	-3.432	^{79}Br	-0.296
^{18}O	-2.690	^{81}Br	-0.306
^{28}Si	-0.035		

Species List

1001	H-ATOM
2001	D-ATOM
3001	HD
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
20001	D2O
25001	CCH
26001	CN
26002	CN-V1
27001	HCN
27002	HNC
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
33001	HO2
34001	O-18-O
34002	H2S
34003	PH3
34004	H2O2
35001	HDS
36001	HCl
38001	HCl-37
40001	CH3CCH
41001	CH3CN
41002	CH3CC-13-H
41003	CH3C-13-CH
41004	C-13-H3CCH
41005	CH3CCD
41006	CH2DCCH
42001	CH3CN-15
42002	CH2CO
43001	CHDCO
44001	CS
44002	SIO
44003	CH3CHO-A
44004	N2O
44005	CH3CHO-E
45001	C-13-S
45002	SI-29-O
45003	NH2CHO
46001	CS-34
46002	SI-30-O
46003	H2CS
46004	C2H5OH
46005	HCOOH
46006	NO2
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
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
51001	HCCCN
51002	CLO
52001	HCCC-13-N
52002	HCC-13-CN
52003	HC-13-CCN
52004	HCCCN-15
52005	DCCCN
52006	HOCL
53001	C2H3CN
53002	CL-37-O
54001	CH2CHC-13-N
54002	CH2C-13-HCN
54003	C-13-H2CHCN
54004	CH2CDCN
54005	HOCL-37
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
64001	S2
64002	SO2
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
80001	HBR-79
82001	HBR-81
95001	BR-79-O
97001	BR-81-O
97002	CL-35-NO3
99001	CL-37-NO3

Species Tag: 1001
Version: 1
Date: Oct 1979
Contributor: H. M. Pickett

Species Name: Hydrogen atom
$^2S_{1/2}$ ground state

Lines Listed = 1
Max. Frequency = 1.42 GHz
Max. J = 1/2
LOGSTR = -9.1
LOGSTR1 =
Isotope Correction = 0.
Minimum Energy = 0.0479 cm^{-1}
Dipoles: μ(a) =
μ(b) =
μ(c) =

Q(300.) = 4.0
Q(225.) = 4.0
Q(150.) = 4.0
Q(75.) = 4.0
Q(37.5) = 3.99
Q(18.25) = 3.99
Q(9.375) = 3.98
A =
B =
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 <u>229</u>, 110). The average spontaneous emission lifetime of the three F = 1 states is 2.876 X 10^{-15} sec $^{-1}$.

Species Tag:	2001	Species Name:	Deuterium atom
Version:	1		
Date:	Oct 1979		$^2S_{1/2}$ ground state
Contributor:	H. M. Pickett		

Lines Listed	= 1	Q(300.) =	6.
Max. Frequency	= 0.3 GHz	Q(225.) =	6.
Max. J	= 1/2	Q(150.) =	6.
LOGSTR	= -10.3	Q(75.) =	6.
LOGSTR1	=	Q(37.5) =	6.
Isotope Correction	= -3.824	Q(18.25) =	6.
Minimum Energy	= 0. cm^{-1}	Q(9.375) =	6.
Dipoles : $\mu(a)$	=	A =	
$\mu(b)$	=	B =	
$\mu(c)$	=	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 X 10^{-17} sec^{-1}.

Species Tag: 3001
Version: 1
Date: Oct. 1979
Contributor: H. M. Pickett

Species Name: HD
Mono-deuterated
molecular hydrogen

Lines Listed = 1
Max. Frequency = 2676. GHz
Max. J = 1
LOGSTR = -5.6
LOGSTR1 = 0.
Isotope Correction = -3.523
Minimum Energy = 0. cm^{-1}
Dipoles: μ(a) =
μ(b) = 0.000585
μ(c) =

Q(300.) = 5.0165
Q(225.) = 3.8583
Q(150.) = 2.7008
Q(75.) = 1.5711
Q(37.5) = 1.0980
Q(18.25) = 1.0032
Q(9.375) = 1.0002
A =
B = 1339100.
C =

The dipole moment is from M. Trefler and H. P. Gush, 1968, Phys. Rev. Letters, 20, 703. The rotational constant is from R. A. Durie and G. Herzberg, 1960, Can. J. Phys. 38, 806. The frequency and its error limits were obtained from the difference of the S_1 (0) and R_1 (1) transitions listed by A. McKellar, 1974, Can. J. Phys. 52, 1144.

Species Tag: 12001
Version: 1
Date: Oct 1979
Contributor: H. M. Pickett

Species Name: Carbon atom
^{3}P ground state

Lines Listed = 2
Max. Frequency = 810 GHz
Max. J = 2
LOGSTR = -5.
LOGSTR1 =
Isotope Correction = 0
Minimum Energy = 0. cm^{-1}
Dipoles: μ(a) =
μ(b) =
μ(c) =

Q(300.) = 7.833
Q(225.) = 7.489
Q(150.) = 6.860
Q(75.) = 5.364
Q(37.5) = 3.543
Q(18.25) = 2.030
Q(9.375) = 1.248
A =
B =
C =

The lines of atomic carbon have been measured by Laser Magnetic Resonance (R. J. Saykally and K. M. Evenson, 1980, Ap. J. 238, L107.) Intensities were calculated using the free electron g factor.

Species Tag:	13001	Species Name:	Carbon atom ^{13}C isotope
Version:	1		
Date:	Oct 1979		
Contributor:	H. M. Pickett		
Lines Listed	= 7	Q(300.) =	15.666
Max. Frequency	= 810. GHz	Q(225.) =	14.978
Max. J	= 2	Q(150.) =	13.720
LOGSTR	= -16.	Q(75.) =	10.727
LOGSTR1	=	Q(37.5) =	7.087
Isotope Correction	= -1.955	Q(18.25) =	4.060
Minimum Energy	= 0. cm^{-1}	Q(9.375) =	2.496
Dipoles: μ(a)	=	A =	
μ(b)	=	B =	
μ(c)	=	C =	

The fine structure intervals of ^{12}C were multiplied by 0.999992967 to account for the isotope effect on the Rydberg constant. The hyperfine invervals of G. Wolber, H. Figger, R. A. Haberstroh and S. Penselin, 1969, Physics Letters A29, 461, were then used to compute the line frequencies. Intensities were calculated using the free electron g value.

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

Lines Listed =	324	Q(300.) =	120.840
Max. Frequency =	10000 GHz	Q(225.) =	91.364
Max. F =	14	Q(150.) =	61.997
LOGSTR =	-10.	Q(75.) =	32.922
LOGSTR1 =	-7.	Q(37.5) =	18.847
Isotope Correction =	0.	Q(18.25) =	12.200
Minimum Energy =	0 cm^{-1}	Q(9.375) =	8.960
Dipoles: $\mu(a)$ =	1.46	A =	
$\mu(b)$ =		B =	425472.8
$\mu(c)$ =		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 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) Ap. J. 268 L51 in a fit to a Hund's case b Hamiltonian with 8 fine structure parameters, B and D and 7 hyperfine parameters. Calculated values are given for the rotational transitions.

The dipole moment was taken from D. H. Phelps and F. W. Dalby, (1966) Phys. Rev. Lett. 16, 3 (1966).

Species Tag: 14001
Version: 1
Date: Oct 1979
Contributor: H. M. Pickett

Species Name: N-atom
$^4S_{3/2}$ ground state

Lines Listed = 2
Max. Frequency = 0.027 GHz
Max. J = 1.5
LOGSTR = -13.
LOGSTR1 =
Isotope Correction = 0.
Minimum Energy = 0. cm^{-1}
Dipoles: $\mu(a)$ =
$\mu(b)$ =
$\mu(c)$ =

Q(300.) = 12.0
Q(225.) = 12.0
Q(150.) = 12.0
Q(75.) = 12.0
Q(37.5) = 12.0
Q(18.25) = 12.0
Q(9.375) = 12.0
A =
B =
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. A 16, 484. Intensities were calculated using the experimental g_J value.

Species Tag:	14002		Species Name:	N-atom ^{2}D state
Version:	2			
Date:	Aug 1983			
Contributor:	H. M. Pickett			

Lines Listed	= 6		Q(300.) =	29.51
Max. Frequency	= 261.	GHz	Q(225.) =	29.35
Max. J	= 2.5		Q(150.) =	29.03
LOGSTR	= -49.		Q(75.) =	28.15
LOGSTR1	=		Q(37.5) =	26.58
Isotope Correction	= 0.		Q(18.25) =	24.13
Minimum Energy	= 19223.	cm^{-1}	Q(9.375) =	21.12
Dipoles: μ(a)	=		A =	
μ(b)	=		B =	
μ(c)	=		C =	

The $^2D_{5/2}$ state is 19223 cm^{-1} above the ground $^4S_{3/2}$ state (C. E. Moore, 1949, Atomic Energy Levels I, Nat. Bureau of Stds.). The $^2D_{3/2}$ - $^2D_{5/2}$ inverted fine structure transition at 260 GHz has a predicted uncertainty of ± 600 MHz, but the hyperfine structure intervals are uncertain by less than 1 MHz. (H. E. Radford and K. M. Evenson, 1968, Phys. Rev. 168, 70). 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 ^3P ground state
Version:	2			
Date:	Mar 1984			
Contributor:	H. M. Pickett			
Lines Listed =	2		Q(300.) =	6.7407
Max. Frequency =	3000	GHz	Q(225.) =	6.3243
Max. J =			Q(150.) =	5.7705
LOGSTR =			Q(75.) =	5.1568
LOGSTR1 =			Q(37.5) =	5.0
Isotope Correction =			Q(18.25) =	5.015
Minimum Energy =		cm^{-1}	Q(9.375) =	5.000
Dipoles: 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
Version: 2
Date: May 1983
Contributor: H. M. Pickett

Species Name: OH
Hydroxyl radical

Lines Listed = 299
Max. Frequency = 9900. GHz
Max. J = 13.5
LOGSTR = -10.
LOGSTR1 = -10.
Isotope Correction = 0.
Minimum Energy = 0. cm^{-1}
Dipoles: $\mu(a)$ = 1.667
$\mu(b)$ =
$\mu(c)$ =

Q(300.) = 81.494
Q(225.) = 60.296
Q(150.) = 40.144
Q(75.) = 22.753
Q(37.5) = 17.034
Q(18.25) = 16.004
Q(9.375) = 15.929
A =
B = 556141.
C =

The microwave data are reported in R. A. Beaudet and R. L. Poynter, 1978, J. Phys. Chem. Ref. Data 7, 311. The predictions of the rotational lines of J. M. Brown et al, Astrophysical J. 258, 899 were included in the fit. The calculation involved fitting the spectra to effective parameters for the two Π states.

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

Species Name: NH_3
Ammonia

Lines Listed = 446
Max. Frequency = 9500. GHz
Max. J = 19
LOGSTR =-17.
LOGSTR1 = 0
Isotope Correction = 0.
Minimum Energy = 0. cm^{-1}
Dipoles: $\mu(a)$ = 0
$\mu(b)$ = 0
$\mu(c)$ = 1.476

Q(300.) = 578.98
Q(225.) = 371.88
Q(150.) = 206.64
Q(75.) = 74.54
Q(37.5) = 26.608
Q(18.25) = 11.251
Q(9.375) = 5.398
A = B
B = 298117.06
C = 186726.36

The computational method and most of the microwave data are given in R. L. Poynter and R. K. Kakar, 1975, Ap. J. Suppl. 29, 87. Additional microwave transitions have been reported by B. V. Shinha and P. D. P. Smith, 1980, J. Mol. Spectrosc. 80, 231.

The rotational transitions and energy levels were taken from R. Poynter and J. S. Margolis, 1983, Mol. Phys. 48, 401. This analysis was based on a very extensive set of accurate ν_2 measurements reported by R. Poynter and J. S. Margolis, 1984, Mol. Phys. 51, 393, and upon a series of "forbidden" transitions in the ν_4 band, reported by E. A. Cohen, W. H. Weber, R. L. Poynter, and J. S. Margolis, 1983, Mol. Phys. 50, 727. The work of Cohen, et al. allowed the C, D_K, H_K, and L_k constants to be determined, thus fixing the energy level scale. The J = 1 → 0, k = 0 rotational transition was taken from P. Helminger, F. C. DeLucia, and W. Gordy, 1971, J. Mol. Spect. 39, 94. Becasuse 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
Version: 1
Date: Feb 1980
Contributor: R. L. Poynter

Species Name: CH_3D
Mono deutero methane

Lines Listed = 80
Max. Frequency = 3000. GHz
Max. J = 13
LOGSTR = -8
LOGSTR1 = 0
Isotope Correction = -3.222
Minimum Energy = 0. cm^{-1}
Dipoles: μ(a) = 0.0056
μ(b) = 0
μ(c) = 0

Q(300.) = 402.17
Q(225.) = 315.14
Q(150.) = 142.69
Q(75.) = 51.09
Q(37.5) = 18.47
Q(18.25) = 7.03
Q(9.375) = 2.98
A = 157412.
B = 115325.
C = B

The J = 0 → 1 line has been measured by H. M. Pickett, E. A. Cohen and T. G. Phillips, 1980, Ap. J. Letters, <u>236</u>, 43. Predicted lines are based upon the constants given by C. Chakerian and G. Guelachvilli, 1980, J. Mol. Spect., <u>84</u>, 447. The dipole moment has been measured by I. Ozier, W. Ho, and G. Birnbaum, 1969, J. Chem. Phys. <u>51</u>, 4873, and by S. C. Wofsey, J. S. Muenter, and W. Klemperer, (1970), J. Chem. Phys. <u>53</u>, 4005.

Species Tag: 17004
Species Name: NH_3, ν_2 - 010 state
Version: 1
Date: Mar 1984
Contributor: R. L. Poynter

Lines Listed = 442
Max. Frequency = 11600 GHz
Max. J = 17
LOGSTR = -12
LOGSTR1 =
Isotope Correction =
Minimum Energy = 0. cm^{-1}
Dipoles: $\mu(a)$ =
$\mu(b)$ =
$\mu(c)$ = 1.253

Q(300.) = 578.98
Q(225.) = 371.88
Q(150.) = 206.64
Q(75.) = 74.54
Q(37.5) = 26.608
Q(18.25) = 11.251
Q(9.375) = 5.397
A = B
B = 299196.11
C = 183595.39

The lines for this species were derived by combination differences from the ν_2 - 010 lnes 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, by S. Urban, et al., 1980, J. Mol. Spect. 79, 455, by E. N. Karyakin, et al., 1977, J. Mol. Spect. 66, 177, and by 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.) =	212.42
Max. Frequency	= 10000.	GHz	Q(225.) =	153.388
Max. J	= 15.5		Q(150.) =	97.477
LOGSTR	= -10.		Q(75.) =	48.966
LOGSTR1	= -10		Q(37.5) =	30.896
Isotope Correction	= -3.824		Q(18.25) =	25.020
Minimum Energy	= 0.	cm^{-1}	Q(9.375) =	24.010
Dipoles: μ(a)	= 1.653		A =	
μ(b)	= 0.		B =	296312.
μ(c)	= 0.		C =	

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

Species Tag: 18002
Version: 2
Date: Jan 1981
Contributor: R. L. Poynter

Species Name: Ammonia, $^{15}NH_3$
15 nitrogen isotope

Lines Listed = 235
Max. Frequency = 3000. GHz
Max. J = 20
LOGSTR = -17
LOGSTR1 =
Isotope Correction = -2.432
Minimum Energy = 0. cm^{-1}
Dipoles: μ(a) = 0
μ(b) = 0.
μ(c) = 1.476

Q(300.) = 575.84
Q(225.) = 451.23
Q(150.) = 206.21
Q(75.) = 74.71
Q(37.5) = 27.669
Q(18.25) = 11.277
Q(9.375) = 5.415
A = B
B = 297390.8
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 IR measurements of M. Carlotti, A. Trombetti, B. Velino, and J. Vrbancich, 1980, J. Mol. Spect. 83, 401. The C rotational constant was assumed to be the same as in $^{14}NH_3$.

The dipole moment was assumed to be the same as $^{14}NH_3$.

Species Tag: 18003
Version: 3
Date: Dec 1983
Contributor: R. L. Poynter and H. M. Pickett

Species Name: H_2O
water

Lines Listed = 424
Max. Frequency = 10000. GHz
Max. J = 12
LOGSTR = -12
LOGSTR1 =
Isotope Correction = 0.
Minimum Energy = 0. cm^{-1}
Dipoles : $\mu(a)$ = 0.
$\mu(b)$ = 1.855
$\mu(c)$ = 0.

Q(300.) = 178.115
Q(225.) = 116.017
Q(150.) = 63.677
Q(75.) = 23.170
Q(37.5) = 8.580
Q(18.25) = 3.033
Q(9.375) = 1.257
A = 835840.29
B = 435351.72
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. DeLucia and P. Helminger (1984), J. Mol. Spect. (in press), and on 720 ground state combination differences derived from the ν_2 data of G. Guelachvilli (1983), J. Opt. Soc. Am. 73, 137. All of the submillimeter/microwave lines fit to within an 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 details of the analysis will be reported shortly. 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. DeLucia, P. Helminger and W. H. Kirchhoff, (1974), J. Phys. Chem. Ref. Data, 3, 211.

The partition function includes contributions from the ν_2 state.

Species Tag:	18004	Species Name:	NH_2D Mono deutero ammonia
Version:	1		
Date:	Jan 1981		
Contributor:	H. M. Pickett		
Lines Listed	= 5036	Q(300.) =	3790.
Max. Frequency	= 3000. GHz	Q(225.) =	2409.
Max. J	= 14	Q(150.) =	1293.
LOGSTR	= -10	Q(75.) =	434.4
LOGSTR1	=	Q(37.5) =	137.0
Isotope Correction	= -3.347	Q(18.25) =	404.3
Minimum Energy	= 0. cm^{-1}	Q(9.375) =	13.24
Dipoles: μ(a)	= -0.18	A =	290124.
μ(b)	= 0	B =	192194.
μ(c)	= 1.463	C =	140797.

The experimental lines were measured by F. C. DeLucia and P. Helminger, 1975, J. Mol. Spec. 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 8-th 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
Version: 2
Date: Mar 1984
Contributor: H. M. Pickett

Species Name: H_2O-ν2 excited bending state (010)

Lines Listed = 292
Max. Frequency = 10000. GHz
Max. J = 10
LOGSTR =-12
LOGSTR1 =
Isotope Correction = 0.
Minimum Energy = 1594.75 cm^{-1}
Dipoles: μ(a) = 0.
μ(b) = 1.855
μ(c) = 0.

Q(300.) = 178.115
Q(225.) = 116.017
Q(150.) = 63.677
Q(75.) = 23.170
Q(37.5) = 8.580
Q(18.25) = 3.033
Q(9.375) = 1.257
A = 933052
B = 440318.
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, Ap. 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
Version: 2
Date: May 1983
Contributor: H. M. Pickett

Species Name: HO-18
Hydroxyl radical

Lines Listed = 295
Max. Frequency = 10000. GHz
Max. J = 13.5
LOGSTR = -10.
LOGSTR1 = -10.
Isotope Correction = -2.690
Minimum Energy = 0. cm^{-1}
Dipoles: μ(a) = 1.667
μ(b) =
μ(c) =

Q(300.) = 81.945
Q(225.) = 60.611
Q(150.) = 40.329
Q(75.) = 22.824
Q(37.5) = 17.054
Q(18.25) = 16.006
Q(9.375) = 15.930
A =
B = 552470.
C =

The microwave data are 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 is available.

Species Tag: 19002
Version: 2
Date: Dec 1983
Contributor: R. L. Poynter

Species Name: HDO
water, mono deuterium isotope

Lines Listed = 461
Max. Frequency = 3013 GHz
Max. J = 17
LOGSTR = -13
LOGSTR1 =
Isotope Correction = -3.523
Minimum Energy = 0. cm^{-1}
Dipoles: $\mu(a)$ = 0.657
$\mu(b)$ = 1.732
$\mu(c)$ = 0

Q(300.) = 146.05
Q(225.) = 95.07
Q(150.) = 52.28
Q(75.) = 18.851
Q(37.5) = 6.952
Q(18.25) = 2.712
Q(9.375) = 1.334
A = 701931.5
B = 272912.6
C = 192055.2

The lines reported here were derived from a fit which included the microwave and submillimeter lines reported by J. K. Messer, F. C. DeLucia and P. Helminger (1984), J. Mol. Spect. (in press), and an extensive set of ground state energy levels obtained from new high resolution FTS measurements of the ν_2 band reported by R. A. Toth, 1984 (private communication). The RMS deviations of the submillimeter lines is almost the same as that reported above by Messer, et al., while the RMS deviations for the fit of the ground state energy levels is 0.00015 cm^{-1} (4 MHz). The dipole moment components are from S. A. Clough, Y. Beers, G. P. Klein and L. S. Rothman (1973), J. Chem. Phys. 59, 2254.

Further references can be found in F. C. DeLucia, P. Helminger, and W. H. Kirchhoff, (1974), J. Phys. and Chem. Ref. Data 3, 211.

Species Tag:	20001	Species Name:	D_2O,
Version:	1		Water, fully substituted
Date:	Feb 1984		with deuterium
Contributor:	R. L. Poynter		deuterium oxide

Lines Listed	= 427		Q(300.) =	1045.3
Max. Frequency	= 3030	GHz	Q(225.) =	679.5
Max. J	= 18		Q(150.) =	371.2
LOGSTR	= -10		Q(75.) =	133.11
LOGSTR1	= 0		Q(37.5) =	48.56
Isotope Correction	= -3.523		Q(18.25) =	18.55
Minimum Energy	= 0.	cm^{-1}	Q(9.375) =	8.64
Dipoles: $\mu(a)$ =			A =	462278.8
$\mu(b)$ =	1.8545		B =	218038.27
$\mu(c)$ =			C =	145258.00

The data used in this fit are based upon the microwave and submillimeter lines reported by

J. Bellet and G. Steenbeckeliers, 1970, Compt. Rend. 271B, 1208

W. S. Benedict, S. A. Clough, L. Frenkel, and T. E. Sullivan, Jr., 1970, J. Chem. Phys. 53, 2565

H. Bluyssen, 1968, 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. Masser, F. C. DeLucia, and P. Helminger, 1984, J. Mol. Spect., (in press)

G. Steenbeckeliers and J. Bellet, 1970, Compt. Rend. 270B, 1039

G. Steenbeckeliers and J. Bellet, 1973, 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

and on the infrared ν_2 data of R. A. Toth, 1984, private communication.

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

Species Tag: 25001

Version: 1

Date: Mar

Contributor: H. M. Pickett

Species Name: Ethynl radical
CCH $X^2\Sigma$ state

Lines Listed = 114
Max. Frequency = 3000 GHz
Max. F = 28
LOGSTR = -10
LOGSTR1 = - 4.
Isotope Correction = 0
Minimum Energy = 0 cm^{-1}
Dipoles : $\mu(a)$ = 0.8
$\mu(b)$ = 0
$\mu(c)$ = 0

Q(300.) = 574.24
Q(225.) = 430.94
Q(150.) = 287.69
Q(75.) = 144.49
Q(37.5) = 72.91
Q(18.25) = 37.14
Q(9.375) = 19.28
A =
B = 43674.534
C =

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

Species Tag: 26001
Version: 1
Date: Apr 1983
Contributor: H. M. Pickett

Species Name: CN radical

Lines Listed = 385
Max. Frequency = 3493. GHz
Max. J = 29.5
LOGSTR = -5.
LOGSTR1 =
Isotope Correction = 0.
Minimum Energy = 0. cm^{-1}
Dipoles : $\mu(a)$ = 3.0
$\mu(b)$ =
$\mu(c)$ =

Q(300.) = 663.88
Q(225.) = 498.44
Q(150.) = 332.91
Q(75.) = 167.43
Q(37.5) = 84.73
Q(18.25) = 43.41
Q(9.375) = 22.80
A =
B = 56693.46
C =

The data and calculational method are from D. D. Skatrud, et al., 1983, J. Molec. Spectroscopy 99, 35.

Species Tag:	26002	Species Name:	CN, v = 1
Version:	1		
Date:	Mar 1984		
Contributor:	H. M. Pickett		

Lines Listed	= 437		Q(300.) =	663.88
Max. Frequency	= 9999	GHz	Q(225.) =	498.44
Max. J	= 29.5		Q(150.) =	332.91
LOGSTR	= -9		Q(75.) =	167.43
LOGSTR1	= 0		Q(37.5) =	84.73
Isotope Correction	= 0.		Q(18.25) =	43.41
Minimum Energy	= 2068.7	cm^{-1}	Q(9.375) =	22.80
Dipoles: 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. Molec. Spectroscopy <u>99</u>, 35.

Species Tag:	27001	Species Name:	HCN
Version:	2		Hydrogen cyanide
Date:	Jan 1984		
Contributor:	R. L. Poynter		

Lines Listed	= 40		Q(300.) =	424.154
Max. Frequency	= 3000.	GHz	Q(225.) =	318.504
Max. J	= 33		Q(150.) =	212.643
LOGSTR	= -4		Q(75.) =	106.811
LOGSTR1	=		Q(37.5) =	53.910
Isotope Correction	= 0		Q(18.25) =	27.472
Minimum Energy	= 0	cm^{-1}	Q(9.375) =	14.272
Dipoles: μ(a)	= 2.984		A =	
μ(b)	=		B =	44315.975
μ(c)	=		C =	

The observed transitions are from F. C. DeLucia 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 Univ.

Species Tag:	27002		Species Name:	HNC
Version:	1			Hydrogen isocyanide
Date:	Dec 1977			
Contributor:	R. L. Poynter			

Lines Listed = 33

Max. Frequency = 3000. GHz

Max. J = 34

LOGSTR = -3

LOGSTR1 =

Isotope Correction = 0

Minimum Energy = 0 cm^{-1}

Dipoles: μ(a) = 2.699

μ(b) =

μ(c) =

Q(300) = 138.223

Q(225.) = 103.801

Q(150.) = 69.302

Q(75.) = 34.814

Q(37.5) = 17.575

Q(18.25) = 8.960

Q(9.375) = 4.659

A =

B = 45332.

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:	28001		Species Name:	CO
Version:	1			Carbon monoxide
Date:	Dec 1979			
Contributor:	R. L. Poynter			

Lines Listed	= 26		Q(300.) =	108.787
Max. Frequency	= 3000.	GHz	Q(225.) =	81.708
Max. J	= 26		Q(150.) =	54.581
LOGSTR	= -5		Q(75.) =	27.454
LOGSTR1	=		Q(37.5) =	13.896
Isotope Correction	= 0		Q(18.25) =	7.122
Minimum Energy	= 0	cm^{-1}	Q(9.375) =	3.744
Dipoles: μ(a)	= 0.1098		A =	
μ(b)	=		B =	57635.97
μ(c)	=		C =	

The experimental measurements were reported by B. Rosenblum, A. H. Nethercot, Jr., and C. H. Townes, 1958, Phys. Rev. 109, 400; W. Gordy and M. J. Cowan, 1957, Bull. Am. Phys. Soc. 2, 212; and by P. Helminger, F. C. De Lucia ad W. Gordy, 1970, Phys. Rev. Lett. 25, 1397.

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, ^{13}C isotope
Date:	Dec 1979			
Contributor:	R. L. Poynter			

Lines Listed	= 45		Q(300.) =	435.38
Max. Frequency	= 3000.	GHz	Q(225.) =	326.93
Max. J	= 34		Q(150.) =	218.26
LOGSTR	= -4		Q(75.) =	109.62
LOGSTR1	=		Q(37.5) =	55.31
Isotope Correction	= -1.955		Q(18.25) =	28.17
Minimum Energy	= 0.	cm^{-1}	Q(9.375) =	14.62
Dipoles: 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 the parent species.

Species Tag: 28003
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: HCN-15
Hydrogen cyanide, ^{15}N isotope

Lines Listed = 35
Max. Frequency = 3000. GHz
Max. J = 35
LOGSTR = -2.6
LOGSTR1 =
Isotope Correction = -2.432
Minimum Energy = 0. cm^{-1}
Dipoles: $\mu(a)$ = 2.984
$\mu(b)$ =
$\mu(c)$ =

Q(300.) = 145.068
Q(225.) = 109.337
Q(150.) = 72.993
Q(75.) = 36.660
Q(37.5) = 18.498
Q(18.25) = 9.421
Q(9.375) = 4.889
A =
B = 43027.69
C =

The measured lines are from E. F. Pearson, R. A. Crewell, M. Winnewisser and G. Winnewisser, (1976), Z. Naturforsch. 31a, 1394.

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

Species Tag:	28004		Species Name:	DCN
Version:	1			Hydrogen cyanide,
Date:	Dec 1979			deuterium isotope
Contributor:	R. L. Poynter			
Lines Listed	= 54		Q(300.) =	518.916
Max. Frequency	= 3000.	GHz	Q(225.) =	389.604
Max. J	= 41		Q(150.) =	260.036
LOGSTR	=-4.2		Q(75.) =	130.504
LOGSTR1	=		Q(37.5) =	65.755
Isotope Correction	= -3.824		Q(18.25) =	33.391
Minimum Energy	= 0.	cm^{-1}	Q(9.375) =	17.224
Dipoles: μ(a)	= 2.984		A =	
μ(b)	=		B =	36207.46
μ(c)	=		C =	

The observed transitions are from F. C. DeLucia and W. Gordy (1969), Phys. Rev. 187, 58. The dipole moment is from G. Tomasevich, (1970), Thesis, Harvard Univ.

Species Tag: 28005
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: $HN^{13}C$
Hydrogen Isocyanide,
^{13}C isotope

Lines Listed = 34
Max. Frequency = 3000. GHz
Max. J = 35
LOGSTR =-2.7
LOGSTR1 =
Isotope Correction = -1.955
Minimum Energy = 0. cm^{-1}
Dipoles: μ(a) = 2.699
μ(b) =
μ(c) =

Q(300.) = 143.880
Q(225.) = 108.047
Q(150.) = 72.132
Q(75.) = 36.228
Q(37.5) = 18.282
Q(18.25) = 9.313
Q(9.375) = 4.835
A =
B = 43545.61
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
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Lines Listed = 33
Max. Frequency = 3000. GHz
Max. J = 33
LOGSTR =-2.7
LOGSTR1 =
Isotope Correction = -2.432
Minimum Energy = 0. cm^{-1}
Dipoles: μ(a) = 2.699
μ(b) =
μ(c) =

Species Name: HN-15-C
Hydrogen isocyanide,
^{15}N isotope

Q(300.) = 141.013
Q(225.) = 105.893
Q(150.) = 70.697
Q(75.) = 35.511
Q(37.5) = 17.924
Q(18.25) = 9.134
Q(9.375) = 4.746
A =
B = 44433.04
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
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: DNC
Hydrogen isocyanide,
deuterium isotope

Lines Listed = 39
Max. Frequency = 3000 GHz
Max. J = 39
LOGSTR = -3
LOGSTR1 =
Isotope Correction = -3.824
Minimum Energy = 0. cm^{-1}
Dipoles: $\mu(a)$ = 2.699
$\mu(b)$ =
$\mu(c)$ =

Q(300.) = 164.169
Q(225.) = 123.269
Q(150.) = 82.279
Q(75.) = 41.301
Q(37.5) = 20.818
Q(18.25) = 10.580
Q(9.375) = 5.467
A =
B = 38152.995
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
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: C-13-O
carbon monoxide,
^{13}C isotope

Lines Listed = 27
Max. Frequency = 3000 GHz
Max. J = 27
LOGSTR = -5.1
LOGSTR1 =
Isotope Correction = -1.955
Minimum Energy = 0. cm^{-1}
Dipoles: $\mu(a)$ = 0.11
$\mu(b)$ =
$\mu(c)$ =

Q(300.) = 113.776
Q(225.) = 85.454
Q(150.) = 57.077
Q(75.) = 28.702
Q(37.5) = 14.520
Q(18.25) = 7.434
Q(9.375) = 3.898
A =
B = 55101.02
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.) =	140.504
Max. Frequency	= 3000.	GHz	Q(225.) =	105.506
Max. J	= 33		Q(150.) =	70.440
LOGSTR	= -3		Q(75.) =	35.384
LOGSTR1	=		Q(37.5) =	17.860
Isotope Correction	= 0.		Q(18.25) =	9.102
Minimum Energy	= 0.	cm^{-1}	Q(9.375) =	4.730
Dipoles: 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
Version: 2
Date: Jan 1981
Contributor: R. L. Poynter

Species Name: CH_2NH
Methyleneimine

Lines Listed = 2957
Max. Frequency = 3000. GHz
Max. J = 33
LOGSTR = -8
LOGSTR1 = -5 above 120 GHz
Isotope Correction = 0.
Minimum Energy = 0. cm^{-1}
Dipoles: $\mu(a)$ = 1.325
$\mu(b)$ = 1.530
$\mu(c)$ = 0.

Q(300.) = 5892.86
Q(225.) = 3800.14
Q(150.) = 2084.97
Q(75.) = 740.46
Q(37.5) = 263.39
Q(18.25) = 94.30
Q(9.375) = 34.20
A = 196211.045
B = 34532.395
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 and G. A. Blake		

Lines Listed	= 2454	Q(300.) =	3024.1
Max. Frequency	= 3000. GHz	Q(225.) =	1963.4
Max. J	= 30	Q(150.) =	1068.1
LOGSTR	=-8	Q(75.) =	378.4
LOGSTR1	=-8.	Q(37.5) =	134.8
Isotope Correction	= 0.	Q(18.25) =	49.0
Minimum Energy	= 0. cm^{-1}	Q(9.375) =	20.3
Dipoles: $\mu(a)$	= 1.3626	A =	7829365.
$\mu(b)$	= 0.700	B =	44788.
$\mu(c)$	= 0	C =	41930.4

The data include some recently measured lines at Duke 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; H. M. Pickett and T. L. Boyd, 1978, Chem. Phys. Lett. 58, 446.

Species Tag:	29005	Species Name:	N_2H^+
Version:	1		
Date:	Jan 1984		
Contributor:	R. L. Poynter		

Lines Listed	= 34		Q(300.) =	1210.8
Max. Frequency	= 3000	GHz	Q(225.) =	909.0
Max. J	= 32		Q(150.) =	607.0
LOGSTR	= -3		Q(75.) =	305.0
LOGSTR1	=		Q(37.5) =	154.0
Isotope Correction	= 0.		Q(18.25) =	78.6
Minimum Energy	= 0.	cm^{-1}	Q(9.375) =	48.9
Dipoles : $\mu(a)$	= 3.40		A =	
$\mu(b)$	=		B =	46586.867
$\mu(c)$	=		C =	

The experimental measurements were reported by R. J. Saykally, T. A. Dixon, T. G. Anderson, P. G. Szanto, and R. C. Woods, (1976), Ap. J. Lett. 205, L101, by K. V. L. N. Sastry, P. Helminger, E. Herbst, and F. C. DeLucia, (1981) Chem. Phys. Lett. 84, 286, and by 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), Ap. J. (Lett), 193, L89.

Species Tag:	30001		Species Name:	CO-18
Version:	1			Carbon monoxide, ^{18}O isotope
Date:	Dec 1979			
Contributor:	R. L. Poynter			

Lines Listed	= 27		Q(300.) =	114.210
Max. Frequency	= 3000.	GHz	Q(225.) =	85.778
Max. J	= 27		Q(150.) =	57.294
LOGSTR	= -5.1		Q(75.) =	28.810
LOGSTR1	=		Q(37.5) =	14.574
Isotope Correction	= -2.690		Q(18.25) =	7.461
Minimum Energy	= 0.	cm^{-1}	Q(9.375) =	3.912
Dipoles: 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. DeLeeuw, and A. Dymanus, 1977, Chem. Phys. 22, 319.

Species Tag: 30002
Version: 2
Date: Dec 1983
Contributor: R. L. Poynter

Species Name: HC-13-O+
Formyl radical cation,
^{13}C isotope

Lines Listed = 34
Max. Frequency = 3000 GHz
Max. J = 34
LOGSTR = -2.7
LOGSTR1 = 0
Isotope Correction = -1.955
Minimum Energy = 0 cm^{-1}
Dipoles: $\mu(a)$ = 3.3
$\mu(b)$ =
$\mu(c)$ =

Q(300.) = 144.486
Q(225.) = 108.459
Q(150.) = 72.407
Q(75.) = 36.367
Q(37.5) = 18.352
Q(18.25) = 9.348
Q(9.375) = 4.852
A =
B = 43377.32
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. Physics 43, 1043. A least squares analysis cannot be done with this limited data. The catalogue entries are therefore just a simple calculation from the B and D rotational constants, and no error estimates can be given beyond the two measured lines. The dipole moment is assumed to be the same as for the parent species.

Species Tag: 30003
Version: 2
Date: Dec 1983
Contributor: R. L. Poynter

Species Name: DCO+
Formyl radical cation,
deuterium isotope

Lines Listed = 41
Max. Frequency = 3000 GHz
Max. J = 41
LOGSTR = -2.7
LOGSTR1 =
Isotope Correction = -3.824
Minimum Energy = 0. cm^{-1}
Dipoles: $\mu(a)$ = 3.3
$\mu(b)$ =
$\mu(c)$ =

Q(300.) = 173.872
Q(225.) = 130.543
Q(150.) = 87.129
Q(75.) = 43.726
Q(37.5) = 22.031
Q(18.25) = 11.186
Q(9.375) = 5.769
A =
B = 36019.76
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, and K. V. L. N. Sastry, E. Herbst, and F. C. DeLucia, (1981), J. Chem. Phys. 75, 4169. The dipole moment was assumed to be the same as the parent species.

Species Tag: 30004
Version: 1
Date: Jan 1980
Contributor: R. L. Poynter

Species Name: H_2CO
formaldehyde

Lines Listed = 611
Max. Frequency = 3000. GHz
Max. J = 40
LOGSTR = -20
LOGSTR1 =
Isotope Correction = 0.
Minimum Energy = 0. cm^{-1}
Dipoles: $\mu(a)$ = 2.331
$\mu(b)$ = 0
$\mu(c)$ =

Q(300.) = 2876.7
Q(225.) = 1868.2
Q(150.) = 1019.7
Q(75.) = 361.7
Q(37.5) = 128.65
Q(18.25) = 44.68
Q(9.375) = 13.80
A = 281925.97
B = 38836.582
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 the following papers:

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

J. S. Chardon and D. Guichon, 1977, J. Phys. (Paris), 38, 113; 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. Spect. (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. Japan, 15, 2265.

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

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

Species Tag: 30005
Version: 1
Date: Jan 1980
Contributor: R. L. Poynter

Species Name: C-13-H_2NH
Methylenimine,
^{13}C isotope

Lines Listed = 439
Max. Frequency = 3000 GHz
Max. J = 10
LOGSTR = -8
LOGSTR1 = 0.
Isotope Correction = -1.955
Minimum Energy = 0. cm^{-1}
Dipoles: μ(a) = 1.325
μ(b) = 1.530
μ(c) = 0.

Q(300.) = 2012.45
Q(225.) = 1307.07
Q(150.) = 711.54
Q(75.) = 251.54
Q(37.5) = 88.94
Q(18.25) = 31.44
Q(9.375) = 11.12
A = 194195.217
B = 33747.87
C = 28707.05

The computational methods 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 has been assumed the same as for the parent species.

Species Tag: 30006
Version: 1
Date: Jan 1980
Contributor: R. L. Poynter

Species Name: CH_2N-15-H
Methylenimine,
^{15}N isotope

Lines Listed = 440
Max. Frequency = 3000 GHz
Max. J = 10
LOGSTR = -8
LOGSTR1 =
Isotope Correction = -2.432
Minimum Energy = 0. cm^{-1}
Dipoles: μ(a) = 1.325
μ(b) = 1.530
μ(c) = 0.

Q(300.) = 2015.79
Q(225.) = 1309.18
Q(150.) = 712.69
Q(75.) = 251.97
Q(37.5) = 89.09
Q(18.25) = 31.50
Q(9.375) = 11.14
A = 195738.07
B = 33736.10
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 has been assumed the same as for the parent species.

Species Tag: 30007
Version: 1
Date: Feb 1981
Contributor: R. L. Poynter

Species Name: CH_2ND
Methylenimine,
deuterium isotope
on nitrogen atom

Lines Listed = 1834
Max. Frequency = 3000. GHz
Max. J = 14
LOGSTR = -5 above 120 GHz
LOGSTR1 =
Isotope Correction = -3.824
Minimum Energy = 0. cm^{-1}
Dipoles: $\mu(a)$ = 1.325
$\mu(b)$ = 1.530
$\mu(c)$ = 0.

Q(300.) = 7181.1
Q(225.) = 4664.3
Q(150.) = 2542.6
Q(75.) = 811.7
Q(37.5) = 297.8
Q(18.25) = 92.62
Q(9.375) = 43.38
A = 157673.877
B = 32069.366
C = 26563.849

The computational method is the same as that used for 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:	30008	Species Name:	NO
Version:	1		Nitric oxide,
Date:	Feb 1980		$^2\Pi$ ground states
Contributor:	H. M. Pickett		

Lines Listed	= 1909		Q(300.) =	1159.46
Max. Frequency	= 3000.	GHz	Q(225.) =	816.88
Max. J	= 35.5		Q(150.) =	492.32
LOGSTR	= -20		Q(75.) =	209.69
LOGSTR1	=		Q(37.5) =	99.48
Isotope Correction	= 0.		Q(18.25) =	51.99
Minimum Energy	= 0	cm^{-1}	Q(9.375) =	28.87
Dipoles: μ(a)	= 0.15872		A =	
μ(b)	=		B =	50849.06
μ(c)	=		C =	

The spectrum of NO was fit 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. Spectroscopy, 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=71/2.

Species Tag: = 30009
Version: = 1
Date: = Jan 1984
Contributor: = R. L. Poynter

Species Name: N_2D^+

Lines Listed = 41
Max. Frequency = 3000 GHz
Max. J = 39
LOGSTR = -4
LOGSTR1 =
Isotope Correction = -3.824
Minimum Energy = 0. cm^{-1}
Dipoles : $\mu(a)$ = 3.40
$\mu(b)$ =
$\mu(c)$ =

Q(300.) = 487.62
Q(225.) = 365.939
Q(150.) = 244.264
Q(75.) = 122.620
Q(37.5) = 61.813
Q(18.25) = 31.421
Q(9.375) = 16.241
A =
B = 38554.719
C =

The experimental measurements were reported by T. G. Angerson, T. A. Dixon, N. D. Piltch, R. J. Saykally, P. G. Szanto, and R. C. Woods, (1977), Ap. J. Lett. 216, L85, and by K. V. L. N. Sastry, P. Helminger, E. Herbst, and F. C. DeLucia, (1981), Chem. Phys. Lett. 84, 286.

The dipole moment was assumed 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.) =	147.16
Max. Frequency	= 3000	GHz	Q(225.) =	110.47
Max. J	= 34		Q(150.) =	73.75
LOGSTR	= -2.7		Q(75.) =	37.04
LOGSTR1	=		Q(37.5) =	18.68
Isotope Correction	= -2.690		Q(18.25) =	9.52
Minimum Energy	= 0.	cm^{-1}	Q(9.375) =	4.94
Dipoles: 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), and by M. Bogey, C. Demuynck, and J. L. Destombes (1981), Mol. Physics 43, 1043. A least squares analysis cannot be done with this limited data. The catalogue entries are therefore just a simple calculation from the B and D rotational constants, and no error estimates can be given. The dipole moment is assumed to be the same as for the parent species.

Species Tag:	31002	Species Name:	H_2C-13-O Formaldehyde, ^{13}C isotope
Version:	1		
Date:	Jan 1980		
Contributor:	R. L. Poynter		

Lines Listed	= 601		Q(300.) =	2949.7
Max. Frequency	= 3000	GHz	Q(225.) =	1925.4
Max. J	= 40		Q(150.) =	1047.6
LOGSTR	= -9.3		Q(75.) =	370.9
LOGSTR1	=		Q(37.5) =	131.9
Isotope Correction	= -1.955		Q(18.25) =	45.78
Minimum Energy	= 0.	cm^{-1}	Q(9.375) =	14.13
Dipoles: μ(a)	= 2.331		A =	281930.85
μ(b)	= 0		B =	37811.92
μ(c)	= 0		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 the following papers:

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, Ap. J., 174, 467.

T. Oka, H. Hirakawa, and K. Shimoda, 1960, J. Phys. Soc. Japan, 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, Ap. J. 174, 463; 1971, Ap. J. 169, 429.

The dipole moment was assumed to be the same as the parent $H_2{}^{12}CO$.

Species Tag: 32001
Version: 2
Date: June 1980
Contributor: H. M. Pickett

Lines Listed = 174
Max. Frequency = 3000. GHz
Max. J = 60
LOGSTR = -32
LOGSTR1 =
Isotope Correction = 0
Minimum Energy = 0 cm^{-1}
Dipoles: $\mu(a)$ = magnetic
$\mu(b)$ =
$\mu(c)$ =

Species Name: O_2
Molecular oxygen,
$^{16}O_2$ v=0 state of the
ground $^3\Sigma_g^-$ electronic
state

Q(300.) = 218.655
Q(225.) = 164.129
Q(150.) = 109.605
Q(75.) = 55.198
Q(37.5) = 28.034
Q(18.25) = 14.515
Q(9.375) = 7.871
A =
B = 43099.795
C =

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. Spectroscopy <u>53</u>, 346. The Raman lines of O_2 (M. Loete and H. Berger, 1977, J. Mol. Spectroscopy <u>68</u>, 317) were used with the millimeter wavelength measurements and the submillimeter-line of W. Steinbach and W. Gordy (1973, Phys. Rev <u>A 8</u>, 1953) in a combined fit of the v = 0 and v = 1 transitions. 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. (Lond.) <u>A251</u>, 565. The zero-frequency absorption is included but the frequency is set to a synthetic frequency of |g|J for the given level.

Species Tag: 32002
Version: 3
Date: Dec. 1983
Contributor: H. M. Pickett

Species Name: O_2 V=1 state of the ground $^3\Sigma_g^-$ electronic state

Lines Listed = 153
Max. Frequency = 3000 GHz
Max. J = 60
LOGSTR = -13.2
LOGSTR1 =
Isotope Correction = 0
Minimum Energy = 1556.33 cm^{-1}
Dipoles: $\mu(a)$ = magnetic
$\mu(b)$ =
$\mu(c)$ =

Q(300.) = 218.655
Q(225.) = 164.129
Q(150.) = 109.605
Q(75.) = 55.198
Q(37.5) = 28.034
Q(18.25) = 14.515
Q(9.375) = 7.871
A =
B = 42626.96
C =

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

Species Tag:	32003	Species Name:	CH_3OH
Version:	2		Methyl alcohol (methanol),
Date:	Nov 1980		lowest A, E_1, and E_2
Contributor:	H. M. Pickett		vibrational states

Lines Listed	= 709		Q(300.) =	6414.25
Max. Frequency	= 3000.	GHz	Q(225.) =	4165.82
Max. J	= 12		Q(150.) =	2267.78
LOGSTR	= -10		Q(75.) =	801.68
LOGSTR1	=		Q(37.5) =	283.47
Isotope Correction	= 0		Q(18.25) =	100.21
Minimum Energy	= 0.	cm^{-1}	Q(9.375) =	39.35
Dipoles: μ(a)	= 0.885		A =	127484.
μ(b)	= 1.440		B =	24679.98
μ(c)	= 0.		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, Ap. J. Suppl., _41_. 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 catalogue 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
Version: 1
Date: Feb 1980
Contributor: R. L. Poynter

Species Name: H_2CO-18
Formaldehyde,
^{18}O isotope

Lines Listed = 449
Max. Frequency = 3000 GHz
Max. J = 20
LOGSTR = -9
LOGSTR1 =
Isotope Correction = -2.690
Minimum Energy = 0. cm^{-1}
Dipoles: μ(a) = 2.331
μ(b) =
μ(c) =

Q(300.) = 3017.23
Q(225.) = 1959.75
Q(150.) = 1066.75
Q(75.) = 379.22
Q(37.5) = 134.86
Q(18.25) = 46.81
Q(9.375) = 14.44
A = 281993.0
B = 36903.6
C = 32514.7

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

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. Japan, 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, Ap. J. 174, 463, 1971, Ap. J., 169, 429.

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

Species Tag:	33001		Species Name:	HO_2
Version:	1			Hydroperoxyl radical
Date:	May 1983			
Contributor:	H. M. Pickett			
Lines Listed	= 6174		Q(300.) =	4344.6
Max. Frequency	= 3000	GHz	Q(225.) =	2837.8
Max. J	= 30		Q(150.) =	1547.0
LOGSTR	= -7.		Q(75.) =	548.4
LOGSTR1	= -7.		Q(37.5) =	195.16
Isotope Correction	= 0.		Q(18.25) =	70.21
Minimum Energy	= 0.	cm^{-1}	Q(9.375) =	27.59
Dipoles: 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. DeLucia, 1982, J. Mol. Spectroscopy 94, 426; Y. Beers and C. J. Howard, 1975, J. Chem. Phys. 63, 4121; S. Saito, 1977, J. Mol. Spectrosc. 65, 229.

The spectrum was computed using a full diagonalization of the spin-rotation Hamiltonian.

Species Tag: 34001
Version: 2
Date: Oct 1980
Contributor: H. M. Pickett

Species Name: O-18-O
Molecular oxygen,
single substituted
^{18}O isotope

Lines Listed = 383
Max. Frequency = 3000 GHz
Max. J = 60
LOGSTR = -10.6
LOGSTR1 =
Isotope Correction = -2.389
Minimum Energy = 0. cm^{-1}
Dipoles: μ(a) = magnetic
μ(b) =
μ(c) =

Q(300.) = 462.32
Q(225.) = 346.96
Q(150.) = 231.67
Q(75.) = 116.45
Q(37.5) = 58.92
Q(18.25) = 30.26
Q(9.375) = 16.12
A =
B = 40708.
C =

The measurements and calculational method are from T. Amano and E. Hirota, 1974, J. Mol. Spectroscopy 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. (Lond.) 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 catalogue.

Species Tag: 34002
Version: 2
Date: July 1980
Contributor: R. L. Poynter

Species Name: H_2S
Hydrogen sulfide

Lines Listed = 311
Max. Frequency = 3000 GHz
Max. J = 15
LOGSTR = -8
LOGSTR1 =
Isotope Correction = 0.
Minimum Energy = 0. cm^{-1}
Dipoles: $\mu(a)$ = 0
$\mu(b)$ = 0.974
$\mu(c)$ = 0.

Q(300.) = 514.197
Q(225.) = 333.981
Q(150.) = 182.164
Q(75.) = 65.525
Q(37.5) = 23.865
Q(18.25) = 8.700
Q(9.375) = 2.911
A = 310182.24
B = 270884.05
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 the following papers:

P. Helminger, R. L. Cook, and F. C. DeLucia, 1972, J. Chem. Phys. 56, 4581.

P. Helminger, F. C. DeLucia, 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
Version: 2
Date: Aug 1983
Contributor: R. L. Poynter

Species Name: PH_3
Phosphine

Lines Listed = 142
Max. Frequency = 3000 GHz
Max. J = 19
LOGSTR = -17
LOGSTR1 =
Isotope Correction = 0.
Minimum Energy = 0. cm^{-1}
Dipoles: $\mu(a)$ = 0.000072*
$\mu(b)$ =
$\mu(c)$ = 0.574

Q(300.) = 405.64
Q(225.) = 263.47
Q(150.) = 143.41
Q(75.) = 51.54
Q(37.5) = 18.59
Q(18.25) = 6.958
Q(9.375) = 2.898
A = B
B = 133480.22
C = 117488.39

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*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; and H. M. Pickett, R. L. Poynter and E. A. Cohen, 1981, J. Quant. Spectrosc. and Radiat. Transfer, 26, 197.

The dipole moment measured by P. B. Davies, et al., above, is 0.57395 ± 0.0003D.

Note that the K=3 energy levels are split by vibrational and distortion interactions with the K=0 level for a given J. (H. H. Nielsen and D. M. Dennison, 1947, Phys. Rev. 72, 1011; J. M. Hoffman, H. H. Nielsen and K. N. Rao, 1960, Z. Elektrochem, 63, 606; J. K. G. Watson, 1971, J. Mol. Spectrosc. 40, 536). We flag the lower of the two K=3 energy levels by a minus sign. Thus, a (J, K) = (4, -3) - (3, +3) designation indicates that the transition is between the upper (J, K) = (4, 3) level. Computations always involve only K = |k|. This choice is similar to, but slightly different from that employed by A. G. Maki, R. L. Sams and W. B. Olson, 1973, J. Chem. Phys. 58, 4502, where further details are discussed.

Species Tag: 34004
Version: 2
Date: Oct 1980
Contributor: H. M. Pickett

Species Name: H_2O_2
Hydrogen peroxide,
ground torsional
states

Lines Listed = 883
Max. Frequency = 3000 GHz
Max. J = 23
LOGSTR = -8
LOGSTR1 =
Isotope Correction = 0
Minimum Energy = 0. cm^{-1}
Dipoles: $\mu(a)$ = 0.
$\mu(b)$ = 0.
$\mu(c)$ = 1.5728

Q(300.) = 7651.8
Q(225.) = 4970.0
Q(150.) = 2705.3
Q(75.) = 916.2
Q(37.5) = 288.7
Q(18.25) = 88.77
Q(9.375) = 26.64
A = 301878.
B = 26211.9
C = 25099.14

The spectral lines and method of calculation are from P. Helminger, W. C. Bowman and F. C. DeLucia, 1981, J. Mol. Spec. 85, 120 and W. Bowman, personal communication. Additional lines and the dipole moment were measured by E. A. Cohen and H. M. Pickett, 1981, J. Mol. Spect. 87, 582. The quantum number designation is $v = 0$ for $\tau = 1, 2$ and $v = 1$ for $\tau = 3, 4$.

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

Lines Listed	= 1138		Q(300.) =	430.90
Max. Frequency	= 3000	GHz	Q(225.) =	280.92
Max. J	= 20		Q(150.) =	153.44
LOGSTR	= -11.4		Q(75.) =	54.75
LOGSTR1	=		Q(37.5) =	19.758
Isotope Correction	= -3.523		Q(18.25) =	7.291
Minimum Energy	= 0.	cm^{-1}	Q(9.375) =	2.829
Dipoles: μ(a)	= 0.470		A =	292351.302
μ(b)	= 0.974		B =	147861.801
μ(c)	= 0.		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. Chem. Phys. 40, 257; P. Helminger, R. L. Cook, and F. C. DeLucia, 1971, J. Mol. Spectrosc. 40, 125; P. Helminger, F. C. DeLucia, and W. H. Kirchhoff, 1973, J. Phys. Chem. Ref. Data 2, 215; and from 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:	HCl35
Version:	1			Hydrochloric acid,
Date:	Feb 1980			^{35}Cl isotope
Contributor:	R. L. Poynter and H. M. Pickett			
Lines Listed	= 17		Q(300.) =	81.232
Max. Frequency	= 3000	GHz	Q(225.) =	60.924
Max. J	= 4		Q(150.) =	40.616
LOGSTR	= -1.3		Q(75.) =	21.249
LOGSTR1	=		Q(37.5) =	11.437
Isotope Correction	= -0.122		Q(18.25) =	6.583
Minimum Energy	= 0.	cm^{-1}	Q(9.375) =	4.488
Dipoles: μ(a)	= 1.109		A =	
μ(b)	= 0.		B =	312989.3
μ(c)	= 0.		C =	

The observed lines were measured by F. C. DeLucia, P. Helminger, and W. Gordy, 1971, Phys. Rev., A 3, 1849.

The dipole moment was measured by F. A. deLeeuw and A. Dymanus, 1971, Symposium on Molec. Spect., Columbus, Ohio.

Species Tag: 38001 Species Name: HCl-37
Version: 1 hydrochloric acid,
Date: Feb 1980 ^{37}Cl isotope
Contributor: R. L. Poynter and H. M. Pickett

Lines Listed = 17 Q(300.) = 81.352
Max. Frequency = 3000. GHz Q(225.) = 61.014
Max. J = 4 Q(150.) = 40.676
LOGSTR = -1.3 Q(75.) = 21.278
LOGSTR1 = Q(37.5) = 11.452
Isotope Correction = -0.611 Q(18.25) = 6.590
Minimum Energy = 0. cm^{-1} Q(9.375) = 4.491
Dipoles: μ(a) = 1.109 A =
μ(b) = B = 312519.12
μ(c) = C =

The observed lines were measured by F. C. De Lucia, P. Helminger, and W. Gordy, 1971, Phys. Rev., A 3, 1849.

The dipole moment was measured by F. A. DeLeeuw and A. Dymanus, 1971, Symposium on Molec. Spect., Columbus, Ohio.

Species Tag:	40001	Species Name:	CH_3CCH propyne
Version:	1		
Date:	Dec 1979		
Contributor:	R. L. Poynter		
Lines Listed	= 813	Q(300.) =	5428.80
Max. Frequency	= 3000 GHz	Q(225.) =	3524.70
Max. J	= 79	Q(150.) =	1920.80
LOGSTR	= -4.5 for J>14	Q(75.) =	679.68
LOGSTR1	=	Q(37.5) =	241.25
Isotope Correction	= 0.	Q(18.25) =	88.27
Minimum Energy	= 0. cm^{-1}	Q(9.375) =	34.42
Dipoles: $\mu(a)$	= 0.75	A =	158590.
$\mu(b)$	= 0.	B =	8545.86
$\mu(c)$	= 0.	C =	B

The experimental measurements were obtained from A. Dubrille, 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:	41001	Species Name:	CH_3CN acetonitrile
Version:	1		
Date:	Dec 1979		
Contributor:	R. L. Poynter		
Lines Listed	= 1441	Q(300.) =	15145.00
Max. Frequency	= 3000. GHz	Q(225.) =	9841.34
Max. J	= 82	Q(150.) =	5359.87
LOGSTR	= -4.5 for J>14	Q(75.) =	1896.38
LOGSTR1	=	Q(37.5) =	673.17
Isotope Correction	= 0.	Q(18.25) =	246.34
Minimum Energy	= 0. cm^{-1}	Q(9.375) =	96.10
Dipoles: μ(a)	= 3.919	A =	158290.
μ(b)	= 0.	B =	9198.9
μ(c)	= 0.	C =	B

The experimental measurements were taken from D. Boucher, J. Burie, J. Demaison, A. Dubrille, 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
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: CH_3CC-13-H propyne, ^{13}C isotope on atom 1.

Lines Listed = 822
Max. Frequency = 3000 GHz
Max. J = 80
LOGSTR = -4.5 for J>14
LOGSTR1 =
Isotope Correction = -1.955
Minimum Energy = 0. cm^{-1}
Dipoles: μ(a) = 0.750
μ(b) = 0
μ(c) = 0

Q(300.) = 5596.1
Q(225.) = 3633.1
Q(150.) = 1979.9
Q(75.) = 700.6
Q(37.5) = 248.7
Q(18.25) = 90.97
Q(9.375) = 35.47
A = 158590.
B = 8290.3
C = B

The experimental measurements were taken from D. Boucher, J. Burie, J. Demaison, A. Dubrille, J. Legrand, and B. Segard, 1977, J. Mol. Spect. 54, 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
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: CH_3C-13-CH
propyne, ^{13}C isotope on atom 2.

Lines Listed = 813
Max. Frequency = 3000 GHz
Max. J = 79
LOGSTR = -4.5 for J>14
LOGSTR1 =
Isotope Correction = -1.955
Minimum Energy = 0. cm^{-1}
Dipoles: μ(a) = 0.75
μ(b) =
μ(c) =

Q(300.) = 5431.06
Q(225.) = 3526.18
Q(150.) = 1921.60
Q(75.) = 679.96
Q(37.5) = 241.35
Q(18.25) = 88.31
Q(9.375) = 34.44
A = 158590.
B = 8542.3
C = B

The experimental measurements were taken from D. Boucher, J. Burie, J. Demaison, A. Dubrille, 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
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: H_3C-13-CCH propyne, ^{13}C isotope on atom 3

Lines Listed = 821
Max. Frequency = 3000 GHz
Max. J = 80
LOGSTR = -4.5 for J>14
LOGSTR1 =
Isotope Correction = -1.955
Minimum Energy = 0. cm^{-1}
Dipoles: μ(a) = 0.750
μ(b) = 0.
μ(c) = 0.

Q(300.) = 5580.65
Q(225.) = 3623.10
Q(150.) = 1974.46
Q(75.) = 698.67
Q(37.5) = 247.97
Q(18.25) = 90.72
Q(9.375) = 35.37
A = 158590.
B = 8313.24
C = B

The experimental measurements were taken from D. Boucher, J. Burie, J. Demaison, A. Dubrille, J. Legrand, and B. Segard, 1977, J. Mol. Spect. 64, 290; A. Bauer and S. Maes, 1969, J. Phys. 30, 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
Version: 2
Date: Jan 1984
Contributor: R. L. Poynter

Species Name: CH$_3$CCD

Lines Listed = 822
Max. Frequency = 405 GHz
Max. J = 40
LOGSTR = -7.8
LOGSTR1 =
Isotope Correction = -3.824
Minimum Energy = 0. cm^{-1}
Dipoles: μ(a) = .77
μ(b) =
μ(c) =

Q(300.) = 17192.04
Q(225.) = 11168.37
Q(150.) = 6139.89
Q(75.) = 2243.60
Q(37.5) = 795.34
Q(18.25) = 290.46
Q(9.375) = 113.17
A = 158590.
B = 7788.170
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. Far. Soc. 51, 619; and 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
Version: 2
Date: Aug 1983
Contributor: R. L. Poynter

Species Name: CH_2DCCH
propyne, deuterium
isotope on methyl
carbon atom

Lines Listed = 223
Max. Frequency = 3000 GHz
Max. J = 15
LOGSTR = -10
LOGSTR1 =
Isotope Correction = -3.347
Minimum Energy = 0. cm^{-1}
Dipoles: $\mu(a)$ = 0.750
$\mu(b)$ =
$\mu(c)$ =

Q(300.) = 4428.44
Q(225.) = 2875.21
Q(150.) = 1633.43
Q(75.) = 904.90
Q(37.5) = 410.30
Q(18.25) = 156.17
Q(9.375) = 55.87
A = 117744.370
B = 8155.784
C = 8025.577

The experimental measurements are from L. F. Thomas, E. I. Sherrard, and J. Sheridan, 1955, Trans. Far. Soc. <u>54</u>, 619.

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

Species Tag: 42001
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: CH_3CN-15, acetonitrile, ^{15}N isotope

Lines Listed = 2755
Max. Frequency = 3000 GHz
Max. J = 99
LOGSTR = -5 for J>14
LOGSTR1 =
Isotope Correction = -2.432
Minimum Energy = 0 cm^{-1}
Dipoles : μ(a) = 3.919
μ(b) =
μ(c) =

Q(300.) = 5226.37
Q(225.) = 3394.69
Q(150.) = 1847.57
Q(75.) = 653.73
Q(37.5) = 232.06
Q(18.25) = 84.86
Q(9.375) = 33.08
A = 158290.
B = 9198.8993
C = B

The experimental measurements were obtained from A. Bauer and S. Maes, 1969, J. de Phys. 30, 169; 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 the parent species.

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

Species Name: CH_2CO, ketene

Lines Listed = 835
Max. Frequency = 3000 GHz
Max. J = 29
LOGSTR = -15
LOGSTR1 =
Isotope Correction = 0.
Minimum Energy = 0. cm^{-1}
Dipoles : μ(a) = 1.422
μ(b) =
μ(c) =

Q(300.) = 10322.85
Q(225.) = 6634.38
Q(150.) = 3433.99
Q(75.) = 1285.88
Q(37.5) = 457.09
Q(18.25) = 157.22
Q(9.375) = 47.58
A = 282473.
B = 10293.80
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 the following papers:

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 E. Fabricant, et al. (above).

Species Tag: 43001
Version: 1
Date: Jan 1980
Contributor: R. L. Poynter

Species Name: CHDCO, ketene,
mono deuterium isotope

Lines Listed = 886
Max. Frequency = 3000 GHz
Max. J = 29
LOGSTR = -23
LOGSTR1 =
Isotope Correction = -3.523
Minimum Energy = 0. cm^{-1}
Dipoles : μ(a) = 1.422
μ(b) =
μ(c) =

Q(300.) = 6682.68
Q(225.) = 4340.53
Q(150.) = 2344.00
Q(75.) = 828.70
Q(37.5) = 295.80
Q(18.25) = 105.15
Q(9.375) = 37.50
A = 194313.
B = 9647.396
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 was assumed the same as the parent species.

Species Tag: 44001
Species Name: CS, carbon monosulfide
Version: 2
Date: Jan 1984
Contributor: R. L. Poynter

Lines Listed = 51
Max. Frequency = 2500 GHz
Max. J = 50
LOGSTR = -5
LOGSTR1 =
Isotope Correction = -0.022
Minimum Energy = 0. cm^{-1}
Dipoles : μ(a) = 1.957
μ(b) =
μ(c) =

Q(300.) = 255.205
Q(225.) = 191.823
Q(150.) = 127.968
Q(75.) = 64.151
Q(37.5) = 32.240
Q(18.25) = 16.286
Q(9.375) = 8.316
A =
B = 24495.562
C =

The experimental data were taken from the following papers:

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:	^{28}SiO, silicon monoxide
Version:	2		
Date:	Jan 1984		
Contributor:	R. L. Poynter		

Lines Listed =	31	Q(300.) =	287.210
Max. Frequency =	1350. GHz	Q(225.) =	215.874
Max. J =	30	Q(150.) =	144.344
LOGSTR =	-4	Q(75.) =	72.327
LOGSTR1 =		Q(37.5) =	36.325
Isotope Correction =	-0.035	Q(18.25) =	18.332
Minimum Energy =	0. cm^{-1}	Q(9.375) =	9.339
Dipoles : μ(a) =	3.098	A =	
μ(b) =		B =	21711.967
μ(c) =		C =	

The experimental data were taken from the following papers:

E. Tiemann, 1974, J. Phys. Chem. Ref. Data, T. Torring, 1968, Z Naturforsch. 23a, 77.

E. L. Manson, W. W. Clark, F. C. De Lucia, and W. Gordy, 1977, Phys. Rev. A15, 223.

The dipole moment was reported by J. W. 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.) =	12111.56
Max. Frequency	=	3000	GHz	Q(225.) =	7866.84
Max. J	=	20		Q(150.) =	4282.08
LOGSTR	=	-9		Q(75.) =	1513.94
LOGSTR1	=			Q(37.5) =	535.26
Isotope Correction	=	0.		Q(18.25) =	190.27
Minimum Energy	=	0.	cm^{-1}	Q(9.375) =	67.76
Dipoles : 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: N_2O

Version: 1

Date: Jan 1980

Contributor: R L. Poynter and H. M. Pickett

Lines Listed = 61
Max. Frequency = 3000 GHz
Max. J = 61
LOGSTR =
LOGSTR1 =
Isotope Correction = 0.
Minimum Energy = 0. cm^{-1}
Dipoles : μ(a) = 0.1608
μ(b) =
μ(c) =

Q(300.) = 497.966
Q(225.) = 373.594
Q(150.) = 249.173
Q(75.) = 124.738
Q(37.5) = 62.546
Q(18.25) = 31.434
Q(9.375) = 15.889
A =
B = 12561.637
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
Version: 1
Date: Dec 1930
Contributor: H. M. Pickett

Species Name: CH_3CHO-E
acetaldehyde,
E state

Lines Listed = 691
Max. Frequency = 3000 GHz
Max. J = 15
LOGSTR = -10
LOGSTR1 =
Isotope Correction = 0.
Minimum Energy = 0. cm^{-1}
Dipoles : $\mu(a)$ = 2.55
$\mu(b)$ = 0.870
$\mu(c)$ =

Q(300.) = 12111.56
Q(225.) = 7866.84
Q(150.) = 4282.08
Q(75.) = 1513.94
Q(37.5) = 535.26
Q(18.25) = 189.46
Q(9.375) = 67.29
A = 56448.5
B = 10160.1
C = 9101.3

The experimental lines of the lowest torsional state of E symmetry are listed in A. Bauder, F. J. Lovas, and D. R. Johnson, 1976, J. Chem. Phys. Ref. Data 5, 53. These lines were fit to a Hamiltonian which included terms up to 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 which were 3.5 times the experimental uncertainties in an rms sense. Calculated values of μ^2 S agree with those of Bauder et al. The reference energy is located at the J=0 level of the A state, but intensities are based on E state concentrations.

Species Tag:	45001	Species Name:	C-13-S
Version:	2		Carbon monosulfide,
Date:	Jan 1984		^{13}C isotope
Contributor:	R. Poynter		

Lines Listed =	29	Q(300.) =	270.65
Max. Frequency =	1340 GHz	Q(225.) =	203.24
Max. J =	28	Q(150.) =	135.550
LOGSTR =	-4	Q(75.) =	67.936
LOGSTR1 =		Q(37.5) =	34.127
Isotope Correction =	-1.977	Q(18.25) =	17.235
Minimum Energy =	0. cm^{-1}	Q(9.375) =	8.790
Dipoles : 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 by M. Bogey, C. Demuynck, and J. L. Destombes, 1982, J. Mol. Spect. 95, 35.

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

The maximum J and frequency were limited by the estimated uncertainty in the predicted lines.

Species Tag: 45002
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: ^{29}SiO
silicon monoxide,
^{29}Si isotope

Lines Listed = 66
Max. Frequency = 3000 GHz
Max. J = 66
LOGSTR = -6
LOGSTR1 =
Isotope Correction = -1.327
Minimum Energy = 0. cm^{-1}
Dipoles : μ(a) = 3.098
μ(b) =
μ(c) =

Q(300.) = 290.870
Q(225.) = 219.180
Q(150.) = 146.184
Q(75.) = 73.2318
Q(37.5) = 36.7790
Q(18.25) = 18.5609
Q(9.375) = 9.4515
A =
B = 21514.07
C =

The experimental data were taken from E. Tiemann, 1974, J. Phys. Chem. Ref. Data, 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.

C - 2

Species Tag: 45003
Version: 2
Date: Jan 1981
Contributor: R. L. Poynter

Species Name: Formamide
NH_2CHO

Lines Listed = 3476
Max. Frequency = 3000 GHz
Max. J = 34
LOGSTR = -8 above 120 GHz
LOGSTR1 =
Isotope Correction = 0.
Minimum Energy = 0. cm^{-1}
Dipoles : $\mu(a)$ = 3.616
$\mu(b)$ = 0.852
$\mu(c)$ =

Q(300.) = 29154.14
Q(225.) = 18479.91
Q(150.) = 10313.37
Q(75.) = 3633.29
Q(37.5) = 1293.30
Q(18.25) = 459.199
Q(9.375) = 163.719
A = 72716.954
B = 11373.453
C = 9333.903

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

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:	46001	Species Name:	C^{34}S, carbon monosulfide ^{34}S isotope
Version:	2		
Date:	Jan 1984		
Contributor:	R. L. Poynter		

Lines Listed =	34	Q(300.) =	259.657
Max. Frequency =	1640 GHz	Q(225.) =	194.939
Max. J =	33	Q(150.) =	130.047
LOGSTR =	-4	Q(75.) =	65.1779
LOGSTR1 =		Q(37.5) =	32.7567
Isotope Correction =	-1.376	Q(18.25) =	16.5463
Minimum Energy =	0. cm^{-1}	Q(9.375) =	8.4470
Dipoles : 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 by M. Bogey, C. Demuynck, and J. L. Destombes, 1982, J. Mol. Spect. 95, 35.

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

The maximum J and frequency were limited by the estimated uncertainty in the predicted lines.

Species Tag: 46002
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: ^{30}Si O,
silicon monoxide,
^{30}Si isotope

Lines Listed = 67
Max. Frequency = 3000 GHz
Max. J = 67
LOGSTR = -6
LOGSTR1 =
Isotope Correction = -1.506
Minimum Energy = 0. cm^{-1}
Dipoles : $\mu(a)$ = 3.098
$\mu(b)$ =
$\mu(c)$ =

Q(300.) = 294.374
Q(225.) = 221.259
Q(150.) = 147.911
Q(75.) = 74.1139
Q(37.5) = 37.2220
Q(18.25) = 18.7759
Q(9.375) = 9.5609
A =
B = 21259.48
C =

The experimental data were taken from E. Tiemann, 1974, J. Phys. Chem. Ref. Data, 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:	H_2CS, thioformaldehyde
Version:	1		
Date:	Jan 1980		
Contributor:	R. L. Poynter		

Lines Listed	=	517	Q(300.)	=	5984.11
Max. Frequency	=	3000 GHz	Q(225.)	=	3760.98
Max. J	=	27	Q(150.)	=	2088.82
LOGSTR	=	-11	Q(75.)	=	750.067
LOGSTR1	=		Q(37.5)	=	265.644
Isotope Correction	=	-0.022	Q(18.25)	=	91.1801
Minimum Energy	=	0. cm^{-1}	Q(9.375)	=	27.5233
Dipoles : (a)	=	1.649	A	=	291291.641
(b)	=		B	=	17699.628
(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 were taken from D. R. Johnson, F. J. Lovas, and W. H. Kirchhoff, 1972, J. Phys. Chem. Ref. Data 1, 1011. Other references were taken from this paper.

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:		C_2H_5OH
Version:		1			ethyl alcohol,
Date:		Jan 1980			ground trans state
Contributor:		R. L. Poynter			
Lines Listed	=	1236	Q(300.)	=	17009.8
Max. Frequency	=	3000 GHz	Q(225.)	=	11048.4
Max. J	=	20	Q(150.)	=	6013.13
LOGSTR	=	-11	Q(75.)	=	2020.23
LOGSTR1	=		Q(37.5)	=	747.653
Isotope Correction	=	0.	Q(18.25)	=	267.547
Minimum Energy	=	0. cm^{-1}	Q(9.375)	=	95.2357
Dipoles : 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. Kirchoff, 1972, J. Mol. Spect. 41, 333. The measurements were taken from the following papers:

J. Michielson-Effinger, 1969, J. de Phys. 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
Version: 1
Date: Jan 1980
Contributor: R. L. Poynter

Species Name: HCOOH
formic acid
ground trans state

Lines Listed = 1888
Max. Frequency = 3000 GHz
Max. J = 20
LOGSTR = -11
LOGSTR1 =
Isotope Correction = 0.
Minimum Energy = 0. cm^{-1}
Dipoles : $\mu(a)$ = 1.396
$\mu(b)$ = 0.260
$\mu(c)$ =

Q(300.) = 8883.82
Q(225.) = 5770.32
Q(150.) = 3141.23
Q(75.) = 1085.67
Q(37.5) = 393.460
Q(18.25) = 139.991
Q(9.375) = 49.9344
A = 77512.25
B = 12055.11
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 the following papers:

J. Bellet, C. Samson, G. Steenbeckeliers, and R. Wertheimer, 1971, J. Mol. Structure 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). Inproved values [μ_a = 1.4214(21)D and μ_b = 0.2096(65)D] have been recently reported by H. Kuze, T. Kuga, and T. Shimizu, 1982, J. Mol. Spect. 93, 248.

Species Tag: 46006
Version: 1
Date: Feb 1980
Contributor: R. L. Poynter

Species Name: nitrogen dioxide, NO_2

Lines Listed = 6360
Max. Frequency = 3000. GHz
Max. J = 50
LOGSTR = -7.
LOGSTR1 = -7.
Isotope Correction = 0.
Minimum Energy = 0. cm^{-1}
Dipoles: $\mu(a)$ =
$\mu(b)$ = 0.316
$\mu(c)$ = 0

Q(300.) = 13402
Q(225.) = 8750.
Q(150.) = 4704.
Q(75.) = 1683.
Q(37.5) = 596.
Q(18.25) = 211.8
Q(9.375) = 75.7
A = 239904.
B = 13002.
C = 12305.

The data are from W. C. Bowman and F. C. DeLucia, 1982, J. Chem. Phys. <u>77</u>, 92. The spectra were calculated using a full diagonalization of the Hamiltonian.

Species Tag: 47001
Version: 1
Date: Jan 1980
Contributor: R. L. Poynter

Species Name: $H_2{}^{13}CS$
thioformaldehyde
^{13}C isotope

Lines Listed = 110
Max. Frequency = 335 GHz
Max. J = 10
LOGSTR = -10
LOGSTR1 =
Isotope Correction = -1.977
Minimum Energy = 0. cm^{-1}
Dipoles : μ(a) = 1.649
μ(b) =
μ(c) =

Q(300.) = 6220.14
Q(225.) = 4040.17
Q(150.) = 2114.95
Q(75.) = 777.678
Q(37.5) = 264.363
Q(18.25) = 94.2540
Q(9.375) = 28.6154
A = 291660.0
B = 16998.342
C = 16030.791

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. <u>41</u>, 333. The measurements were taken from the following papers:

D. R. Johnson, F. J. Lovas, and W. H. Kirchhoff, 1972, J. Phys. Chem. Ref. Data <u>1</u>, 1011.

Other references were taken from this paper.

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

Species Tag:	47002	Species Name:	$H^{13}COOH$
Version:	1		formic acid,
Date:	Jan 1980		^{13}C isotope
Contributor:	R. L. Poynter		

Lines Listed	=	1194	Q(300.)	=	8896.12
Max. Frequency	=	3000 GHz	Q(225.)	=	6672.68
Max. J	=	20	Q(150.)	=	3144.85
LOGSTR	=	-10	Q(75.)	=	1094.21
LOGSTR1	=		Q(37.5)	=	399.209
Isotope Correction	=	-1.955	Q(18.25)	=	142.037
Minimum Energy	=	0. cm^{-1}	Q(9.375)	=	50.6640
Dipoles : 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. <u>41</u>, 333. The measurements were taken from the following papers:

J. Bellet, A. Deldalle, C. Samson, G. Steenbeckeliers, and R. Wertheimer, 1971, J. Mol. Structure, 9, 65.

R. G. Lerner, B. P. Dailey, and J. P. Friend, 1957, J. Chem. Phys. 26, 680.

The dipole moment was assumed the same as the parent species, tag #46005.

Species Tag: 47003
Version: 1
Date: Jan 1980
Contributor: R. L. Poynter

Species Name: DCOOH
formic acid,
deuterium isotope
on C atom

Lines Listed = 628
Max. Frequency = 3000 GHz
Max. J = 20
LOGSTR = -10
LOGSTR1 =
Isotope Correction = -3.824
Minimum Energy = 0. cm^{-1}
Dipoles : $\mu(a)$ = 1.396
$\mu(b)$ = 0.260
$\mu(c)$ =

Q(300.) = 10531.2
Q(225.) = 6840.2
Q(150.) = 3626.47
Q(75.) = 1251.4
Q(37.5) = 466.123
Q(18.25) = 165.882
Q(9.375) = 59.1562
A = 57709.33
B = 12055.971
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 the following papers:

J. Bellet, A. Deldalle, C. Samson, G. Steenbeckeliers, and R. Wertheimer, 1971, J. Mol. Structure, 9, 65.

R. G. Lerner, B. P. Dailey, and J. P. Friend, 1957, J. Chem. Phys. 26, 680.

The dipole moment was assumed the same as the parent species, tag #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.) =	9954.87
Max. Frequency =	3000 GHz	Q(225.) =	6465.87
Max. J =	20	Q(150.) =	3519.57
LOGSTR =	-9	Q(75.) =	1213.13
LOGSTR1 =		Q(37.5) =	440.555
Isotope Correction =	-3.824	Q(18.25) =	156.820
Minimum Energy =	0. cm^{-1}	Q(9.375) =	55.9114
Dipoles : μ(a) =	1.396	A =	66100.14
μ(b) =	0.260	B =	11762.577
μ(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 the following papers:

J. Bellet, A. Deldalle, C. Samson, G. Steenbeckeliers, and P. Wertheimer, 1971, J. Mol. Structure, 9, 65.

R. G. Lerner, B. P. Dailey, and J. P. Friend, 1957, J. Chem. Phys. 26, 680.

The dipole moment was assumed the same as the parent species, tag #46005.

Species Tag: 48001
Version: 1
Date: Dec 1979
Contributor: H. M. Pickett

Species Name: SO, sulfur monoxide, $^3\Sigma$ ground state

Lines Listed	= 330	Q(300.) =	850.159
Max. Frequency	= 3000 GHz	Q(225.) =	632.266
Max. J	= 50	Q(150.) =	414.477
LOGSTR	= -6	Q(75.) =	197.515
LOGSTR1	=	Q(37.5) =	90.3441
Isotope Correction	= -0.022	Q(18.25) =	38.8776
Minimum Energy	= 0. cm^{-1}	Q(9.375) =	15.9038
Dipoles : 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. Molec. Spectroscopy 53, 346. The data used is from W. W. Clark and F. C. DeLucia, 1976, J. Molec. Spectroscopy 60, 332. Both electric dipole and magnetic dipole transitions are listed.

Species Tag:	48002	Species Name:	SO, sulfur monoxide $^3\Sigma$ ground state, v=1 vibrational state
Version:	1		
Date:	Dec 1979		
Contributor:	H. M. Pickett		

Lines Listed	= 261	Q(300.) =	850.159
Max. Frequency	= 3000 GHz	Q(225.) =	632.266
Max. J	= 50	Q(150.) =	414.477
LOGSTR	= -8	Q(75.) =	197.615
LOGSTR1	=	Q(37.5) =	90.3441
Isotope Correction	= -0.022	Q(18.75) =	38.8776
Minimum Energy	= 1111.5 cm^{-1}	Q(9.375) =	15.9038
Dipoles : 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. Molec. Spectroscopy <u>53</u>, 346. The data are from T. Amano, E. Hirota, and Y. Morino, 1967, J. Phys. Soc. Japan <u>22</u>, 399. All centrifugal distortion constants were fixed to their ground state values. Magnetic and electric dipole transitions are included.

This state is 1111.5 cm^{-1} above v=0 (G. Herzberg, 1950, Spectra of Diatomic Molecules, Van Nostrand, New York).

Species Tag: 48003
Version: 1
Date: Jan 1980
Contributor: R. L. Poynter

Species Name: $H_2C^{34}S$
thioformaldehyde,
^{34}S isotope

Lines Listed = 111
Max. Frequency = 343 GHz
Max. J = 10
LOGSTR = -9
LOGSTR1 =
Isotope Correction = -1.376
Minimum Energy = 0. cm^{-1}
Dipoles : (a) = 1.647
(b) =
(c) =

Q(300.) = 6084.16
Q(225.) = 4563.52
Q(150.) = 2150.80
Q(75.) = 760.502
Q(37.5) = 259.239
Q(18.25) = 92.2997
Q(9.375) = 28.0092
A = 291660.
B = 17387.949
C = 16376.922

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. R. Johnson, F. J. Lovas and W. H. Kirchhoff, 1972, J. Phys. Chem. Ref. Data 1, 1011. Other references were taken from this paper.

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

Species Tag:	48004	Species Name:	$^{16}O_3$, ozone
Version:	2		
Date:	Mar 1984		
Contributor:	H. M. Pickett		
Lines Listed =	6471	Q(300.) =	3553.04
Max. Frequency =	10000 GHz	Q(225.) =	2263.60
Max. J =	80.	Q(150.) =	1198.67
LOGSTR =	-10.	Q(75.) =	423.448
LOGSTR1 =	-10.	Q(37.5) =	150.037
Isotope Correction =	0.	Q(18.25) =	53.2967
Minimum Energy =	0. cm^{-1}	Q(9.375) =	19.0371
Dipoles : μ(a) =		A =	106535.234
μ(b) =	0.5324	B =	13349.090
μ(c) =		C =	11834.524

The catalog of the ozone lines is based on the work of M. J. C. Depannemaecker, B. Duterage, and M. J. Bellet, 1977, J. Quant. Spect. Radiat. Transfer 17, 519. Additional lines are cited in F. J. Lovas, 1978, J. Phys. Chem. Ref. Data 7, 1445. Further lines were measured at JPL by E. A. Cohen. The ground state lines were fit with the ν_1 and ν_3 lines and infrared lines in the 10μ region simultaneously. The maximum value of K_a is 20.

The dipole moment was reported by M. Lichtenstein, J. J. Gallagher, and S. A. Clough, (1971), J. Mol. Spectrosc. 40, 10.

The partition function includes contributions from all vibrational states.

Species Tag:	48005	Species Name:	O_3
Version:	2		ν_2 vibrational
Date:	Mar 1984		state (010)
Contributor:	H. M. Pickett		

Lines Listed	= 4337	Q(300.) =	3553.04
Max. Frequency	= 3000 GHz	Q(225.) =	2263.60
Max. J	= 60	Q(150.) =	1198.67
LOGSTR	= -10.	Q(75.) =	423.448
LOGSTR1	= -10.	Q(37.5) =	150.037
Isotope Correction	= 0.	Q(18.25) =	53.2967
Minimum Energy	= 700.9 cm^{-1}	Q(9.375) =	19.0371
Dipoles : μ(a)	=	A =	108137.979
μ(b)	= 0.5324	B =	13311.143
μ(c)	=	C =	11765.222

The ν_2 ozone lines were derived from a fit of the data given by M. J. C. Depannemaecker, B. Duterage, and M. J. Bellet, 1977, J. Quant. Spect. and Radiat. Transfer 17, 519. Additional lines are listed in F. J. Lovas, 1978, J. Phys. Chem. Ref. Data., 7, 1445. Further lines were measured at JPL by E. A. Cohen. The maximum valued K is 15.

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

Species Tag: 48006
Version: 2
Date: Mar 1984
Contributor: H. M. Pickett

Species Name: O_3
ν_1, ν_3 vibrational
states (100)
and (001)

Lines Listed = 9459
Max. Frequency = 10000 GHz
Max. J = 80
LOGSTR = -10.
LOGSTR1 = -10.
Isotope Correction = 0.
Minimum Energy = 1042. cm^{-1}
Dipoles : $\mu(a)$ =
$\mu(b)$ = .5324
$\mu(c)$ =

Q(300.) = 3553.04
Q(225.) = 2263.60
Q(150.) = 1198.67
Q(75.) = 423.448
Q(37.5) = 150.037
Q(18.25) = 53.2967
Q(9.375) = 19.0371
A = 104944.
B = 13229.7
C = 11726.6

The rotational lines were measured by T. Tanaka and Y. Morino, 1970, J. Mol. Spec. 33, 538 and A. Barbe, *et al.*, 1977, J. Mol. Spec. 64, 343. The rotational lines of the ground, ν_1 and ν_3 states were fit along with infrared lines in the 10μ region simultaneously. The maximum value of K_a is 20.

The (100) state has a vibrational label of 1, and the (001) state has a vibrational label of 3.

Species Tag: 48007
Version: 1
Date: Mar 1984
Contributor: H. M. Pickett

Species Name: O_3 ν_2 = 2 state
(0,2,0)

Lines Listed = 1779
Max. Frequency = 9999 GHz
Max. J = 50
LOGSTR = -10.
LOGSTR1 = -10.
Isotope Correction = -0
Minimum Energy = 1400. cm^{-1}
Dipoles : $\mu(a)$ =
$\mu(b)$ = 0.5324
$\mu(c)$ =

Q(300.) = 3553.04
Q(225.) = 2263.60
Q(150.) = 1198.67
Q(75.) = 423.448
Q(37.5) = 150.037
Q(18.25) = 53.2967
Q(9.375) = 19.0371
A = 109796.
B = 13273.
C = 11694.

Data measured at JPL were combined with that of T. Tanaka and Y. Morino, 1970, J. Mol. Spectroscop. 33, 538.

Species Tag: 49001
Version: 1
Date: Mar 1984
Contributor: H. M. Pickett

Species Name: $^{16}O-^{17}O-O^{16}$
Ozone symmetric
^{17}O substitution

Lines Listed = 13277
Max. Frequency = 999. GHz
Max. J = 37
LOGSTR = -7.2
LOGSTR1 = -7.2
Isotope Correction = -3.432
Minimum Energy = 0. cm^{-1}
Dipoles : $\mu(a)$ =
$\mu(b)$ = 0.5324
$\mu(c)$ =

Q(300.) = 19114.5
Q(225.) = 13038.6
Q(150.) = 7299.7
Q(75.) = 2597.63
Q(37.5) = 920.348
Q(18.25) = 327.0
Q(9.375) = 116.8
A = 102351.
B = 13350.8
C = 11781.9

The spectra and calculation are from E. A. Cohen and H. M. Pickett, 1983, J. Molec. Str. 97, 97-100.

Species Tag:		49002	Species Name:	^{17}O-^{16}O-^{16}O
Version:		1		Ozone asymmetric
Date:		Mar 1984		^{17}O substitution
Contributor:		H. M. Pickett		
Lines Listed	=	24138	Q(300.) =	40541.5
Max. Frequency	=	9999. GHz	Q(225.) =	2732.5
Max. J	=	37	Q(150.) =	14831.8
LOGSTR	=	-7.5	Q(75.) =	5257.0
LOGSTR1	=	-7.5	Q(37.5) =	1862.4
Isotope Correction	=	-3.131	Q(18.25) =	661.58
Minimum Energy	=	0. cm^{-1}	Q(9.375) =	236.21
Dipoles : μ(a)	=	0.0034	A =	105491.
μ(b)	=	0.5324	B =	12951.
μ(c)	=		C =	11508.

The spectra and calculation are from E. A. Cohen and H. M. Pickett, 1983, J. Molec. Str. 97, 97-100. Additional lines have been measured by E. A. Cohen and K. Hillig. The calculation includes quadrupole interactions of $\Delta N = 0, \pm 1, \pm 2$.

Species Tag:	50001	Species Name:	^{34}SO, sulfur monoxide, $^3\Sigma$ ground state, ^{34}S isotope
Version:	1		
Date:	Dec 1979		
Contributor:	H. M. Pickett		
Lines Listed =	280	Q(300.) =	866.963
Max. Frequency =	3000 GHz	Q(225.) =	644.615
Max. J =	50	Q(150.) =	422.669
LOGSTR =	-6	Q(75.) =	201.326
LOGSTR1 =		Q(37.5) =	92.0449
Isotope Correction =	-1.376	Q(18.25) =	39.5549
Minimum Energy =	0 cm^{-1}	Q(9.375) =	16.1473
Dipoles : 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. Molec. Spectroscopy 53, 346. The data used is reported in E. Tiemann, 1974, J. Phys. Chem. Ref. Data 3, 259. Both electric dipole and magnetic dipole transitions are listed in the catalogue.

Species Tag: 50002 Species Name: $S^{18}O$, sulfur monoxide
Version: 1 $^3\Sigma$ ground state
Date: Dec 1979
Contributor: H. M. Pickett

Lines Listed = 179
Max. Frequency = 3000 GHz
Max. J = 50
LOGSTR = -5
LOGSTR1 =
Isotope Correction = -2.712
Minimum Energy = 0. cm^{-1}
Dipoles : $\mu(a)$ = 1.55
$\mu(b)$ =
$\mu(c)$ =

Q(300.) = 917.488
Q(225.) = 675.460
Q(150.) = 446.684
Q(75.) = 212.814
Q(37.5) = 97.1180
Q(18.25) = 41.6007
Q(9.375) = 16.8850
A =
B = 19929.
C =

The calculational method is described in T. Amano and E. Hirota, 1974, J. Molec. Spectroscopy 53, 346. The value of μ was fixed at -156.51 MHz and $\mu(1)$ was set to zero. Both electric dipole and magnetic dipole transitions are listed in the catalogue. The data used is listed in E. Tiemann, 1974, J. Phys. Chem. Ref. Data. 3, 259.

Species Tag:	50003	Species Name:	$^{16}O^{18}O^{16}O$
Version:	2		ozone, ground state,
Date:	Mar 1984		symmetric ^{18}O isotope
Contributor:	H. M. Pickett and R. L. Poynter		

Lines Listed =	3184	Q(300.) =	3525.34
Max. Frequency =	9999. GHz	Q(225.) =	2445.129
Max. J =	50	Q(150.) =	1247.107
LOGSTR =	-9	Q(75.) =	441.8769
LOGSTR1 =	-9	Q(37.5) =	156.5677
Isotope Correction =	-2.690	Q(18.25) =	55.6161
Minimum Energy =	0. cm^{-1}	Q(9.375) =	19.8610
Dipoles : $\mu(a)$ =		A =	98646.687
$\mu(b)$ =	0.5324	B =	13352.732
$\mu(c)$ =		C =	11731.767

The catalog of symmetric ^{18}O ozone is based on the work of J. Depannemaecker and J. Bellet (1977, J. Mol. Specty. 66, 106). The dipole moment used is the $^{16}O_3$ value. The new version extends the calculation in frequency and J.

Species Tag:	50004	Species Name:	$^{18}O^{16}O^{16}O$,
Version:	2		asymmetric ^{18}O
Date:	Mar 1984		ozone, ground state
Contributor:	H. M. Pickett and R. L. Poynter		

Lines Listed	= 7304	Q(300.) =	7214.414
Max. Frequency	= 9999 GHz	Q(225.) =	4994.599
Max. J	= 40	Q(150.) =	2549.761
LOGSTR	= -9	Q(75.) =	904.0679
LOGSTR1	= -9	Q(37.5) =	320.2580
Isotope Correction	= -2.389	Q(18.25) =	113.7639
Minimum Energy	= 0. cm^{-1}	Q(9.375) =	40.6069
Dipoles : $\mu(a)$	= 0.0068	A =	104573.161
$\mu(b)$	= 0.5324	B =	12591.48
$\mu(c)$	=	C =	11212.5057

The catalog of asymmetric ^{18}O ozone is based on the work of J. Depannemaecker and J. Bellet (1977, J. Mol. Specty. 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 version extends the calculation in frequency and J.

Species Tag:	50005	Species Name:	O_3 symmetric O^{18}
Version:	1		$\nu_2=1$
Date:	Mar 1984		
Contributor:	C. Chiu and E. A. Cohen		

Lines Listed =	2387	Q(300.) =	3525.34
Max. Frequency =	9999 GHz	Q(225.) =	2445.129
Max. J =	50	Q(150.) =	1247.107
LOGSTR =	-8.9	Q(75.) =	441.8769
LOGSTR1 =	-8.9	Q(37.5) =	156.5677
Isotope Correction =	2.690	Q(18.25) =	55.6161
Minimum Energy =	678. cm^{-1}	Q(9.375) =	19.8610
Dipoles : 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 assumed dipoles are based on the ground state. The vibrational energy is an assumed value.

Species: 50006
Version: 1
Date: Mar 1984
Contributor: C. Chiu and E. A. Cohen

Species Name: O_3 asymmetric
^{18}O $\nu_2 = 1$

Lines Listed = 423
Max. Frequency = 9999 GHz
Max. J = 50
LOGSTR = -9.
LOGSTR1 = -9.
Isotope Correction =
Minimum Energy = 693 cm^{-1}
Dipoles : μ(a) = 0.0068
μ(b) = 0.5324
μ(c) =

Q(300.) = 7214.414
Q(225.) = 4994.599
Q(150.) = 2549.761
Q(75.) = 904.0679
Q(37.5) = 320.2580
Q(18.75) = 113.7639
Q(9.375) = 40.6069
A = 106071.8
B = 12556.0
C = 11150.6

New spectra were measured at JPL and were fit to a Watson "S" set Hamiltonian. The assumed dipoles are based on the ground state. The vibrational energy is an assumed value.

Species Tag: 51001

Version: 2

Date: Mar 1984

Contributor: R. L. Poynter

Species Name: HCCCN, cyanoacetylene

Lines Listed = 154
Max. Frequency = 1000 GHz
Max. J = 99
LOGSTR = -7
LOGSTR1 =
Isotope Correction = 0.
Minimum Energy = 0. cm^{-1}
Dipoles : $\mu(a)$ = 3.724
$\mu(b)$ =
$\mu(c)$ =

Q(300.) = 4122.88
Q(225.) = 3093.14
Q(150.) = 2062.53
Q(75.) = 1031.57
Q(37.5) = 516.416
Q(18.25) = 258.643
Q(9.375) = 129.8381
A =
B = 4549.059
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.

Species Tag:	51002	Species Name:	^{35}ClO, chlorine monoxide $^{2}\Pi$ states, ν =0
Version:	2		
Date:	Oct 1980		
Contributor:	H. M. Pickett		

Lines Listed =	2610	Q(300.) =	3291.54
Max. Frequency =	3000 GHz	Q(225.) =	2297.20
Max. J =	87.5	Q(150.) =	1424.30
LOGSTR =	-10	Q(75.) =	689.287
LOGSTR1 =		Q(37.5) =	351.318
Isotope Correction =	-0.122	Q(18.25) =	183.316
Minimum Energy =	0. cm^{-1}	Q(9.375) =	99.7011
Dipoles : $\mu(a)$ =	1.239	A =	
$\mu(b)$ =		B =	18602.865
$\mu(c)$ =		C =	

The experimental lines below 200 GHz are from R. K. Kakar, E. A. Cohen, and M. Geller, 1978, J. Mol. Spec. 70, 243. Lines above 200 GHz were measured at JPL by E. A. Cohen and H. M. Pickett. The lines were fit to a fine structure Hamiltonian which included p_D and q_D terms and centrifugal distortion on B to sixth power in J. The hyperfine terms in the Hamiltonian included all off-diagonal matrix elements for a, b, c, d, η_1, η_2, and η_3. The partition function was determined by a sum over states to F = 86 for both the Ω =3/2 and Ω =1/2 states.

Species Tag: 52001
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: H^{13}CCCN
cyanoacetylene
^{13}C isotope on
atom 1

Lines Listed = 152
Max. Frequency = 1000 GHz
Max. J = 99
LOGSTR = -7
LOGSTR1 =
Isotope Correction = -1.955
Minimum Energy = 0. cm^{-1}
Dipoles : μ(a) = 3.724
μ(b) =
μ(c) =

Q(300.) = 4140.00
Q(225.) = 3105.99
Q(150.) = 2071.10
Q(75.) = 1035.86
Q(37.5) = 518.442
Q(18.25) = 259.717
Q(9.375) = 130.377
A =
B = 4530.198
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 as 3.724D.

Species Tag:	52002	Species Name:	HC^{13}CCN
Version:	1		cyanoacetylene
Date:	Dec 1979		^{13}C isotope on
Contributor:	R. L. Poynter		atom 2

Lines Listed =	146	Q(300.) =	4140.95
Max. Frequency =	1000 GHz	Q(225.) =	3106.71
Max. J =	99	Q(150.) =	2071.10
LOGSTR =	-7	Q(75.) =	1036.10
LOGSTR1 =		Q(37.5) =	518.561
Isotope Correction =	-1.955	Q(18.25) =	259.777
Minimum Energy =	0. cm^{-1}	Q(9.375) =	130.377
Dipoles : 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 as 3.724D.

Species Tag:	52003	Species Name:	$H^{13}CCCN$ cyanoacetylene ^{13}C isotope atom 3
Version:	1		
Date:	Dec 1979		
Contributor:	R. L. Poynter		

Lines Listed =	144	Q(300.) =	4255.01
Max. Frequency =	1000 GHz	Q(225.) =	3192.27
Max. J =	99	Q(150.) =	2128.14
LOGSTR =	-7	Q(75.) =	1064.63
LOGSTR1 =		Q(37.5) =	532.721
Isotope Correction =	-1.955	Q(18.25) =	266.870
Minimum Energy =	0. cm^{-1}	Q(9.375) =	133.937
Dipoles: 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 as 3.724D.

Species Tag:	52004	Species Name:	$HCCC^{15}N$ cyanoacetylene ^{15}N isotope
Version:	1		
Date:	Dec 1979		
Contributor:	R. L. Poynter		
Lines Listed =	99	Q(300.) =	1415.47
Max. Frequency =	1000 GHz	Q(225.) =	1061.94
Max. J =	99	Q(150.) =	708.109
LOGSTR =	-6	Q(75.) =	354.161
LOGSTR1 =		Q(37.5) =	177.256
Isotope Correction =	-2.432	Q(18.25) =	83.7973
Minimum Energy =	0. cm^{-1}	Q(9.375) =	44.5656
Dipoles: $\mu(a)$ =	3.724	A =	
$\mu(b)$ =		B =	4416.75
$\mu(c)$ =		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 as 3.724D.

Species Tag:	52005	Species Name:	DCCCN, cyanoacetylene, deuterium isotope
Version:	1		
Date:	Dec. 1979		
Contributor:	R. L. Poynter		
Lines Listed =	156	Q(300.) =	4443.2393
Max. Frequency =	1000 GHz	Q(225.) =	3332.7310
Max. J =	99	Q(150.) =	2222.2842
LOGSTR =	-7	Q(75.) =	1111.7319
LOGSTR1 =		Q(37.5) =	556.2878
Isotope Correction =	-3.824	Q(18.25) =	278.6121
Minimum Energy =	0. cm^{-1}	Q(9.375) =	139.8297
Dipoles: $\mu(a)$ =	3.724	A =	
$\mu(b)$ =		B =	4221.58
$\mu(c)$ =		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, <u>7</u>, 441.

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Species Tag:	52006	Species Name:	$HO^{35}Cl$, hypochlorous acid
Version:	2		
Date:	Jan 1984		
Contributor:	H. M. Pickett		
Lines Listed =	3919	Q(300.) =	2380.4
Max. Frequency =	10000 GHz	Q(225.) =	1545.4
Max. J =	60	Q(150.) =	840.9
LOGSTR =	-8	Q(75.) =	297.5
LOGSTR1 =	-8	Q(37.5) =	105.5
Isotope Correction =	-0.122	Q(18.25) =	37.66
Minimum Energy =	0. cm^{-1}	Q(9.375) =	14.59
Dipoles: 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. Molec. Spectr. 103, 466. Chrlorine hyperfine structure is omitted in this version of the catalogue since the splittings are generally smaller than the width of lower stratospheric lines. Maximum value of K in the calculation is 20.

Species Tag:	53001	Species Name:	C_2H_3CN, acrylonitrile
Version:	1		
Date:	Jan 1980		
Contributor:	R. L. Poynter		

Lines Listed =	3697		Q(300.) =	26198.1
Max. Frequency =	3000	GHz	Q(225.) =	17016.2
Max. J =	40		Q(150.) =	9262.4
LOGSTR =	-9		Q(75.) =	3243.7
LOGSTR1 =			Q(37.5) =	1159.8
Isotope Correction =	0		Q(18.25) =	410.9
Minimum Energy =	0.	cm^{-1}	Q(9.375) =	145.8
Dipoles: $\mu(a)$ =	3.68		A =	49850.712
$\mu(b)$ =	1.25		B =	4971.0849
$\mu(c)$ =			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 the following papers:

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:	^{37}ClO, chlorine monoxide, ^{37}Cl isotope
Version:	2		
Date:	Oct 1980		
Contributor:	H. M. Pickett		
Lines Listed =	2649	Q(300.) =	3348.1118
Max. Frequency =	3000 GHz	Q(225.) =	2336.6826
Max. J =	85	Q(150.) =	1448.4390
LOGSTR =	-10	Q(75.) =	700.9711
LOGSTR1 =		Q(37.5) =	357.1905
Isotope Correction =	-0.611	Q(18.25) =	186.3374
Minimum Energy =	0. cm^{-1}	Q(9.375) =	101.2744
Dipoles: $\mu(a)$ =	1.239	A =	
$\mu(b)$ =		B =	1828.70
$\mu(c)$ =		C =	

The experimental lines below 200 GHz are from R. K. Kakar, E. A. Cohen, and M. Geller, 1978, J. Mol. Spec. 70, 243. Lines above 200 GHz were measured at JPL by E. A. Cohen and H. M. Pickett. The lines were fit to a fine structure Hamiltonian which included p_D and q_D terms and centrifugal distortion on B to sixth power in J. The hyperfine terms in the Hamiltonian included all off-diagonal matrix elements for a, b, c, d, η_1, η_2, and η_3. The partition function was determined by a sum over states to F = 86 for both the Ω = 1/2 and Ω =3/2 states.

Species Tag:	54001	Species Name:	$CH_2CH^{13}CN$, acrylonitrile, ^{13}C isotope on atom 1
Version:	1		
Date:	Jan 1980		
Contributor:	R. L. Poynter		
Lines Listed =	118	Q(300.) =	26332.9770
Max. Frequency =	3000 GHz	Q(225.) =	17104.0740
Max. J =	10	Q(150.) =	9311.0723
LOGSTR =	-9	Q(75.) =	3291.5420
LOGSTR1 =		Q(37.5) =	1163.8567
Isotope Correction =	-1.955	Q(18.2	358.5091
Minimum Energy =	0. cm^{-1}	Q(9.37	138.3247
Dipoles: μ(a) =	3.68		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 #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 the parent species.

Species Tag:	54002	Species Name:	$CH_2{}^{13}CHCN$, acrylonitrile, ^{13}C isotope on atom 2
Version:	1		
Date:	Jan 1980		
Contributor:	R. L. Poynter		
Lines Listed =	117	Q(300.) =	26662.4960
Max. Frequency =	3000 GHz	Q(225.) =	17318.0740
Max. J =	10	Q(150.) =	9427.5684
LOGSTR =	-9	Q(75.) =	3332.7310
LOGSTR1 =		Q(37.5) =	1178.4197
Isotope Correction =	-1.955	Q(18.25) =	362.9110
Minimum Energy =	0. cm^{-1}	Q(9.375) =	140.0232
Dipoles: 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 #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 the parent species.

Species Tag:	54003	Species Name:	$^{13}CH_2CHCN$, acrylonitrile, ^{13}C isotope on atom 3
Version:	1		
Date:	Jan 1980		
Contributor:	R. L. Poynter		

Lines Listed =	116	Q(300.) =	27089.4530
Max. Frequency =	178 GHz	Q(225.) =	26631.7500
Max. J =	10	Q(150.) =	9578.5527
LOGSTR =	-9	Q(75.) =	3386.0991
LOGSTR1 =		Q(37.5) =	1197.2913
Isotope Correction =	-1.955	Q(18.25) =	366.8595
Minimum Energy =	0. cm^{-1}	Q(9.375) =	141.7098
Dipoles: 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 #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 the parent species.

Species Tag:	54004	Species Name:	CH_2CDCN, acrylonitrile, deuterium isotope on atom 2
Version:	1		
Date:	Jan 1980		
Contributor:	R. L. Poynter		
Lines Listed =	322	Q(300.) =	29696.1680
Max. Frequency =	3000 GHz	Q(225.) =	19288.6940
Max. J =	10	Q(150.) =	10500.2640
LOGSTR =	-10	Q(75.) =	3711.9375
LOGSTR1 =		Q(37.5) =	1312.5034
Isotope Correction =	-3.824	Q(18.25) =	402.1610
Minimum Energy =	0. cm^{-1}	Q(9.375) =	155.4532
Dipoles: $\mu(a)$ =	3.68	A =	40198.6
$\mu(b)$ =	1.25	B =	4934.35
$\mu(c)$ =		C =	4388.41

The methods used on this species were the same as for the parent species, given in tag #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 the parent species.

Species Tag: 54005
Version: 2
Date: Jan 1984
Contributor: H. M. Pickett

Species Name: $HO^{37}Cl$,
hypochlorous acid,
^{37}Cl isotope

Lines Listed = 3923
Max. Frequency = 10000 GHz
Max. J = 60
LOGSTR = -8
LOGSTR1 = -8
Isotope Correction = -0.611
Minimum Energy = 0. cm^{-1}
Dipoles: $\mu(a)$ = 0.3627
$\mu(b)$ = 1.471
$\mu(c)$ =

Q(300.) = 2422.5
Q(225.) = 1572.7
Q(150.) = 855.8
Q(75.) = 302.8
Q(37.5) = 107.33
Q(18.25) = 38.32
Q(9.375) = 14.84
A = 613461.
B = 14850.441
C = 14472.895

The data and calculational method are given in H. E. Singbeil, et al, 1984, J. Molec. Spectr. 103, 466. Chlorine hyperfine structure is omitted in this version of the catalogue since the splittings are generally smaller than the width of lower stratospheric lines. Maximum value of K in the calculation is 20.

Species Tag: 55001
Version: 2
Date: Jan 1981
Contributor: R. L. Poynter

Species Name: C_2H_5CN,
ethyl cyanide

Lines Listed = 3684
Max. Frequency = 3000 GHz
Max. J = 21
LOGSTR = -5 above 160 GHz
LOGSTR1 =
Isotope Correction = 0
Minimum Energy = 0 cm^{-1}
Dipoles: $\mu(a)$ = 3.85
$\mu(b)$ = 1.23
$\mu(c)$ =

Q(300.) = 111840.8900
Q(225.) = 70892.5160
Q(150.) = 39554.9140
Q(75.) = 12589.2560
Q(37.5) = 4595.1553
Q(18.25) = 1406.3713
Q(9.375) = 650.8787
A = 27663.66
B = 4714.144
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 the following papers:

J. Burie, J. Demaison, A. Dubrille, 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, Ap. 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:		$CH_3CH_2{}^{13}CN$, ethyl cyanide,. ^{13}C isotope on atom 1
Version:		2			
Date:		Jan 1981			
Contributor:		R. L. Poynter			
Lines Listed	=	1183	Q(300.)	=	112460.3700
Max. Frequency	=	3000 GHz	Q(225.)	=	71285.1870
Max. J	=	10	Q(150.)	=	39774.0860
LOGSTR	=	-5 above 160 GHz	Q(75.)	=	12659.0120
LOGSTR1	=		Q(37.5)	=	4620.6172
Isotope Correction	=	-1.955	Q(18.25)	=	1414.1650
Minimum Energy	=	0 cm^{-1}	Q(9.375)	=	654.4858
Dipoles: (a)	=	3.84	A	=	27634.94
(b)	=	1.37	B	=	4689.805
(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 the same as in the parent species, tag #55001.

Species Tag: 56002 Species Name: $CH_3{}^{13}CH_2CN$, ^{13}C isotope on atom 2
Version: 2
Date: Jan 1981
Contributor: R. L. Poynter

Lines Listed =	1252	Q(300.) =	113684.2800
Max. Frequency =	3000 GHz	Q(225.) =	72060.9840
Max. J =	10	Q(150.) =	40206.7970
LOGSTR =	-9 below 160 GHz	Q(75.) =	12796.7320
LOGSTR1 =	-5 above 160 GHz	Q(37.5) =	4670.8945
Isotope Correction =	-1.955	Q(18.25) =	1429.5522
Minimum Energy =	0 cm^{-1}	Q(9.375) =	661.6073
Dipoles: (a) =	3.84	A =	27045.40
(b) =	1.37	B =	4697.868
(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 the same as in the parent species, tag #55001.

Species Tag:	56003	Species Name:	$^{13}CH_3CH_2CN$, ethyl cyanide, ^{13}C isotope on atom 3
Version:	2		
Date:	Jan 1981		
Contributor:	R. L. Poynter		
Lines Listed =	1183	Q(300.) =	115292.3300
Max. Frequency =	3000 GHz	Q(225.) =	73080.2660
Max. J =	10	Q(150.) =	40775.6020
LOGSTR =	-9 below 160 GHz	Q(75.) =	12977.7660
LOGSTR1 =	-5 above 160 GHz	Q(37.5) =	4736.9639
Isotope Correction =	-1.955	Q(18.25) =	1449.4407
Minimum Energy =	0 cm^{-1}	Q(9.375) =	670.9657
Dipoles: (a) =	3.84	A =	27342.174
(b) =	1.37	B =	4597.939
(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 the same as in the parent species, tag #55001.

Species Tag:	56004	Species Name:	$CH_3CH_2C^{15}N$, ethyl cyanide, ^{15}N isotope
Version:	1		
Date:	Jan 1980		
Contributor:	R. L. Poynter		
Lines Listed =	1621	Q(300.) =	38458.0
Max. Frequency =	3000 GHz	Q(225.) =	24980.4
Max. J =	20	Q(150.) =	13598.7
LOGSTR =	-9	Q(75.) =	3966.4
LOGSTR1 =		Q(37.5) =	1542.4
Isotope Correction =	-2.432	Q(18.25) =	598.1
Minimum Energy =	0 cm^{-1}	Q(9.375) =	213.9
Dipoles: 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 the same as in the parent species, tag #55001.

Species Tag:	56005	Species Name:	CH_2DCH_2CN-s, ethyl cyanide, deuterium isotope on methyl carbon trans to CN group
Version:	2		
Date:	Jan 1981		
Contributor:	R. L. Poynter		
Lines Listed =	1166	Q(300.) =	118795.
Max. Frequency =	3000 GHz	Q(225.) =	75300.
Max. J =	10	Q(150.) =	42000.
LOGSTR =	-9 below 160 GHz	Q(75.) =	14849.
LOGSTR1 =	-5 above 160 GHz	Q(37.5) =	5250.
Isotope Correction =	-3.347	Q(18.25) =	1787.8
Minimum Energy =	0 cm^{-1}	Q(9.375) =	607.95
Dipoles: 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 the parent species.

Species Tag:	56006	Species Name:	CH_2DCH_2CN-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.) =	121059.9
Max. Frequency =	3000 GHz	Q(225.) =	76736.2
Max. J =	10	Q(150.) =	42815.4
LOGSTR =	-9 below 160 GHz	Q(75.) =	15132.5
LOGSTR1 =	-5 above 160 GHz	Q(37.5) =	5350.1
Isotope Correction =	-3.347	Q(18.25) =	1827.2
Minimum Energy =	0. cm^{-1}	Q(9.375) =	623.25
Dipoles: 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, H. M. Heise, and H. Dreizler, 1973, Z. Naturforsch. 29a, 164.

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

Species Tag:	60001	Species Name:	OCS carbonyl sulfide
Version:	2		
Date:	Jan 1981		
Contributor:	R. L. Poynter		

Lines Listed	= 99	Q(300.) =	1028.2539
Max. Frequency	= 3000 GHz	Q(225.) =	771.6135
Max. J	= 99	Q(150.) =	514.3989
LOGSTR	= -7	Q(75.) =	257.2764
LOGSTR1	=	Q(37.5) =	128.8250
Isotope Correction	= -0.022	Q(18.25) =	64.5803
Minimum Energy	= 0. cm^{-1}	Q(9.375) =	32.4565
Dipoles: $\mu(a)$	= 0.715	A =	
$\mu(b)$	=	B =	6081.4921
$\mu(c)$	=	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:	$^{28}Si^{32}S$ silicon monosulfide
Version:	1		
Date:	Dec 1979		
Contributor:	R. L. Poynter		
Lines Listed =	97	Q(300.) =	688.9700
Max. Frequency =	3000 GHz	Q(225.) =	517.1307
Max. J =	97	Q(150.) =	344.8263
LOGSTR =	-5	Q(75.) =	172.5440
LOGSTR1 =		Q(37.5) =	86.4172
Isotope Correction =	-0.057	Q(18.25) =	43.3711
Minimum Energy =	0. cm^{-1}	Q(9.375) =	21.8575
Dipoles: $\mu(a)$ =	1.730	A =	
$\mu(b)$ =		B =	9077.45
$\mu(c)$ =		C =	

The experimental measurements are summarized in E. Tiemann, 1976, J. Phys. Chem. Ref. Data, 5, 1147.

The dipole moment was measured by J. Hoeft, F. J. Lovas, E. Tiemann, and T. Törring, 1969, Z. Naturforsch. 24a, 1422.

Species Tag: 61001
Version: 2
Date: Jan 1981
Contributor: R. L. Poynter

Species Name: $O^{13}CS$
carbonyl sulfide,
^{13}C isotopic species

Lines Listed = 99
Max. Frequency = 3000 GHz
Max. J = 99
LOGSTR = -6.4
LOGSTR1 =
Isotope Correction = -1.977
Minimum Energy = 0. cm^{-1}
Dipoles: μ(a) = 0.715
μ(b) =
μ(c) =

Q(300.) = 1031.5737
Q(225.) = 773.9269
Q(150.) = 515.9410
Q(75.) = 258.1666
Q(37.5) = 129.2409
Q(18.25) = 64.7888
Q(9.375) = 32.5612
A =
B = 6061.924
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 the parent species.

Species Tag: 61002
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: $^{29}\mathrm{Si}^{32}\mathrm{S}$
silicon monoxide
$^{29}\mathrm{Si}$ isotopic species

Lines Listed = 98
Max. Frequency = 3000 GHz
Max. J = 98
LOGSTR = -5
LOGSTR1 =
Isotope Correction = -1.349
Minimum Energy = 0 cm^{-1}
Dipoles: μ(a) = 1.730
μ(b) =
μ(c) =

Q(300.) = 701.7784
Q(225.) = 526.8662
Q(150.) = 351.2369
Q(75.) = 175.7521
Q(37.5) = 88.0239
Q(18.25) = 44.1774
Q(9.375) = 22.2587
A =
B = 8910.66
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 the parent species.

Species Tag: 62001
Version: 2
Date: Jan 1981
Contributor: R. L. Poynter

Species Name: OC^{34}S
carbonyl sulfide
^{34}S isotopic species

Lines Listed = 99
Max. Frequency = 3000 GHz
Max. J = 99
LOGSTR = -6.4
LOGSTR1 =
Isotope Correction = -1.376
Minimum Energy = 0. cm^{-1}
Dipoles: μ(a) = 0.715
μ(b) =
μ(c) =

Q(300.) = 1053.9019
Q(225.) = 777.6780
Q(150.) = 527.2301
Q(75.) = 263.7545
Q(37.5) = 132.0383
Q(18.25) = 66.1911
Q(9.375) = 33.2583
A =
B = 5932.8338
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 the parent species.

Species Tag:	62002	Species Name:	^{18}OCS, carbonyl sulfide, ^{18}O isotopic species
Version:	2		
Date:	Jan 1981		
Contributor:	R. L. Poynter		

Lines Listed =	99	Q(300.) =	1095.9731
Max. Frequency =	3000 GHz	Q(225.) =	822.4320
Max. J =	99	Q(150.) =	548.1509
LOGSTR =	-6.4	Q(75.) =	274.2837
LOGSTR1 =		Q(37.5) =	137.3093
Isotope Correction =	-2.712	Q(18.25) =	68.8176
Minimum Energy =	0 cm^{-1}	Q(9.375) =	34.5780
Dipoles: $\mu(a)$ =	0.715	A =	
$\mu(b)$ =		B =	5704.8574
$\mu(c)$ =		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 the parent species.

Species Tag:	62003	Species Name:	$^{30}Si^{32}S$, silicon monosulfide, ^{30}Si isotopic species
Version:	1		
Date:	Dec 1979		
Contributor:	R. L. Poynter		
Lines Listed =	99	Q(300.) =	714.3315
Max. Frequency =	3000 GHz	Q(225.) =	536.1669
Max. J =	99	Q(150.) =	357.4372
LOGSTR =	-5	Q(75.) =	178.8546
LOGSTR1 =		Q(37.5) =	89.5984
Isotope Correction =	-1.528	Q(18.25) =	44.9573
Minimum Energy =	0 cm^{-1}	Q(9.375) =	22.6465
Dipoles: 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 the parent species.

Species Tag:	62004	Species Name:	$^{28}Si^{34}S$, silicon monosulfide, ^{34}S isotopic species
Version:	1		
Date:	Dec 1979		
Contributor:	R. L. Poynter		
Lines Listed =	99	Q(300.) =	708.2720
Max. Frequency =	3000 GHz	Q(225.) =	531.7408
Max. J =	99	Q(150.) =	354.4869
LOGSTR =	-5	Q(75.) =	177.3781
LOGSTR1 =		Q(37.5) =	88.8383
Isotope Correction =	1.411	Q(18.25) =	44.5862
Minimum Energy =	0. cm^{-1}	Q(9.375) =	22.4647
Dipoles: $\mu(a)$ =	1.730	A =	
$\mu(b)$ =		B =	8828.86
$\mu(c)$ =		C =	

The measurements were taken from the data set given in F. J. Lovas, 1978, J. Phys. Chem. Ref. Data, 7, 1445.

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

Species Tag:	63001	Species Name:	HNO_3,
Version:	2		nitric acid
Date:	Jun 1983		
Contributor:	H. M. Pickett and R. L. Poynter		

Lines Listed =	24767		Q(300.) =	27938.3360
Max. Frequency =	3000	GHz	Q(225.) =	18150.9490
Max. J =	80		Q(150.) =	9878.7090
LOGSTR =	-6.5		Q(75.) =	3493.8193
LOGSTR1 =	-6.5		Q(37.5) =	1236.8015
Isotope Correction =	0		Q(18.25) =	438.3291
Minimum Energy =	0.	cm^{-1}	Q(9.375) =	155.8116
Dipoles: $\mu(a)$ =	1.986		A =	13010.9867
$\mu(b)$ =	0.882		B =	12099.9025
$\mu(c)$ =			C =	6260.6680

The data set used in this fit includes the microwave and submillimeter lines reported by G. Cazzoli and F. C. DeLucia, (1979), J. Mol. Spectrosc. 76, 131, by W. C. Bowman, F. C. DeLucia, and P. Helminger, (1981), J. Mol. Spectrosc. 88, 431, by P. N. Ghosh, C. E. Blom, and A. Bauder, (1981), J. Mol. Spectrosc. 89, 159, and the far infrared lines measured by K. M. Evenson, (1983), private communication. Inclusion of the data from this last source produces a more reliable prediction of the far infrared transitions.

The dipole moment was taken from the remeasurements reported by A. P. Cox and J. M. Riveros, (1965), J. Chem. Phys. 42, 3106. Very small quadrupole splittings were resolvable for only the $J = 1 \leftarrow 0$ 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:	64001	Species Name:	S_2 ,
Version:	1		
Date:	Oct 1979		diatomic sulfur
Contributor:	H. M. Pickett		
			v=0, $^3\Sigma_g^-$
			ground state

Lines Listed	=	34		Q(300.) =	588.1659
Max. Frequency	=	3000	GHz	Q(225.) =	478.8508
Max. J	=	35		Q(150.) =	340.0165
LOGSTR	=	-8.4		Q(75.) =	174.3814
LOGSTR1	=			Q(37.5) =	87.7608
Isotope Correction	=	-0.044		Q(18.25) =	44.4836
Minimum Energy	=	0.	cm^{-1}	Q(9.375) =	22.9087
Dipoles: μ(a)	=			A =	
magnetic 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. Specty. 75, 53. The calculational method used is from T. Amano and E. Hirota, 1974, J. Mol. Specty. 53, 346. For S_2, the parameter μ(1) is assumed to be zero. Only transitions between states with J = N and J = N - 1 are listed because the energies of the J = N + 1 states are uncertain by more than 1 GHz. All the neglected transitions from J = N + 1 states lie above 450 GHz for J < 35.

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 Σ = 0 and the J = N - 1 and J = N states correlate with Σ = ± 1 states of $p = \pm (-1)^J$ inversion parity, respectively.

The value of Q is determined from a sum over states to J = 50.

Species Tag: 64002
Version: 2
Date: Jun 1983
Contributor: R. L. Poynter

Species Name: SO$_2$,
sulfur dioxide

Lines Listed = 9622
Max. Frequency = 10000 GHz
Max. J = 74
LOGSTR = -10
LOGSTR1 = -10
Isotope Correction = -0.022
Minimum Energy = 0 cm^{-1}
Dipoles: $\mu(a)$ =
$\mu(b)$ = 1.633
$\mu(c)$ =

Q(300.) = 5899.2969
Q(225.) = 3765.3037
Q(150.) = 2075.8706
Q(75.) = 738.9240
Q(37.5) = 261.6373
Q(18.25) = 92.8325
Q(9.375) = 33.0674
A = 60778.558
B = 10317.913
C = 8799.652

The experimental measurements are summarized in F. J. Lovas, 1978, J. Phys. Chem. Ref. Data 7, 1445. Selected additional lines were taken from M. Carlotti, et al., 1984, J. Molec. Spec., (submitted).

The dipole moment was taken from D. Patel, D. Margolese, and T. R. Dyke, 1979, J. Chem. Phys. 70, 2740.

This version is a refit of all lines up through J = 74, using a new fitting program. The prediction only includes lines up through K=28.

Species Tag:	75001	Species Name:	HC_5N ,
Version:	1		cyanodiacetylene
Date:	Dec 1979		
Contributor:	R. L. Poynter		

Lines Listed	=	99		Q(300.) =	4695.6914
Max. Frequency	=	300	GHz	Q(225.) =	3315.8906
Max. J	=	99		Q(150.) =	2314.7271
LOGSTR	=	-6.6		Q(75.) =	1174.0852
LOGSTR1	=			Q(37.5) =	587.2181
Isotope Correction	=	0		Q(18.25) =	293.7650
Minimum Energy	=	0	cm^{-1}	Q(9.375) =	147.0618
Dipoles: μ(a)	=	4.330		A =	
μ(b)	=			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 the same authors.

Species Tag: 76001
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: HCCCC^{13}CN, cyanodiacetylene, ^{13}C isotope on atom 1

Lines Listed = 99
Max. Frequency = 300 GHz
Max. J = 99
LOGSTR = -6.6
LOGSTR1 =
Isotope Correction = -1.933
Minimum Energy = 0. cm^{-1}
Dipoles: $\mu(a)$ = 4.330
$\mu(b)$ =
$\mu(c)$ =

Q(300.) = 4742.4238
Q(225.) = 3448.2642
Q(150.) = 2336.6826
Q(75.) = 1185.7676
Q(37.5) = 593.0616
Q(18.25) = 296.6880
Q(9.375) = 148.5251
A =
B = 1318.18
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 the parent species.

Species Tag:	76002	Species Name:	HCCC^{13}CCN, cyanodiacetylene, ^{13}C isotope on atom 2
Version:	1		
Date:	Dec 1979		
Contributor:	R. L. Poynter		

Lines Listed	=	99		Q(300.) =	4700.0195
Max. Frequency	=	300	GHz	Q(225.) =	3417.4316
Max. J	=	99		Q(150.) =	2316.8604
LOGSTR	=	-6.6		Q(75.) =	1174.8972
LOGSTR1	=	-1.955		Q(37.5) =	587.7594
Isotope Correction	=	0		Q(18.25) =	294.0357
Minimum Energy	=		cm^{-1}	Q(9.375) =	147.1974
Dipoles: $\mu(a)$	=	4.329		A =	
$\mu(b)$	=			B =	1330.11
$\mu(c)$	=			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 the parent species.

Species Tag: 76003
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: HCC^{13}CCCN,
cyanodiacetylene,
^{13}C isotope
on atom 3

Lines Listed = 99
Max. Frequency = 300 GHz
Max. J = 99
LOGSTR = -6.6
LOGSTR1 =
Isotope Correction = -1.955
Minimum Energy = 0 cm^{-1}
Dipoles: $\mu(a)$ = 4.329
$\mu(b)$ =
$\mu(c)$ =

Q(300.) = 4700.0195
Q(225.) = 3417.4316
Q(150.) = 2317.3931
Q(75.) = 1175.1672
Q(37.5) = 587.8950
Q(18.25) = 294.1033
Q(9.375) = 147.2313
A =
B = 1329.95
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 the parent species.

Species Tag: 76004
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: $HC^{13}CCCCN$, cyanodiacetylene, ^{13}C isotope on atom 4

Lines Listed = 99
Max. Frequency = 300 GHz
Max. J = 99
LOGSTR = -6.6
LOGSTR1 =
Isotope Correction = -1.955
Minimum Energy = 0 cm^{-1}
Dipoles: $\mu(a)$ = 4.329
$\mu(b)$ =
$\mu(c)$ =

Q(300.) = 4744.6045
Q(225.) = 3449.8496
Q(150.) = 2337.2217
Q(75.) = 1186.0413
Q(37.5) = 593.3350
Q(18.25) = 296.8244
Q(9.375) = 148.5935
A =
B = 1317.689
C =

The experimental measurements were taken from A. J. Alexander, H. W. Kroto, and D. R. M. Walton, 1976, J. Mol. Spect. <u>62</u>, 175.

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

Species Tag:	76005	Species Name:	H^{13}CCCCCN,
Version:	1		cyanodiacetylene,
Date:	Dec 1979		^{13}C isotope
Contributor:	R. L. Poynter		on atom 5

Lines Listed =	99	Q(300.) =	4820.5898
Max. Frequency =	300 GHz	Q(225.) =	3500.2559
Max. J =	99	Q(150.) =	2372.4639
LOGSTR =	-6.6	Q(75.) =	1205.3130
LOGSTR1 =		Q(37.5) =	602.9758
Isotope Correction =	-1.955	Q(18.25) =	301.6474
Minimum Energy =	0 cm^{-1}	Q(9.375) =	150.9731
Dipoles: 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 the parent species.

Species Tag:	76006	Species Name:	HC$_5$^{15}N, cyanodiacetylene, ^{15}N isotopic species
Version:	1		
Date:	Dec 1979		
Contributor:	R. L. Poynter		

Lines Listed =	99	Q(300.) =	4813.9287
Max. Frequency =	300 GHz	Q(225.) =	3495.4258
Max. J =	99	Q(150.) =	2369.7368
LOGSTR =	-6.6	Q(75.) =	1203.3718
LOGSTR1 =		Q(37.5) =	602.0048
Isotope Correction =	-2.432	Q(18.25) =	301.1616
Minimum Energy =	0 cm^{-1}	Q(9.375) =	150.7648
Dipoles: 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
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: DC_5N,
cyanodiacetylene,
D isotopic species

Lines Listed = 99
Max. Frequency = 300 GHz
Max. J = 99
LOGSTR = -6.6
LOGSTR1 =
Isotope Correction = -3.824
Minimum Energy = 0 cm^{-1}
Dipoles: μ(a) = 4.329
μ(b) =
μ(c) =

Q(300.) = 4918.1348
Q(225.) = 3564.5166
Q(150.) = 2417.1284
Q(75.) = 1229.4199
Q(37.5) = 615.0352
Q(18.25) = 307.6805
Q(9.375) = 153.9927
A =
B = 1271.056
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 the parent species.

Species Tag:	80001	Species Name:	$H^{79}Br$,
Version:	1		Hydrogen Bromide,
Date:	Feb 1980		^{79}Br isotopic species
Contributor:	R. L. Poynter and H. M. Pickett		

Lines Listed	=	19		Q(300.)	=	101.2045
Max. Frequency	=	10000	GHz	Q(225.)	=	73.3500
Max. J	=	6		Q(150.)	=	50.3732
LOGSTR	=	-2.2		Q(75.)	=	26.3512
LOGSTR1	=			Q(37.5)	=	13.9123
Isotope Correction	=	-2.96		Q(18.25)	=	.7732
Minimum Energy	=	0	cm^{-1}	Q(9.375)	=	4.9340
Dipoles: $\mu(a)$	=	0.828		A	=	
$\mu(b)$	=			B	=	250357.6
$\mu(c)$	=			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:	$H^{81}Br$, Hydrogen Bromide, ^{81}Br isotopic species
Version:	1		
Date:	Feb 1980		
Contributor:	R. L. Poynter and H. M. Pickett		

Lines Listed =	19	Q(300.) =	101.2511
Max. Frequency =	10000 GHz	Q(225.) =	73.3668
Max. J =	6	Q(150.) =	50.3848
LOGSTR =	-2.2	Q(75.) =	26.3573
LOGSTR1 =		Q(37.5) =	13.9155
Isotope Correction =	-0.306	Q(18.25) =	7.7750
Minimum Energy =	0. cm^{-1}	Q(9.375) =	4.9351
Dipoles: 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:	^{79}BrO ,
Version:	1		Bromine Monoxide,
Date:	Feb 1980		^{79}Br isotopic species,
Contributor:	H. M. Pickett		$^{2}\Pi_{3/2}$ state

Lines Listed =	850	Q(300.) =	3897.6226
Max. Frequency =	1300 GHz	Q(225.) =	2938.3271
Max. J =	49	Q(150.) =	1965.1685
LOGSTR =	-9	Q(75.) =	989.4642
LOGSTR1 =		Q(37.5) =	501.9954
Isotope Correction =	-0.296	Q(18.25) =	259.5374
Minimum Energy =	0 cm^{-1}	Q(9.375) =	136.8043
Dipoles: μ(a) =	1.765	A =	
μ(b) =		B =	12830.4
μ(c) =		C =	

The 63 GHz spectrum of BrO is referenced in F. J. Lovas and E. Tiemann, 1974, J. Phys. Chem. Ref. Data 3, 653. The other lines were measured at JPL by E. A. Cohen and H. M. Pickett, and a new fit was made which included these lines.

Species Tag:	97001	Species Name:	^{81}BrO , Bromine Monoxide, ^{81}Br isotopic species, $^{2}\Pi_{3/2}$ state
Version:	1		
Date:	Feb 1980		
Contributor:	H. M. Pickett		
Lines Listed =	850	Q(300.) =	3913.8101
Max. Frequency =	1500 GHz	Q(225.) =	2950.5308
Max. J =	49	Q(150.) =	1973.3323
LOGSTR =	-9	Q(75.) =	993.5737
LOGSTR1 =		Q(37.5) =	503.9649
Isotope Correction =	-0.306	Q(18.75) =	259.2984
Minimum Energy =	0 cm^{-1}	Q(9.375) =	137.2459
Dipoles: μ(a) =	1.794	A =	
μ(b) =		B =	12777.08
μ(c) =		C =	

The 63 GHz spectrum of BrO is referenced in F. J. Lovas and E. Tiemann, 1974, J. Phys. Chem. Ref. Data 3, 653. The other lines were measured at JPL by E. A. Cohen and H. M. Pickett, and a new fit was made which included these lines.

Species Tag: 97002
Version: 1
Date: Mar 1984
Contributor: H. M. Pickett

Species Name: $^{35}ClNO_3$
Chlorine nitrate

Lines Listed = 4198
Max. Frequency = 3000 GHz
Max. J = 60
LOGSTR = -6
LOGSTR1 = -6
Isotope Correction = -0.122
Minimum Energy = 0 cm^{-1}
Dipoles: $\mu(a)$ = 0.72
$\mu(b)$ = 0.28
$\mu(c)$ = 0

Q(300.) = 100540.
Q(225.) = 65303.
Q(150.) = 35546.
Q(75.) = 12567.
Q(37.5) = 4447.
Q(18.25) = 1574.
Q(9.375) = 557.
A = 12105.8
B = 2777.0
C = 2258.1

The data are taken from R. D. Suenram and F. J. Lovas, 1977, J. Molec. Spectrosc. 65, 239 (1977), and chlorine hyperfine structure is omitted in this version of the catalogue since the splittings are generally smaller than the width of lower stratospheric lines.

Species Tag: 99001
Version: 1
Date: Mar 1984
Contributor: H. M. Pickett

Species Name: $^{37}\mathrm{ClNO_3}$
Chlorine nitrate

Lines Listed = 4182
Max. Frequency = 3000 GHz
Max. J = 60
LOGSTR = -6
LOGSTR1 = -6
Isotope Correction = -0.611
Minimum Energy = 0 cm^{-1}
Dipoles: $\mu(a)$ = 0.72
$\mu(b)$ = 0.28
$\mu(c)$ = 0

Q(300.) = 103108.
Q(225.) = 66971.
Q(150.) = 36454.
Q(75.) = 12888.
Q(37.5) = 4561.
Q(18.25) = 1614.
Q(9.375) = 572.
A = 12105.4
B = 2707.6
C = 2207.6

The data are taken from R. D. Suenram and F. J. Lovas, 1977, J. Molec. Spectrosc. 65, 239 (1977), and chlorine hyperfine structure is omitted in this version of the catalogue since the splittings are generally smaller than the width of lower stratospheric lines.