

JPL PUBLICATION 80-23, REVISION 2

(NASA-CR-173899) SUBMILLIMETER, MILLIMETER,
AND MICROWAVE SPECTRAL LINE CATALOGUE (Jet
Propulsion Lab.) 171 p HC AC8/MF A01

N84-32448

CSSL 07D

Unclas

G3/25 23826

Submillimeter, Millimeter, and Microwave Spectral Line Catalogue

R.L. Poynter
H.M. Pickett



June 1, 1984



National Aeronautics and
Space Administration

Jet Propulsion Laboratory
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The research described in this publication was carried out by the Jet Propulsion Laboratory, California Institute of Technology, under contract with the National Aeronautics and Space Administration.

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	TAG NAME	TAG NAME
13002 CH	29004 HCU	49001 03-SYM-0-17
17004 NH3-V2	29005 NNH+	49002 03-ASYM-0-17
20001 D2O	30009 NND+	50005 03-S-018-V2
25001 CCH	33001 HO2	50006 03-A-018-V2
26001 CN	46006 NO2	97002 CL-35-NO3
26002 CN-V1	48007 03-2V2	99001 CL-37-NO3

Revised Species, Rev. 2 (30)

TAG NAME	TAG NAME	TAG NAME
16001 O-ATOM	30002 HC-13-0+	46001 CS-34
17001 OH	30003 DCO+	48004 O3
17002 NH3	31001 HCO-18+	48005 03-V2
18001 OD	32001 O2	48006 03-V1,3
18003 H2O	32002 O2-V1	50003 03-SYM-0-18
18005 H2O-V2	34001 O-18-0	50004 03-ASYM-0-18
19001 HO-18	41005 CH3CCD	52006 HOCL
19002 HDO	44001 CS	54005 HOCL-37
27001 HCN	44002 SIO	63001 HNO3
29002 HCO+	45001 C-13-S	64002 SO2

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	TAG NAME	TAG NAME
18004 NH2D	44005 CH3CHO-E	52006 HOCL
18005 H2O-V2	48005 03-V2	54005 HOCL-37
34004 H2O2	48006 03-V1,3	63001 HNO3

Revised Species, Rev. 1 (24)

TAG NAME	TAG NAME	TAG NAME
17002 NH3	34001 O-18-0	56002 CH3C-13-H2CN
18002 N-15-H3	34002 H2S	56003 C-13-H3CH2CN
18003 H2O	34003 PH3	56005 CH2DCH2CN-S
29003 CH2NH	45003 NH2CHO	56006 CH2DCH2CN-A
30007 CH2ND	51002 CLO	60001 OCS
32001 O2	53002 CL-37-0	61001 OC-13-S
32002 O2-V1	55001 C2H5CN	62001 OC-34-S
32003 CH3OH	56001 CH3CH2C-13-N	62002 O-18-CS

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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 30 μ m). 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
( 16,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 logarithm 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, $\text{nm}^2 \text{ MHz}$, 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 $\text{cm}^{-1}/(\text{molecule}/\text{cm}^2)$. The latter is obtainable by dividing the catalogue intensity by 2.9979×10^{18} .

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

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

where ν_{ba} is the line frequency, 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 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 $T=300\text{K}$.

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

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

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

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

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

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

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

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

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

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

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

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

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

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:

$$\epsilon_n^2 = \sum_{kj} \frac{\partial \nu_n}{\partial p_k} \frac{\partial \nu_n}{\partial p_j} V_{kj} \quad (7)$$

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

$$(V^{-1})_{kj} = \sum_m \frac{\partial \nu_m}{\partial p_k} \frac{\partial \nu_m}{\partial p_j} \epsilon_m^{-2} \quad (8)$$

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 because every author starts with a different viewpoint of the problem. In our case, we have tried to develop a program that will treat a wide variety of problems with a minimum of adaptation. This saves a great deal of time in the initial 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 consistency can be maintained, facilitating comparisons between different molecules. The particular model needed to analyze a specific problem is treated as a subroutine. For certain problems, this subroutine can be quite simple, 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

$$\text{QNFORM} = \text{Q} \cdot 100 + \text{H} \cdot 10 + \text{NQN}$$

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 not 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:

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

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 H₂O and O₃.) 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)
^1H	0.	^{29}Si	-1.327
^2H	-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	32002 O2-V1	50003 O3-SYM-0-18
2001 D-ATOM	32003 CH3OH	50004 O3-ASYM-0-18
3001 HD	32004 H2CO-18	50005 O3-S-018-V2
12001 C-ATOM	33001 H02	50006 O3-A-018-V2
13001 C-13-ATOM	34001 O-18-0	51001 HCCCN
13002 CH	34002 H2S	51002 CLO
14001 N-ATOM	34003 PH3	52001 HCCC-13-N
14002 N-ATOM-D-STATE	34004 H2O2	52002 HCC-13-CN
16001 O-ATOM	35001 HDS	52003 HC-13-CCN
17001 OH	36001 HCl	52004 HCCCN-15
17002 NH3	38001 HCl-37	52005 DCCCN
17003 CH3D	40001 CH3CCH	52006 HOCL
17004 NH3-V2	41001 CH3CN	53001 C2H3CN
18001 O2	41002 CH3CC-13-H	53002 CL-37-0
18002 N-15-H3	41003 CH3C-13-CH	54001 CH2CHC-13-N
18003 H2O	41004 C-13-H3CCH	54002 CH2C-13-HCN
18004 NH2D	41005 CH3CCD	54003 C-13-H2CHCN
18005 H2O-V2	41006 CH2DCCH	54004 CH2CDCN
19001 HO-18	42001 CH3CN-15	54005 HOCL-37
19002 HDO	42002 CH2CO	55001 C2H5CN
20001 D2O	43001 CHDCO	56001 CH3CH2C-13-N
25001 CCH	44001 CS	56002 CH3C-13-H2CN
26001 CN	44002 SiO	56003 C-13-H3CH2CN
26002 CN-V1	44003 CH3CHO-A	56004 C2H5CN-15
27001 HCN	44004 N2O	56005 CH2DCH2CN-S
27002 HNC	44005 CH3CHO-E	56006 CH2DCH2CN-A
28001 CO	45001 C-13-S	60001 OCS
28002 HC-13-N	45002 Si-29-0	60002 SIS
28003 HCN-15	45003 NH2CHO	61001 OC-13-S
28004 DCN	46001 CS-34	61002 Si-29-S
28005 HNC-13	46002 Si-30-0	62001 OC-34-S
28006 HN-15-C	46003 H2CS	62002 O-18-CS
28007 DNC	46004 C2H5OH	62003 Si-30-S
29001 C-13-0	46005 HCOOH	62004 SIS-34
29002 HCO+	46006 NO2	63001 HN03
29003 CH2NH	47001 H2C-13-S	64001 S2
29004 HCO	47002 HC-13-00H	64002 S02
29005 NNH+	47003 DC00H	75001 HCCCCCN
30001 CO-18	47004 HCOOD	76001 HCCCCC-13-N
30002 HC-13-0+	48001 SO	76002 HCCCC-13-CN
30003 DCO+	48002 SO-V1	76003 HCCC-13-CCN
30004 H2CO	48003 H2CS-34	76004 HCC-13-CCCN
30005 C-13-H2NH	48004 O3	76005 HC-13-CCCN
30006 CH2N-15-H	48005 O3-V2	76006 HCCCCCN-15
30007 CH2ND	48006 O3-V1,3	76007 DCCCCCN
30008 NO	48007 O3-2V2	80001 HBR-79
30009 NND+	49001 O3-SYM-0-17	82001 HBR-81
31001 HCO-18+	49002 O3-ASYM-0-17	95001 BR-79-0
31002 H2C-13-0	50001 S-34-0	97001 BR-81-0
32001 O2	50002 SO-18	97002 CL-35-N03
		99001 CL-37-N03

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

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

Lines Listed	= 1		Q(300.) =	4.0
Max. Frequency	= 1.42	GHz	Q(225.) =	4.0
Max. J	= 1/2		Q(150.) =	4.0
LOGSTR	= -9.1		Q(75.) =	4.0
LOGSTR1	=		Q(37.5) =	3.99
Isotope Correction	= 0.		Q(18.25) =	3.99
Minimum Energy	= 0.0479	cm ⁻¹	Q(9.375) =	3.98
Dipoles:	$\mu(a)$ =		A =	
	$\mu(b)$ =		B =	
	$\mu(c)$ =		C =	

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

Species Tag:	2001	Species Name:	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 4.695×10^{-17} sec⁻¹.

Species Tag:	3001	Species Name:	HD
Version:	1		Mono-deuterated
Date:	Oct. 1979		molecular hydrogen
Contributor:	H. M. Pickett		
Lines Listed	= 1	Q(300.) =	5.0165
Max. Frequency	= 2676. GHz	Q(225.) =	3.8583
Max. J	= 1	Q(150.) =	2.7008
LOGSTR	= -5.6	Q(75.) =	1.5711
LOGSTR1	= 0.	Q(37.5) =	1.0980
Isotope Correction	= -3.523	Q(18.25) =	1.0032
Minimum Energy	= 0. cm^{-1}	Q(9.375) =	1.0002
Dipoles:	$\mu(a) =$	A =	
	$\mu(b) = 0.000585$	B =	1339100.
	$\mu(c) =$	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
3P ground state

Lines Listed	= 2		Q(300.)	=	7.833
Max. Frequency	= 810	GHz	Q(225.)	=	7.489
Max. J	= 2		Q(150.)	=	6.860
LOGSTK	= -5.		Q(75.)	=	5.364
LOGSTR1	=		Q(37.5)	=	3.543
Isotope Correction	= 0		Q(18.25)	=	2.030
Minimum Energy	= 0.	cm ⁻¹	Q(9.375)	=	1.248
Dipoles:	$\mu(a)$	=	A	=	
	$\mu(b)$	=	B	=	
	$\mu(c)$	=	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
Version: 1
Date: Oct 1979
Contributor: H. M. Pickett

Species Name: Carbon atom
¹³C isotope

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:	$\mu(a)$ =	A =	
	$\mu(b)$ =	B =	
	$\mu(c)$ =	C =	

The fine structure intervals of ¹²C were multiplied by 0.999992967 to account for the isotope effect on the Rydberg constant. The hyperfine intervals 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
Version: 1
Date: Feb 1984
Contributor: H. M. Pickett

Species Name: CH radical
 2π states

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. Demuyne 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		Q(300.) =	12.0
Max. Frequency	= 0.027	GHz	Q(225.) =	12.0
Max. J	= 1.5		Q(150.) =	12.0
LOGSTR	= -13.		Q(75.) =	12.0
LOGSTR1	=		Q(37.5) =	12.0
Isotope Correction	=		Q(18.25) =	12.0
Minimum Energy	= 0.	cm ⁻¹	Q(9.375) =	12.0
Dipoles:	$\mu(a)$ =		A =	
	$\mu(b)$ =		B =	
	$\mu(c)$ =		C =	

The hyperfine transitions of atomic nitrogen at 14.6 and 26.1 MHz were obtained from J. M. Hirsch, G. H. Zimmerman, III, D. J. Larson, and N. F. Ramsey, 1977, Phys. Rev. A 16, 484. Intensities were calculated using the experimental g_J value.

Species Tag: 14002
 Version: 2
 Date: Aug 1983
 Contributor: H. M. Pickett

Species Name: N-atom 2D state

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:	$\mu(a)$ =		A =	
	$\mu(b)$ =		B =	
	$\mu(c)$ =		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 $\pm 600 \text{ MHz}$, 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 $1.06 \times 10^{-6} \text{ sec.}^{-1}$. In contrast, the spontaneous emission rate from $^2D_{3/2} F = 5/2$ to $^2D_{5/2} F = 7/2$ is $3.15 \times 10^{-9} \text{ sec}^{-1}$.

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

Species Name: O atom
 3p ground state

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:	$\mu(a)$ =		A =	
	$\mu(b)$ =		B =	
	$\mu(c)$ =		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		Q(300.) =	81.494
Max. Frequency	= 9900.	GHz	Q(225.) =	60.296
Max. J	= 13.5		Q(150.) =	40.144
LOGSTR	= -10.		Q(75.) =	22.753
LOGSTR1	= -10.		Q(37.5) =	17.034
Isotope Correction	= 0.		Q(18.25) =	16.004
Minimum Energy	= 0.	cm ⁻¹	Q(9.375) =	15.929
Dipoles:	$\mu(a)$ = 1.667		A =	
	$\mu(b)$ =		B =	556141.
	$\mu(c)$ =		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		Q(300.) =	578.98
Max. Frequency	= 9500.	GHz	Q(225.) =	371.88
Max. J	= 19		Q(150.) =	206.64
LOGSTR	= -17.		Q(75.) =	74.54
LOGSTR1	= 0		Q(37.5) =	26.608
Isotope Correction	= 0.		Q(18.25) =	11.251
Minimum Energy	= 0.	cm^{-1}	Q(9.375) =	5.398
Dipoles:	$\mu(a)$ = 0		A =	B
	$\mu(b)$ = 0		B =	298117.06
	$\mu(c)$ = 1.476		C =	186726.36

The computational method and most of the microwave data are given in R. L. Poynter and R. K. Kakar, 1975, 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 $J = 1 \rightarrow 0$, $k = 0$ rotational transition was taken from P. Helminger, F. C. DeLucia, and W. Gordy, 1971, J. Mol. Spect. 39, 94. Because of the important applications of these rotational lines, the upper frequency limit has been extended to 335 cm^{-1} (9.5 THz). Hyperfine splittings have not been included.

Species Tag:	17003	Species Name:	CH ₃ D
Version:	1		Mono deuterio methane
Date:	Feb 1980		
Contributor:	R. L. Poynter		

Lines Listed	= 80	Q(300.) =	402.17
Max. Frequency	= 3000. GHz	Q(225.) =	315.14
Max. J	= 13	Q(150.) =	142.69
LOGSTR	= -8	Q(75.) =	51.09
LOGSTR1	= 0	Q(37.5) =	18.47
Isotope Correction	= -3.222	Q(18.25) =	7.03
Minimum Energy	= 0. cm ⁻¹	Q(9.375) =	2.98
Dipoles:	$\mu(a)$ = 0.0056	A =	157412.
	$\mu(b)$ = 0	B =	116325.
	$\mu(c)$ = 0	C =	B

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

Species Tag: 17004
 Version: 1
 Date: Mar 1984
 Contributor: R. L. Poynter

Species Name: NH₃, v₂ - 010 state

Lines Listed	= 442		Q(300.) =	578.98
Max. Frequency	= 11600	GHz	Q(225.) =	371.88
Max. J	= 17		Q(150.) =	206.64
LOGSTR	= -12		Q(75.) =	74.54
LOGSTR1	=		Q(37.5) =	26.608
Isotope Correction	=		Q(18.25) =	11.251
Minimum Energy	= 0.	cm ⁻¹	Q(9.375) =	5.397
Dipoles:	μ(a) =		A =	B
	μ(b) =		B =	299196.11
	μ(c) = 1.253		C =	183595.39

The lines for this species were derived by combination differences from the v₂ - 010 lines reported by R. L. Poynter and J. S. Margolis, 1984, Mol. Phys. 81, 393. Some measurements have been reported by F. Y. Chu and S. M. Freund, 1973, J. Mol. Spect. 48, 183, 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
Version: 1
Date: May 1983
Contributor: H. M. Pickett

Species Name: OD
Hydroxyl radical,
deuterium isotope

Lines Listed	= 912		Q(30.) =	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:	$\mu(a)$ = 1.653		A =	
	$\mu(b)$ = 0.		B =	296312.
	$\mu(c)$ = 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, $^{15}\text{NH}_3$
 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: $\mu(a) = 0$
 $\mu(b) = 0.$
 $\mu(c) = 1.476$

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 $^{14}\text{NH}_3$. 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 $^{14}\text{NH}_3$.

The dipole moment was assumed to be the same as $^{14}\text{NH}_3$.

Species Tag: 18003 Species Name: H₂O
 Version: 3 water
 Date: Dec 1983
 Contributor: R. L. Poynter and H. M. Pickett

Lines Listed	= 424		Q(300.) =	178.115
Max. Frequency	= 10000.	GHz	Q(225.) =	116.017
Max. J	= 12		Q(150.) =	63.677
LOGSTR	= -12		Q(75.) =	23.170
LOGSTR1	=		Q(37.5) =	8.580
Isotope Correction	= 0.		Q(18.25) =	3.033
Minimum Energy	= 0.	cm ⁻¹	Q(9.375) =	1.257
Dipoles : $\mu(a)$	= 0.		A =	835840.29
$\mu(b)$	= 1.855		B =	435351.72
$\mu(c)$	= 0.		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. Muentzer, (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 ₂ D
Version:	1		Mono deuterio
Date:	Jan 1981		ammonia
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:		A =	290124.
μ(a)	= -0.18	B =	112194.
μ(b)	= 0	C =	110797.
μ(c)	= 1.463		

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 $P_a P_c + P_c P_a$ 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: H₂O-v₂
excited bending
state (010)

Lines Listed	= 292		Q(300.) = 178.115
Max. Frequency	= 10000.	GHz	Q(225.) = 116.017
Max. J	= 10		Q(150.) = 63.677
LOGSTR	= -12		Q(75.) = 23.170
LOGSTR1	=		Q(37.5) = 8.580
Isotope Correction	= 0.		Q(18.25) = 3.033
Minimum Energy	= 1594.75	cm ⁻¹	Q(9.375) = 1.257
Dipoles:	$\mu(a)$ = 0.		A = 933052
	$\mu(b)$ = 1.855		B = 440318.
	$\mu(c)$ = 0.		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		Q(300.) = 81.945
Max. Frequency	= 10000.	GHz	Q(225.) = 60.611
Max. J	= 13.5		Q(150.) = 40.329
LOGSTR	= -10.		Q(75.) = 22.824
LOGSTR1	= -10.		Q(37.5) = 17.054
Isotope Correction	= -2.690		Q(18.25) = 16.006
Minimum Energy	= 0.	cm ⁻¹	Q(9.375) = 15.930
Dipoles:	$\mu(a)$ = 1.667		A =
	$\mu(b)$ =		B = 552470.
	$\mu(c)$ =		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	Species Name:	HDO
Version:	2		water, mono deuterium
Date:	Dec 1983		isotope
Contributor:	R. L. Poynter		

Lines Listed	= 461		Q(300.) = 146.05
Max. Frequency	= 3013	GHz	Q(225.) = 95.07
Max. J	= 17		Q(150.) = 52.28
LOGSTR	= -13		Q(75.) = 18.851
LOGSTR1	=		Q(37.5) = 6.952
Isotope Correction	= -3.523		Q(18.25) = 2.712
Minimum Energy	= 0.	cm ⁻¹	Q(9.375) = 1.334
Dipoles:	$\mu(a)$ = 0.657		A = 701931.5
	$\mu(b)$ = 1.732		B = 272912.6
	$\mu(c)$ = 0		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 ₂ O,
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. Bluysen, 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. 15, 10
- D. A. Stephenson and R. G. Strauch, 1970, J. Mol. Spect. 35, 494
- J. Verhoeven, H. Bluysen, 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. Muentzer, 1973, J. Chem. Phys. 59, 3125.

Species Tag: 25001
 Version: 1
 Date: Mar
 Contributor: H. M. Pickett

Species Name: Ethynl radical
 CCH X²Σ state

Lines Listed	=	114		Q(300.)	=	574.24
Max. Frequency	=	3000	GHz	Q(225.)	=	430.94
Max. F	=	28		Q(150.)	=	287.69
LOGSTR	=	-10		Q(75.)	=	144.49
LOGSTR1	=	- 4.		Q(37.5)	=	72.91
Isotope Correction	=	0		Q(18.25)	=	37.14
Minimum Energy	=	0	cm ⁻¹	Q(9.375)	=	19.28
Dipoles : μ(a)	=	0.8		A	=	
μ(b)	=	0		B	=	43674.534
μ(c)	=	0		C	=	

The spectral data and Hamiltonian are from C. A. Gottlieb, E. W. Gottlieb, 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		Q(300.)	= 663.88
Max. Frequency	= 3493.	GHz	Q(225.)	= 498.44
Max. J	= 29.5		Q(150.)	= 332.91
LOGSTR	= -5.		Q(75.)	= 167.43
LOGSTR1	=		Q(37.5)	= 84.73
Isotope Correction	= 0.		Q(18.25)	= 43.41
Minimum Energy	= 0.	cm ⁻¹	Q(9.375)	= 22.80
Dipoles : $\mu(a)$	= 3.0		A	=
$\mu(b)$	=		B	= 56693.46
$\mu(c)$	=		C	=

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

Species Tag: 26002
Version: 1
Date: Mar 1984
Contributor: H. M. Pickett

Species Name: CN, v = 1

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:	$\mu(a)$ = 3.0		A =	
	$\mu(b)$ =		B =	56693.46
	$\mu(c)$ =		C =	

The data and calculational method are from D. D. Skatrud, et al.,
1983, J. Molec. Spectroscopy 99, 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:	$\mu(a)$ = 2.984		A =	
	$\mu(b)$ =		B =	44315.975
	$\mu(c)$ =		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
Version: 1
Date: Dec 1977
Contributor: R. L. Poynter

Species Name: HNC
Hydrogen isocyanide

Lines Listed	= 33		Q(300.) =	138.223
Max. Frequency	= 3000.	GHz	Q(225.) =	103.801
Max. J	= 34		Q(150.) =	69.302
LOGSTR	= -3		Q(75.) =	34.814
LOGSTR1	=		Q(37.5) =	17.575
Isotope Correction	= 0		Q(18.25) =	8.960
Minimum Energy	= 0	cm ⁻¹	Q(9.375) =	4.659
Dipoles:	$\mu(a)$ = 2.699		A =	
	$\mu(b)$ =		B =	45332.
	$\mu(c)$ =		C =	

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

Species Tag: 28001
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: CO
Carbon monoxide

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:	$\mu(a)$	= 0.1098	A	=
	$\mu(b)$	=	B	= 57635.97
	$\mu(c)$	=	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 and W. Gordy, 1970, Phys. Rev. Lett. 25, 1397.

The dipole moment was measured by J. S. Muentzer, 1975, J. Mol. Spect. 55, 490.

Species Tag:	28002	Species Name:	HC-13-N
Version:	1		Hydrogen cyanide,
Date:	Dec 1979		¹³ C isotope
Contributor:	R. L. Poynter		

Lines Listed	= 45		Q(300.) =	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:	$\mu(a)$ = 2.984		A =	
	$\mu(b)$ =		B =	43170.137
	$\mu(c)$ =		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	Species Name:	HCN-15
Version:	1		Hydrogen cyanide,
Date:	Dec 1979		¹⁵ N isotope
Contributor:	R. L. Poynter		
Lines Listed	= 35	Q(300.) =	145.068
Max. Frequency	= 3000. GHz	Q(225.) =	109.337
Max. J	= 35	Q(150.) =	72.993
LOGSTR	= -2.6	Q(75.) =	36.660
LOGSTR1	=	Q(37.5) =	18.498
Isotope Correction	= -2.432	Q(18.25) =	9.421
Minimum Energy	= 0. cm ⁻¹	Q(9.375) =	4.889
Dipoles:	$\mu(a)$ = 2.984	A =	
	$\mu(b)$ =	B =	43027.69
	$\mu(c)$ =	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
 Version: 1
 Date: Dec 1979
 Contributor: R. L. Poynter

Species Name: DCN
 Hydrogen cyanide,
 deuterium isotope

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:	$\mu(a)$ =	2.984	A =	
	$\mu(b)$ =		B =	30207.46
	$\mu(c)$ =		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	Species Name:	HN ¹³ C
Version:	1		Hydrogen Isocyanide,
Date:	Dec 1979		¹³ C isotope
Contributor:	R. L. Poynter		

Lines Listed	= 34		Q(300.) = 143.880
Max. Frequency	= 3000.	GHz	Q(225.) = 108.047
Max. J	= 35		Q(150.) = 72.132
LOGSTR	= -2.7		Q(75.) = 36.228
LOGSTR1	=		Q(37.5) = 18.282
Isotope Correction	= -1.955		Q(18.25) = 9.313
Minimum Energy	= 0.	cm ⁻¹	Q(9.375) = 4.835
Dipoles:	$\mu(a)$ = 2.699		A =
	$\mu(b)$ =		B = 43545.61
	$\mu(c)$ =		C =

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

Species Tag: 28006
 Version: 1
 Date: Dec 1979
 Contributor: R. L. Poynter

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

Lines Listed	= 33		Q(300.) =	141.013
Max. Frequency	= 3000.	GHz	Q(225.) =	105.893
Max. J	= 33		Q(150.) =	70.697
LOGSTR	= -2.7		Q(75.) =	35.511
LOGSTR1	=		Q(37.5) =	17.924
Isotope Correction	= -2.432		Q(18.25) =	9.134
Minimum Energy	= 0.	cm ⁻¹	Q(9.375) =	4.746
Dipoles:	$\mu(a)$ = 2.699		A =	
	$\mu(b)$ =		B =	44433.04
	$\mu(c)$ =		C =	

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

Species Tag: 28007
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: DNC
Hydrogen isocyanide,
deuterium isotope

Lines Listed	= 39		Q(300.) =	164.169
Max. Frequency	= 3000	GHz	Q(225.) =	123.269
Max. J	= 39		Q(150.) =	82.279
LOGSTR	= -3		Q(75.) =	41.301
LOGSTR1	=		Q(37.5) =	20.818
Isotope Correction	= -3.824		Q(18.25) =	10.580
Minimum Energy	= 0.	cm ⁻¹	Q(9.375) =	5.467
Dipoles:	$\mu(a)$ = 2.699		A =	
	$\mu(b)$ =		B =	38152.995
	$\mu(c)$ =		C =	

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

Species Tag: 29001
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: C-13-0
carbon monoxide,
¹³C isotope

Lines Listed	= 27		Q(300.) =	113.776
Max. Frequency	= 3000	GHz	Q(225.) =	85.454
Max. J	= 27		Q(150.) =	57.077
LOGSTR	= -5.1		Q(75.) =	28.702
LOGSTR1	=		Q(37.5) =	14.520
Isotope Correction	= -1.955		Q(18.25) =	7.434
Minimum Energy	= 0.	cm ⁻¹	Q(9.375) =	3.898
Dipoles:	$\mu(a)$ = 0.11		A =	
	$\mu(b)$ =		B =	55101.02
	$\mu(c)$ =		C =	

The experimental measurement was reported by B. Rosenblum, A. H. Nethercot, Jr. and C. H. Townes, 1958, Phys. Rev. 109, 400.

The dipole moment was measured by W. L. Meerts, F. H. De Leeuw, and A. Dymanus, 1977, Chem. Phys. 22, 319.

Species Tag:	29002	Species Name:	HCO+
Version:	2		Formyl radical
Date:	Jan 1984		cation
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:	$\mu(a)$ = 3.30	A =	
	$\mu(b)$ =	B =	44594.419
	$\mu(c)$ =	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: CH₂NH
Methyleneimine

Lines Listed	= 2957	Q(300.) =	5892.86
Max. Frequency	= 3000. GHz	Q(225.) =	3800.14
Max. J	= 33	Q(150.) =	2084.97
LOGSTR	= -8	Q(75.) =	740.46
LOGSTR1	= -5 above 120 GHz	Q(37.5) =	263.39
Isotope Correction	= 0.	Q(18.25) =	94.30
Minimum Energy	= 0. cm ⁻¹	Q(9.375) =	34.20
Dipoles: $\mu(a)$	= 1.325	A =	196211.045
$\mu(b)$	= 1.530	B =	34532.395
$\mu(c)$	= 0.	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.	CHz	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
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: CO-18
Carbon monoxide,
180 isotope

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:	$\mu(a)$ = 0.11		A =	
	$\mu(b)$ =		B =	54891.425
	$\mu(c)$ =		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	Species Name:	HC-13-0+
Version:	2		Formyl radical cation,
Date:	Dec 1983		¹³ C isotope
Contributor:	R. L. Poynter		

Lines Listed	= 34	Q(300.) =	144.486
Max. Frequency	= 3000	Q(225.) =	108.459
			GHz
Max. J	= 34	Q(150.) =	72.407
LOGSTR	= -2.7	Q(75.) =	36.367
LOGSTR1	= 0	Q(37.5) =	18.352
Isotope Correction	= -1.955	Q(18.25) =	9.348
Minimum Energy	= 0	Q(9.375) =	4.852
			cm ⁻¹
Dipoles:	$\mu(a)$ = 3.3	A =	
	$\mu(b)$ =	B =	43377.32
	$\mu(c)$ =	C =	

Only two lines of this molecule have been measured by R. C. Woods, R. J. Saykally, T. A. Dixon, P. G. Szanto and T. Anderson (1976), 31st Symposium on Molecular Spectroscopy, Columbus, Ohio, and by M. Bogey, C. Demuyck, 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: DC0+
Formyl radical cation,
deuterium isotope

Lines Listed	= 41		Q(300.) =	173.872
Max. Frequency	= 3000	GHz	Q(225.) =	130.543
Max. J	= 41		Q(150.) =	87.129
LOGSTR	= -2.7		Q(75.) =	43.726
LOGSTR1	=		Q(37.5) =	22.031
Isotope Correction	= -3.824		Q(18.25) =	11.186
Minimum Energy	= 0.	cm ⁻¹	Q(9.375) =	5.769
Dipoles:	$\mu(a)$ = 3.3		A =	
	$\mu(b)$ =		B =	36019.76
	$\mu(c)$ =		C =	

The observed lines are from R. C. Woods, R. J. Saykally, T. A. Dixon, P. G. Szanto, and T. Anderson (1976), 31st Symposium on Molecular Spectroscopy, Columbus, Ohio, M. Bogey, C. Demuyneck, 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: H₂CO
formaldehyde

Lines Listed	= 611		Q(300.) =	2876.7
Max. Frequency	= 3000.	GHz	Q(225.) =	1868.2
Max. J	= 40		Q(150.) =	1019.7
LOGSTR	= -20		Q(75.) =	361.7
LOGSTR1	=		Q(37.5) =	128.65
Isotope Correction	= 0.		Q(18.25) =	44.68
Minimum Energy	= 0.	cm ⁻¹	Q(9.375) =	13.80
Dipoles:	$\mu(a)$ = 2.331		A =	281925.97
	$\mu(b)$ = 0		B =	38836.582
	$\mu(c)$ =		C =	34001.673

The experimental data were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333. The measurements were taken from 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: ?
 Date: Jan 1980
 Contributor: R. L. Poynter

Species Name: C-13-H₂NH
 Methyleneimine,
¹³C isotope

Lines Listed	=	439		Q(300.)	=	2012.45
Max. Frequency	=	3000	GHz	Q(225.)	=	1307.07
Max. J	=	10		Q(150.)	=	711.54
LOGSTR	=	-8		Q(75.)	=	251.54
LOGSTR1	=	0.		Q(37.5)	=	88.94
Isotope Correction	=	-1.955		Q(18.25)	=	31.44
Minimum Energy	=	0.	cm ⁻¹	Q(9.375)	=	11.12
Dipoles: $\mu(a)$	=	1.325		A	=	194195.217
$\mu(b)$	=	1.530		B	=	33747.87
$\mu(c)$	=	0.		C	=	28707.05

The computational methods is the same as that used on the parent species, CH₂NH. 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: CH₂N-15-H
Methylenimine,
15N isotope

Lines Listed	= 440		Q(300.) =	2015.79
Max. Frequency	= 3000	GHz	Q(225.) =	1309.18
Max. J	= 10		Q(150.) =	712.69
LOGSTR	= -8		Q(75.) =	251.97
LOGSTR1	=		Q(37.5) =	89.09
Isotope Correction	= -2.432		Q(18.25) =	31.50
Minimum Energy	= 0.	cm ⁻¹	Q(9.375) =	11.14
Dipoles:	$\mu(a)$ = 1.325		A =	195738.07
	$\mu(b)$ = 1.530		B =	33736.10
	$\mu(c)$ = 0.		C =	28688.61

The computational method is the same as that used on the parent species, CH₂NH. 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: CH₂ND
Methylenimine,
deuterium isotope
on nitrogen atom

Lines Listed	= 1834	Q(300.) =	7181.1
Max. Frequency	= 3000. GHz	Q(225.) =	4664.3
Max. J	= 14	Q(150.) =	2542.6
LOGSTR	= -5 above 120 GHz	Q(75.) =	811.7
LOGSTR1	=	Q(37.5) =	297.8
Isotope Correction	= -3.824	Q(18.25) =	92.62
Minimum Energy	= 0. cm ⁻¹	Q(9.375) =	43.38
Dipoles:	$\mu(a) = 1.325$	A =	157673.877
	$\mu(b) = 1.530$	B =	32069.366
	$\mu(c) = 0.$	C =	26563.849

The computational method is the same as that used for the parent species, CH₂NH. 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 2Π 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:	$\mu(a)$ = 0.15872		A =	
	$\mu(b)$ =		B =	50849.06
	$\mu(c)$ =		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 $J=7\frac{1}{2}$.

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

Species Name: N_2D^+

Lines Listed	= 41		Q(300.) =	487.62
Max. Frequency	= 3000	GHz	Q(225.) =	365.939
Max. J	= 39		Q(150.) =	244.264
LOGSTR	= -4		Q(75.) =	122.620
LOGSTR1	=		Q(37.5) =	61.813
Isotope Correction	= -3.824		Q(18.25) =	31.421
Minimum Energy	= 0.	cm^{-1}	Q(9.375) =	16.241
Dipoles : $\mu(a)$	= 3.40		A =	
$\mu(b)$	=		B =	38554.719
$\mu(c)$	=		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:	$\mu(a)$ = 3.30		A =
	$\mu(b)$ =		B = 42581.21
	$\mu(c)$ =		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. Demuyck, 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: 3100%
Version: 1
Date: Jan. 1980
Contributor: R. L. Poynter

Species Name: H₂C-13-0
Formaldehyde,
13C isotope

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:	$\mu(a)$	= 2.331	A	= 281930.85
	$\mu(b)$	= 0	B	= 37811.92
	$\mu(c)$	= 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 H₂¹²C¹⁶O.

Species Tag:	32001	Species Name:	O ₂
Version:	2		Molecular oxygen,
Date:	June 1980		¹⁶ O ₂ v=0 state of the
Contributor:	H. M. Pickett		ground ³ Σ _g ⁻ electronic
			state
Lines Listed	= 174	Q(300.) =	218.655
Max. Frequency	= 3000. GHz	Q(225.) =	164.129
Max. J	= 60	Q(150.) =	109.605
LOGSTR	= -3?	Q(75.) =	55.198
LOGSTR1	=	Q(37.5) =	28.034
Isotope Correction	= 0	Q(18.25) =	14.515
Minimum Energy	= 0 cm ⁻¹	Q(9.375) =	7.871
Dipoles:	μ(a) = magnetic	A =	
	μ(b) =	B =	43099.795
	μ(c) =	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 53, 346. The Raman lines of O₂ (M. Loete and H. Berger, 1977, J. Mol. Spectroscopy 68, 317) were used with the millimeter wavelength measurements and the submillimeter-line of W. Steinbach and W. Gordy (1973, Phys. Rev A 8, 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.) A251, 565. The zero-frequency absorption is included but the frequency is set to a synthetic frequency of |g|J for the given level.

Species Tag:	32002	Species Name:	O ₂ v=1 state
Version:	3		of the ground
Date:	Dec. 1983		³ Σ _g ⁻ electronic
Contributor:	H. M. Pickett		state
Lines Listed	= 153	Q(300.) =	218.655
Max. Frequency	= 3000 GHz	Q(225.) =	164.129
Max. J	= 60	Q(150.) =	109.605
LOGSTR	= -13.2	Q(75.) =	55.198
LOGSTR1	=	Q(37.5) =	28.034
Isotope Correction	= 0	Q(18.25) =	14.515
Minimum Energy	= 1556.33 cm ⁻¹	Q(9.375) =	7.871
Dipoles:	μ(a) = magnetic	A =	
	μ(b) =	B =	42626.96
	μ(c) =	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. Spectry. 68, 317). Intensities were calculated using the ground state g values.

Species Tag:	32003	Species Name:	CH ₃ OH
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:	$\mu(a)$ = 0.885	A =	127484.
	$\mu(b)$ = 1.440	B =	24679.98
	$\mu(c)$ = 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:

<u>v</u>	<u>species</u>	<u>asymmetric rotor correspondence</u>
1	A+	upper K state for K even, lower for K odd
2	A-	upper K state for K odd, lower for K even
3	E ₁	no direct correspondence
4	E ₂	no direct correspondence

Species Tag:	32004	Species Name:	H ₂ CO-18
Version:	1		Formaldehyde,
Date:	Feb 1980		¹⁸ O isotope
Contributor:	R. L. Poynter		

Lines Listed	= 449		Q(300.) = 3017.23
Max. Frequency	= 3000	GHz	Q(225.) = 1959.75
Max. J	= 20		Q(150.) = 1066.75
LOGSTR	= -9		Q(75.) = 379.22
LOGSTR1	=		Q(37.5) = 134.86
Isotope Correction	= -2.690		Q(18.25) = 46.81
Minimum Energy	= 0.	cm ⁻¹	Q(9.3.) = 14.44
Dipoles:	$\mu(a)$ = 2.331		A = 281993.0
	$\mu(b)$ =		B = 36903.6
	$\mu(c)$ =		C = 32514.7

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

- D. Dangoisse, E. Willemot, and J. Bellet, 1973, 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		Hydroperoxy! 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:	$\mu(a)$ = 1.412		A =	610273.
	$\mu(b)$ = 1.541		B =	33514.
	$\mu(c)$ =		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-18-0
Molecular oxygen,
single substituted
18O isotope

Lines Listed	= 383		Q(300.) =	462.32
Max. Frequency	= 3000	GHz	Q(225.) =	346.96
Max. J	= 60		Q(150.) =	231.67
LOGSTR	= -10.6		Q(75.) =	116.45
LOGSTR1	=		Q(37.5) =	58.92
Isotope Correction	= -2.389		Q(18.25) =	30.26
Minimum Energy	= 0.	cm ⁻¹	Q(9.375) =	16.12
Dipoles:	$\mu(a)$	= magnetic	A =	
	$\mu(b)$	=	B =	40708.
	$\mu(c)$	=	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: H₂S
Hydrogen sulfide

Lines Listed	= 311		Q(300.) =	514.197
Max. Frequency	= 3000	GHz	Q(225.) =	333.981
Max. J	= 15		Q(150.) =	182.164
LOGSTR	= -8		Q(75.) =	65.525
LOGSTR1	=		Q(37.5) =	23.865
Isotope Correction	= 0.		Q(18.25) =	8.700
Minimum Energy	= 0.	cm ⁻¹	Q(9.375) =	2.911
Dipoles:	$\mu(a)$ = 0		A =	310182.24
	$\mu(b)$ = 0.974		B =	270884.05
	$\mu(c)$ = 0.		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: PH₃
 Phosphine

Lines Listed	= 142		Q(300.) =	405.64
Max. Frequency	= 3000	GHz	Q(225.) =	263.47
Max. J	= 19		Q(150.) =	143.41
LOGSTR	= -17		Q(75.) =	51.54
LOGSTR1	=		Q(37.5) =	18.59
Isotope Correction	= 0.		Q(18.25) =	6.958
Minimum Energy	= 0.	cm ⁻¹	Q(9.375) =	2.898
Dipoles:	$\mu(a)$ = 0.000072*		A =	B
	$\mu(b)$ =		B =	133480.22
	$\mu(c)$ = 0.574		C =	117488.39

*centrifugally induced

The measured lines are taken from D. Helms and W. Gordy, 1971, J. Mol. Spect., 66, 206; F. Y. Chu and T. Oka, 1974, J. Chem. Phys. 60, 4612; P. B. Davies, R. M. Newman, S. C. Wofsy, and W. Klemperer, 1971, J. Chem. Phys. 55, 3564; A. F. Krupnov, A. A. Melnikov, and V. A. Skvortsov, 1979, Opt. Spectrosc. (USSR) 46, (5), 570; 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	Species Name:	H ₂ O ₂
Version:	2		Hydrogen peroxide,
Date:	Oct 1980		ground torsional
Contributor:	H. M. Pickett		states
Lines Listed	= 883	Q(300.) =	7651.8
Max. Frequency	= 3000 GHz	Q(225.) =	4970.0
Max. J	= 23	Q(150.) =	2705.3
LOGSTR	= -8	Q(75.) =	916.2
LOGSTR1	=	Q(37.5) =	288.7
Isotope Correction	= 0	Q(18.25) =	88.77
Minimum Energy	= 0. cm ⁻¹	Q(9.375) =	26.64
Dipoles:	μ(a) = 0.	A =	301878.
	μ(b) = 0.	B =	26211.9
	μ(c) = 1.5728	C =	25099.14

The spectral lines and method of calculation are from P. Helminger, W. C. Bowman and F. C. 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.) =	280.9?
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:	$\mu(a)$ = 0.470		A =	292351.302
	$\mu(b)$ = 0.974		B =	147861.801
	$\mu(c)$ = 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: HC135
 Version: 1 Hydrochloric acid,
 Date: Feb 1980 ³⁵Cl 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:	$\mu(a)$ = 1.109		A =	
	$\mu(b)$ = 0.		B =	312989.3
	$\mu(c)$ = 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 ³⁷Cl 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:	$\mu(a)$ = 1.109		A =	
	$\mu(b)$ =		B =	312519.12
	$\mu(c)$ =		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 ₃ CCH
Version:	1		propyne
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. Muentzer and V. W. Laurie, 1966, J. Chem. Phys. 45, 855.

Species Tag: 47001
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: CH₃CN
acetonitrile

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: $\mu(a)$	= 3.91 μ	A =	158290.
$\mu(b)$	= 0.	B =	9198.9
$\mu(c)$	= 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. Bier and S. Maes, 1969, J. Phys. 30, 169; S. G. Kukolich, D. J. Ruben, J. H. S. Wang, and J. R. Williams, 1973, J. Chem. Phys. 58, 3155.

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

Species Tag:	41002	Species Name:	CH ₃ CC-13-H
Version:	1		propyne, ¹³ C
Date:	Dec 1979		isotope on
Contributor:	R. L. Poynter		atom 1.

Lines Listed	= 822	Q(300.)	= 5596.1
Max. Frequency	= 3000 GHz	Q(225.)	= 3633.1
Max. J	= 80	Q(150.)	= 1979.9
LOGSTR	= -4.5 for J>14	Q(75.)	= 700.6
LOGSTR1	=	Q(37.5)	= 248.7
Isotope Correction	= -1.955	Q(18.25)	= 90.97
Minimum Energy	= 0. cm ⁻¹	Q(9.375)	= 35.47
Dipoles:	$\mu(a) = 0.750$	A	= 158590.
	$\mu(b) = 0$	C	= 8290.3
	$\mu(c) = 0$	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. 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: CH₃C-13-CH
propyne, ¹³C isotope on
atom 2.

Lines Listed	= 813	Q(300.) =	5431.06
Max. Frequency	= 3000 GHz	Q(225.) =	3526.18
Max. J	= 79	Q(150.) =	1921.60
LOGSTR	= -4.5 for J>14	Q(75.) =	679.96
LOGSTR1	=	Q(37.5) =	241.35
Isotope Correction	= -1.955	Q(18.25) =	88.31
Minimum Energy	= 0. cm ⁻¹	Q(9.375) =	34.44
Dipoles:	$\mu(a)$ = 0.75	A =	158590.
	$\mu(b)$ =	B =	8542.3
	$\mu(c)$ =	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: H₃C-13-CCH
propyne, ¹³C
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: $\mu(a)$ = 0.750
 $\mu(b)$ = 0.
 $\mu(c)$ = 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 Species Name: CH₃CCD
 Version: 2
 Date: Jan 1984
 Contributor: R. L. Poynter

Lines Listed	= 822		Q(300.) =	17192.04
Max. Frequency	= 405	GHz	Q(225.) =	11168.37
Max. J	= 40		Q(150.) =	6139.89
LOGSTR	= -7.8		Q(75.) =	2243.60
LOGSTR1	=		Q(37.5) =	795.34
Isotope Correction	= -3.824		Q(18.25) =	290.46
Minimum Energy	= 0.	cm ⁻¹	Q(9.375) =	113.17
Dipoles:	$\mu(a)$ =	.77	A =	158590.
	$\mu(b)$ =		B =	7788.170
	$\mu(c)$ =		C =	B

The experimental measurements are from J. S. Muentner 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 Muentner and Laurie, above.

Species Tag:	41006	Species Name:	CH ₂ DCCH
Version:	2		propyne, deuterium
Date:	Aug 1983		isotope on methyl
Contributor:	R. L. Poynter		carbon atom

Lines Listed	= 223		Q(300.) = 4428.44
Max. Frequency	= 3000	GHz	Q(225.) = 2875.21
Max. J	= 15		Q(150.) = 1633.43
LOGSTR	= -10		Q(75.) = 904.90
LOGSTR1	=		Q(37.5) = 410.30
Isotope Correction	= -3.347		Q(18.25) = 156.17
Minimum Energy	= 0.	cm ⁻¹	Q(9.375) = 55.87
Dipoles:	$\mu(a)$ = 0.750		A = 117744.370
	$\mu(b)$ =		B = 8155.784
	$\mu(c)$ =		C = 8025.577

The experimental measurements are from L. F. Thomas, E. I. Sherrard, and J. Sheridan, 1955, Trans. Far. Soc. 54, 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: CH₃CN-15,
acetonitrile,
¹⁵N isotope

Lines Listed	=	2755	Q(300.)	=	5226.37
Max. Frequency	=	3000 GHz	Q(225.)	=	3394.69
Max. J	=	99	Q(150.)	=	1847.57
LOGSTR	=	-5 for J>14	Q(75.)	=	653.73
LOGSTR1	=		Q(37.5)	=	232.06
Isotope Correction	=	-2.432	Q(18.25)	=	84.86
Minimum Energy	=	0 cm ⁻¹	Q(9.375)	=	33.08
Dipoles : $\mu(a)$	=	3.919	A	=	158290.
$\mu(b)$	=		B	=	9198.8993
$\mu(c)$	=		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	Species Name:	CH ₂ CO, ketene
Version:	1		
Date:	Jan 1980		
Contributor:	R. L. Poynter		
Lines Listed	= 835	Q(300.) =	10322.85
Max. Frequency	= 3000 GHz	Q(225.) =	6634.38
Max. J	= 29	Q(150.) =	3433.99
LOGSTR	= -15	Q(75.) =	1285.88
LOGSTR1	=	Q(37.5) =	457.09
Isotope Correction	= 0.	Q(18.25) =	157.22
Minimum Energy	= 0. cm ⁻¹	Q(9.375) =	47.58
Dipoles : $\mu(a)$	= 1.422	A =	282473.
$\mu(b)$	=	B =	10293.80
$\mu(c)$	=	C =	9916.38

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

B. Fabricant, D. Krieger, and J. S. Muentner, 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. F. 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	Q(300.)	=	6682.68
Max. Frequency	=	3000 GHz	Q(225.)	=	4340.53
Max. J	=	29	Q(150.)	=	2344.00
LOGSTR	=	-23	Q(75.)	=	828.70
LOGSTR1	=		Q(37.5)	=	295.80
Isotope Correction	=	-3.523	Q(18.25)	=	105.15
Minimum Energy	=	0. cm ⁻¹	Q(9.375)	=	37.50
Dipoles : $\mu(a)$	=	1.422	A	=	194313.
$\mu(b)$	=		B	=	9647.396
$\mu(c)$	=		C	=	9174.975

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333. The measurements were taken from L. Nemes and M. Winnewisser, 1976, Z. Naturforsch. 31a, 272.

The dipole moment 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	Q(300.)	=	255.205
Max. Frequency	=	2500 GHz	Q(225.)	=	191.823
Max. J	=	50	Q(150.)	=	127.968
LOGSTR	=	-5	Q(75.)	=	64.151
LOGSTR1	=		Q(37.5)	=	32.240
Isotope Correction	=	-0.022	Q(18.25)	=	16.286
Minimum Energy	=	0. cm ⁻¹	Q(9.375)	=	8.316
Dipoles : $\mu(a)$	=	1.957	A	=	
$\mu(b)$	=		B	=	24495.562
$\mu(c)$	=		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. Demuyneck, 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
Version: 2
Date: Jan 1984
Contributor: R. L. Poynter

Species Name: ^{28}SiO , silicon monoxide

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 : $\mu(a)$	= 3.098	A =	
$\mu(b)$	=	B =	21711.967
$\mu(c)$	=	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. Muentzer, and W. A. Klemperer, 1970, J. Chem. Phys. 52, 3458.

Species Tag: 44003
Version: 1
Date: Jan 1980
Contributor: R. L. Poynter

Species Name: CH₃CHO-A, acetaldehyde,
ground vibrational state,
A species.

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 : $\mu(a)$	=	2.550	A	=	56609.474
$\mu(b)$	=	0.870	B	=	10162.766
$\mu(c)$	=		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 ₂ O
Version:	1		
Date:	Jan 1980		
Contributor:	R L. Poynter and H. M. Pickett		
Lines Listed	= 61	Q(300.)	= 497.966
Max. Frequency	= 3000 GHz	Q(225.)	= 373.594
Max. J	= 61	Q(150.)	= 249.173
LOGSTR	=	Q(75.)	= 124.738
LOGSTR1	=	Q(37.5)	= 62.546
Isotope Correction	= 0.	Q(18.25)	= 31.434
Minimum Energy	= 0. cm ⁻¹	Q(9.375)	= 15.889
Dipoles : $\mu(a)$	= 0.1608	A	=
$\mu(b)$	=	B	= 12561.637
$\mu(c)$	=	C	=

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

The dipole moment was measured by L. H. Scharpen, J. S. Muentert, and V. W. Laurie, 1970, J. Chem. Phys. 53, 2513.

Species Tag: 44005
 Version: 1
 Date: Dec 1930
 Contributor: H. M. Pickett

Species Name: CH₃CHO-E
 acetaldehyde,
 E state

Lines Listed	=	691		Q(300.)	=	12111.56
Max. Frequency	=	3000	GHz	Q(225.)	=	7866.84
Max. J	=	15		Q(150.)	=	4282.08
LOGSTR	=	-10		Q(75.)	=	1513.94
LOGSTR!	=			Q(37.5)	=	535.26
Isotopic Correction	=	0.		Q(18.25)	=	189.46
Minimum Energy	=	0.	cm ⁻¹	Q(9.375)	=	67.29
Dipoles : $\mu(a)$	=	2.55		A	=	56448.5
$\mu(b)$	=	0.870		B	=	10160.1
$\mu(c)$	=			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_a^2 , P_a^4 , P_a^3 , $P_a^3 P^2$, 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 $\mu^2 S$ 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
Version: 2
Date: Jan 1984
Contributor: R. Poynter

Species Name: C-13-S
Carbon monosulfide,
¹³C isotope

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 : $\mu(a)$	=	1.957		A	=	
$\mu(b)$	=			B	=	23123.856
$\mu(c)$	=			C	=	

The experimental measurements were reported by R. C. Mockler and G. R. Bird, 1955, Phys. Rev. 98, 1837, and by M. Bogey, C. Demuyneck, 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	Species Name:	^{29}SiO
Version:	1		silicon monoxide,
Date:	Dec 1979		^{29}Si isotope
Contributor:	R. L. Poynter		

Lines Listed	=	66	Q(300.)	=	290.870
Max. Frequency	=	3000 GHz	Q(225.)	=	219.180
Max. J	=	66	Q(150.)	=	146.184
LOGSTR	=	-6	Q(75.)	=	73.2318
LOGSTR1	=		Q(37.5)	=	36.7790
Isotope Correction	=	-1.327	Q(18.25)	=	18.5609
Minimum Energy	=	0. cm^{-1}	Q(9.375)	=	9.4515
Dipoles : $\mu(a)$	=	3.098	A	=	
$\mu(b)$	=		B	=	21514.07
$\mu(c)$	=		C	=	

The experimental data were taken from E. Tiemann, 1974, J. Phys. Chem. Ref. Data, and T. Ljrring, 1968, Z. Naturforsch, 23a, 777.

The dipole moment was reported by J. W. Raymonda, J. S. Muentner, and W. A. Klemperer, 1970, J. Chem. Phys. 52, 3458.

c - 2

Species Tag:	45003	Species Name:	Formamide
Version:	2		NH ₂ CHO
Date:	Jan 1981		
Contributor:	R. L. Poynter		

Lines Listed	=	3476	Q(300.)	=	29154.14
Max. Frequency	=	3000 GHz	Q(225.)	=	18479.91
Max. J	=	34	Q(150.)	=	10313.37
LOGSTR	=	-8 above 120 GHz	Q(75.)	=	3633.29
LOGSTR1	=		Q(37.5)	=	1293.30
Isotope Correction	=	0.	Q(18.25)	=	459.199
Minimum Energy	=	0. cm ⁻¹	Q(9.375)	=	163.719
Dipoles : $\mu(a)$	=	3.616	A	=	72716.954
$\mu(b)$	=	0.852	B	=	11373.453
$\mu(c)$	=		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
 Version: 2
 Date: Jan 1984
 Contributor: R. L. Poynter

Species Name: C³⁴S, carbon
 monosulfide ³⁴S
 isotope

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 : $\mu(a)$	=	1.957	A	=	
$\mu(b)$	=		B	=	24103.541
$\mu(c)$	=		C	=	

The experimental measurements were reported by R. C. Mockler and G. R. Bird, 1955, Phys. Rev. 98, 1837, and by M. Bogey, C. Demuyneck, 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: $^{30}\text{Si O}$,
silicon monoxide,
 ^{30}Si isotope

Lines Listed	=	67		Q(300.)	=	294.374
Max. Frequency	=	3000	GHz	Q(225.)	=	221.259
Max. J	=	67		Q(150.)	=	147.911
LOGSTR	=	-6		Q(75.)	=	74.1139
LOGSTR1	=			Q(37.5)	=	37.2220
Isotope Correction	=	-1.506		Q(18.25)	=	18.7759
Minimum Energy	=	0.	cm^{-1}	Q(9.375)	=	9.5609
Dipoles : $\mu(a)$	=	3.098		A	=	
$\mu(b)$	=			B	=	21259.48
$\mu(c)$	=			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. Muentzer, and W. A. Klemperer, 1970, J. Chem. Phys. 52, 3458.

Species Tag: 46003
Version: 1
Date: Jan 1980
Contributor: R. L. Poynter

Species Name: H₂CS, thioformaldehyde

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. Muentner, 1977, J. Chem. Phys. 67, 1576.

Species Tag:	46004	Species Name:	C ₂ H ₅ OH
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 : $\mu(a)$	=	0.046	A =	34891.75
$\mu(b)$	=	1.438	B =	9350.635
$\mu(c)$	=		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	Species Name:	HCOOH
Version:	1		formic acid
Date:	Jan 1980		ground trans state
Contributor:	R. L. Poynter		

Lines Listed	=	1888	Q(300.) =	8883.82
Max. Frequency	=	3000 GHz	Q(225.) =	5770.32
Max. J	=	20	Q(150.) =	3141.23
LOGSTR	=	-11	Q(75.) =	1085.67
LOGSTR1	=		Q(37.5) =	393.460
Isotope Correction	=	0.	Q(18.25) =	139.991
Minimum Energy	=	0. cm ⁻¹	Q(9.375) =	49.9344
Dipoles : $\mu(a)$	=	1.396	A =	77512.25
$\mu(b)$	=	0.260	B =	12055.11
$\mu(c)$	=		C =	10416.12

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333. The measurements were taken from 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. Irambarulo, A. Clark, and C. Hearn, 1958, J. Chem. Phys. 28, 736.

The dipole moment used in the present work was measured by H. Kim, R. Kelle, and W. D. Gwinn, 1962, J. Chem. Phys. 37, 2748, and was adjusted to the new OCS standard, (J. S. Muentzer, 1968, J. Chem. Phys. 48, 4544).

Improved values [$\mu_a = 1.4214(21)D$ and $\mu_b = 0.2096(65)D$] 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,
NO₂

Lines Listed	= 6360		Q(300.) =	13402
Max. Frequency	= 3000.	GHz	Q(225.) =	8750.
Max. J	= 50		Q(150.) =	4704.
LOGSTR	= -7.		Q(75.) =	1683.
LOGSTR1	= -7.		Q(37.5) =	596.
Isotope Correction	= 0.		Q(18.25) =	211.8
Minimum Energy	= 0.	cm ⁻¹	Q(9.375) =	75.7
Dipoles:	$\mu(a)$ =		A =	239904.
	$\mu(b)$ = 0.316		B =	13002.
	$\mu(c)$ = 0		C =	12305.

The data are from W. C. Bowman and F. C. DeLucia, 1982, J. Chem. Phys. 77, 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: H₂¹³C
thioformaldehyde
¹³C isotope

Lines Listed	=	110	Q(300.)	=	6220.14
Max. Frequency	=	335 GHz	Q(225.)	=	4040.17
Max. J	=	10	Q(150.)	=	2114.95
LOGSTR	=	-10	Q(75.)	=	777.678
LOGSTR1	=		Q(37.5)	=	264.363
Isotope Correction	=	-1.977	Q(18.25)	=	94.2540
Minimum Energy	=	0. cm ⁻¹	Q(9.375)	=	28.6154
Dipoles : $\mu(a)$	=	1.649	A	=	291660.0
$\mu(b)$	=		B	=	16998.342
$\mu(c)$	=		C	=	16030.791

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

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: 47002
Version: 1
Date: Jan 1980
Contributor: R. L. Poynter

Species Name: H¹³COOH
formic acid,
¹³C isotope

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 : $\mu(a)$	=	1.396	A	=	77580.494
$\mu(b)$	=	0.260	B	=	12053.567
$\mu(c)$	=		C	=	10378.997

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333. The measurements were taken from 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: i
Date: Jan 1980
Contributor: R. L. Poynter

Species Name: DC00H
formic acid,
deuterium isotope
on C atom

Lines Listed	=	628		Q(300.)	=	10531.2
Max. Frequency	=	3000	GHz	Q(225.)	=	6840.2
Max. J	=	20		Q(150.)	=	3626.47
LOGSTR	=	-10		Q(75.)	=	1251.4
LOGSTR1	=			Q(37.5)	=	466.123
Isotope Correction	=	-3.824		Q(18.25)	=	165.882
Minimum Energy	=	0.	cm ⁻¹	Q(9.375)	=	59.1562
Dipoles : $\mu(a)$	=	1.396		A	=	57709.33
$\mu(b)$	=	0.260		B	=	12055.971
$\mu(c)$	=			C	=	9955.609

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

J. Bellet, A. Deldalle, C. Samson, G. Steenbeckeliers, and K. 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
 Version: 1 formic acid,
 Date: Jan 1980 deuterium isotope
 Contributor: R. L. Poynter on O atom

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 : $\mu(a)$	=	1.396		A	=	66100.14
$\mu(b)$	=	0.260		B	=	11762.577
$\mu(c)$	=			C	=	9969.943

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333. The measurements were taken from 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 : $\mu(a)$	=	1.55	A	=	
$\mu(b)$	=		B	=	21523.02
$\mu(c)$	=		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
Version:	1		monoxide
Date:	Dec 1979		³ Σ ground state,
Contributor:	H. M. Pickett		v=1 vibrational state
Lines Listed	= 251	Q(300.) =	850.159
Max. Frequency	= 3000 GHz	Q(225.) =	632.266
Max. J	= 50	Q(150.) =	414.477
LOGSTR	= -8	Q(75.) =	197.515
LOGSTR1	=	Q(37.5) =	90.3441
Isotope Correction	= -0.022	Q(18 25) =	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 53, 346. The data are from T. Amano, E. Hirota, and Y. Morino, 1967, J. Phys. Soc. Japan 22, 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	Species Name:	H ₂ C ³⁴ S
Version:	1		
Date:	Jan 1980		thioformaldehyde,
Contributor:	R. L. Poynter		³⁴ S isotope
Lines Listed	= 111	Q(300.) =	6084.16
Max. Frequency	= 343 GHz	Q(225.) =	4563.52
Max. J	= 10	Q(150.) =	2150.80
LOGSTR	= -9	Q(75.) =	760.502
LOGSTR1	=	Q(37.5) =	259.239
Isotope Correction	= -1.376	Q(18.25) =	92.2997
Minimum Energy	= 0. cm ⁻¹	Q(9.375) =	28.0092
Dipoles :	{(a) = 1.647	A =	291660.
	{(b) =	B =	17387.949
	{(c) =	C =	16376.922

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333. The measurements 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
 Version: 2
 Date: Mar 1984
 Contributor: H. M. Pickett

Species Name: $^{16}\text{O}_3$, ozone

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 : $\mu(a)$	=		A	=	106535.234
$\mu(b)$	=	0.5324	B	=	13349.090
$\mu(c)$	=		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
Version: 2
Date: Mar 1984
Contributor: H. M. Pickett

Species Name: O₃
v₂ vibrational
state (010)

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 : $\mu(a)$	=		A	=	108137.979
$\mu(b)$	=	0.5324	B	=	13311.143
$\mu(c)$	=		C	=	11765.222

The v₂ 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	Species Name:	O ₃
Version:	2		v ₁ , v ₃ vibrational
Date:	Mar 1984		states (100)
Contributor:	H. M. Pickett		and (001)
Lines Listed	= 9459	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	= 1042. cm ⁻¹	Q(9.375) =	19.0371
Dipoles : μ(a)	=	A =	104944.
μ(b)	= .5324	B =	13229.7
μ(c)	=	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, v₁ and v₃ 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 $v_2 = 2$ state
(0,2,0)

Lines Listed	=	1779	Q(300.)	=	3553.04
Max. Frequency	=	9999 GHz	Q(225.)	=	2263.60
Max. J	=	50	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	=	1400. cm^{-1}	Q(9.375)	=	19.0371
Dipoles : $\mu(a)$	=		A	=	109796.
$\mu(b)$	=	0.5324	B	=	13273.
$\mu(c)$	=		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: 16O-17O-016
Ozone symmetric
17O substitution

Lines Listed	=	13277	Q(300.)	=	19114.5
Max. Frequency	=	999. GHz	Q(225.)	=	13038.6
Max. J	=	37	Q(150.)	=	7299.7
LOGSTR	=	-7.2	Q(75.)	=	2597.63
LOGSTR1	=	-7.2	Q(37.5)	=	920.348
Isotope Correction	=	-3.432	Q(18.25)	=	327.0
Minimum Energy	=	0. cm ⁻¹	Q(9.375)	=	116.8
Dipoles : $\mu(a)$	=		A	=	102351.
$\mu(b)$	=	0.5324	B	=	13350.8
$\mu(c)$	=		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
Version: 1
Date: Mar 1984
Contributor: H. M. Pickett

Species Name: 17O-16O-16O
Ozone asymmetric
17O substitution

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 : $\mu(a)$	=	0.0034	A	=	105491.
$\mu(b)$	=	0.5324	B	=	12951.
$\mu(c)$	=		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:	$^{34}\text{S}^{16}\text{O}$, sulfur monoxide,
Version:	1		$^3\Sigma$ ground state,
Date:	Dec 1979		^{34}S isotope
Contributor:	H. M. Pickett		
Lines Listed	= 280	Q(300.) =	856.963
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 : $\mu(a)$	= 1.55	A =	
$\mu(b)$	=	B =	21102.72
$\mu(c)$	=	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
 Version: 1
 Date: Dec 1979
 Contributor: H. M. Pickett

Species Name: $S^{18}O$, sulfur monoxide
 3Σ ground state

Lines Listed	=	179	Q(300.)	=	917.488
Max. Frequency	=	3000 GHz	Q(225.)	=	675.460
Max. J	=	50	Q(150.)	=	446.684
LOGSTR	=	-5	Q(75.)	=	212.814
LOGSTR1	=		Q(37.5)	=	97.1180
Isotope Correction	=	-2.712	Q(18.25)	=	41.6007
Minimum Energy	=	0. cm^{-1}	Q(9.375)	=	16.8850
Dipoles : $\mu(a)$	=	1.55	A	=	
$\mu(b)$	=		B	=	19929.
$\mu(c)$	=		C	=	

The calculational method is described in T. Amano and E. Hirota, 1974, J. Molec. Spectroscopy 53, 346. The value of ν 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. Depanneaecker 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: 18O16O16O,
 Version: 2 asymmetric 18O
 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 ¹⁸O ozone is based on the work of J. Depannemaecker and J. Bellet (1977, J. Mol. Spectry. 66, 106). The dipole moment used is the ¹⁶O₃ value rotated to the inertial axes of asymmetric ¹⁸O ozone (based on the equilibrium structure). The new version extends the calculation in frequency and J.

Species Tag:	50005	Species Name:	O ₃ symmetric 0 ¹⁸
Version:	1		v 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	=	2.090	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 Species Name: O₃ asymmetric
 Version: 1
 Date: Mar 1984 ¹⁸O v₂ = 1
 Contributor: C. Chiu and E. A. Cohen

Lines Listed	=	42.3	Q(300.)	=	7214.414
Max. Frequency	=	9999 GHz	Q(225.)	=	4994.599
Max. J	=	50	Q(150.)	=	2549.761
LOGSTR	=	-9.	Q(75.)	=	904.0679
LOGSTR1	=	-9.	Q(37.5)	=	320.2580
Isotope Correction	=		Q(18.75)	=	113.7639
Minimum Energy	=	693 cm ⁻¹	Q(9.375)	=	40.6069
Dipoles : μ(a)	=	0.0068	A	=	106071.8
μ(b)	=	0.5324	B	=	12556.0
μ(c)	=		C	=	11150.6

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

Species Tag: 51001 Species Name: HCCCN, cyanoacetylene
Version: 2
Date: Mar 1984
Contributor: R. L. Poynter

Lines Listed	=	154	Q(300.)	=	4122.88
Max. Frequency	=	1000 GHz	Q(225.)	=	3093.14
Max. J	=	99	Q(150.)	=	2062.53
LOGSTR	=	-7	Q(75.)	=	1031.57
LOGSTR1	=		Q(37.5)	=	516.416
Isotope Correction	=	0.	Q(18.25)	=	258.643
Minimum Energy	=	0. cm ⁻¹	Q(9.375)	=	129.8381
Dipoles : $\mu(a)$	=	3.724	A	=	
$\mu(b)$	=		B	=	4549.059
$\mu(c)$	=		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.

Species Tag:	51002	Species Name:	^{35}ClO , chlorine monoxide
Version:	2		$^2\Pi$ states, $v=0$
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, n_1 , n_2 , and n_3 . The partition function was determined by a sum over states to $F = 86$ for both the $\Omega = 3/2$ and $\Omega = 1/2$ states.

Species Tag:	52001	Species Name:	H ¹³ CCCN
Version:	1		cyanoacetylene
Date:	Dec 1979		¹³ C isotope on
Contributor:	R. L. Poynter		atom 1
Lines Listed	= 152	Q(300.) =	4140.00
Max. Frequency	= 1000 GHz	Q(225.) =	3105.99
Max. J	= 99	Q(150.) =	2071.10
LOGSTR	= -7	Q(75.) =	1035.86
LOGSTR1	=	Q(37.5) =	518.442
Isotope Correction	= -1.955	Q(18.25) =	259.717
Minimum Energy	= 0. cm ⁻¹	Q(9.375) =	130.377
Dipoles : $\mu(a)$	= 3.724	A =	
$\mu(b)$	=	B =	4530.198
$\mu(c)$	=	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: 52002
 Version: 1
 Date: Dec 1979
 Contributor: R. L. Poynter

Species Name: HC¹³CCN
 cyanoacetylene
¹³C isotope on
 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 : $\mu(a)$	=	3.724	A	=	
$\mu(b)$	=		B	=	4529.76
$\mu(c)$	=		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: 52003
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: H¹³CCCN
cyanoacetylene
¹³C isotope atom 3

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: $\mu(a)$	=	3.724	A	=	
$\mu(b)$	=		B	=	4408.44
$\mu(c)$	=		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 3.7240.

Species Tag: 52004
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: HC^{15}N
cyanoacetylene
 ^{15}N isotope

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) =	88.7973
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
Version: 1
Date: Dec. 1979
Contributor: R. L. Poynter

Species Name: DCCCN,
cyanoacetylene,
deuterium isotope

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:				A	=	
	$\mu(a)$	=	3.724	B	=	4221.58
	$\mu(b)$	=		C	=	
	$\mu(c)$	=				

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: 52006
Version: 2
Date: Jan 1984
Contributor: H. M. Pickett

Species Name: H³⁵OCl,
hypochlorous acid

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:			A	=	613483.8
	$\mu(a)$	= 0.3627	B	=	15116.795
	$\mu(b)$	= 1.471	C	=	14725.78
	$\mu(c)$	=			

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: 53001
Version: 1
Date: Jan 1980
Contributor: R. L. Poynter

Species Name: C₂H₃CN,
acrylonitrile

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:				A	=	49850.712
	$\mu(a)$	=	3.68	B	=	4971.0849
	$\mu(b)$	=	1.25	C	=	4513.8005
	$\mu(c)$	=				

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
 Version: 2
 Date: Oct 1980
 Contributor: H. M. Pickett

Species Name: ³⁷ClO,
 chlorine monoxide,
³⁷Cl isotope

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:				A	=	
	μ(a)	=	1.239	B	=	1828.70
	μ(b)	=		C	=	
	μ(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_0 and q_0 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, n_1 , n_2 , and n_3 . The partition function was determined by a sum over states to $F = 86$ for both the $\Omega = 1/2$ and $\Omega = 3/2$ states.

Species Tag:	54001	Species Name:	CH ₂ CH ¹³ CN,
Version:	1		acrylonitrile,
Date:	Jan 1980		¹³ C isotope on
Contributor:	R. L. Poynter		atom 1
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(9.3) =	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,
Version:	1		acrylonitrile,
Date:	Jan 1980		¹³ C isotope on
Contributor:	R. L. Poynter		atom 2
<hr/>			
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
Version: 1
Date: Jan 1980
Contributor: R. L. Poynter

Species Name: $^{13}\text{CH}_2\text{CHCN}$,
acrylonitrile,
 ^{13}C isotope on
atom 3

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:	$\mu(\text{a})$	=	3.68	A	=	49180.
	$\mu(\text{b})$	=	1.25	B	=	4837.34
	$\mu(\text{c})$	=		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
Version: 1
Date: Jan 1980
Contributor: R. L. Poynter

Species Name: CH₂DCN,
acrylonitrile,
deuterium isotope
on atom 2

Lines Listed	=	322	Q(300.) =	29696.1680
Max. Frequency	=	3000 GHz	Q(225.) =	19299.5940
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:			A =	40198.6
	$\mu(a)$	= 3.68	B =	4934.35
	$\mu(b)$	= 1.25	C =	4388.41
	$\mu(c)$	=		

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	Species Name:	HO ³⁷ Cl,
Version:	2		hypochlorous acid,
Date:	Jan 1984		³⁷ Cl isotope
Contributor:	H. M. Pickett		
Lines Listed	= 3923	Q(300.) =	2422.5
Max. Frequency	= 10000 GHz	Q(225.) =	1572.7
Max. J	= 60	Q(150.) =	855.8
LOGSTR	= -8	Q(75.) =	302.8
LOGSTR1	= -8	Q(37.5) =	107.33
Isotope Correction	= -0.611	Q(18.25) =	38.32
Minimum Energy	= 0. cm ⁻¹	Q(9.375) =	14.84
Dipoles:	$\mu(a)$ = 0.3627	A =	613461.
	$\mu(b)$ = 1.471	B =	14850.441
	$\mu(c)$ =	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 Species Name: C₂H₅CN,
 Version: 2 ethyl cyanide
 Date: Jan 1981
 Contributor: R. L. Poynter

Lines Listed	=	3684	Q(300.)	=	111840.8900
Max. Frequency	=	3000 GHz	Q(225.)	=	70892.5160
Max. J	=	21	Q(150.)	=	39554.9140
LOGSTR	=	-5 above 160 GHz	Q(75.)	=	12589.2560
LOGSTR1	=		Q(37.5)	=	4595.1553
Isotope Correction	=	0	Q(18.25)	=	1406.3713
Minimum Energy	=	0 cm ⁻¹	Q(9.375)	=	650.8787
Dipoles:			A	=	27663.66
	μ(a)	= 3.85	B	=	4714.144
	μ(b)	= 1.23	C	=	4235.041
	μ(c)	=			

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 ₃ CH ₂ ¹³ CN,
Version:	2		ethyl cyanide,
Date:	Jan 1981		¹³ C isotope on
Contributor:	R. L. Poynter		atom 1
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. 29z, 1345.

The dipole moment was assumed the same as in the parent species, tag #55001.

Species Tag: 56002
 Version: 2
 Date: Jan 1981
 Contributor: R. L. Poynter

Species Name: $\text{CH}_3^{13}\text{CH}_2\text{CN}$,
 ^{13}C isotope on
 atom 2

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:	$^{13}\text{CH}_3\text{CH}_2\text{CN}$,
Version:	2		ethyl cyanide,
Date:	Jan 1981		^{13}C isotope on
Contributor:	R. L. Poynter		atom 3
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:	$\text{CH}_3\text{CH}_2\text{C}^{15}\text{N}$,
Version:	1		ethyl cyanide,
Date:	Jan 1980		^{15}N isotope
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:	$\mu(a)$	=	3.84	A	=	27541.953
	$\mu(b)$	=	1.37	B	=	4574.771
	$\mu(c)$	=		C	=	4119.430

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333. The measurements were taken from H. M. Heise, H. 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 ₂ DCH ₂ CN-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:	$\mu(a)$ = 3.84	A =	27650.795
	$\mu(b)$ = 1.37	B =	4425.061
	$\mu(c)$ =	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 ₂ DCH ₂ CN-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
Version: 2
Date: Jan 1981
Contributor: R. L. Poynter

Species Name: OCS
carbonyl sulfide

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:	$^{28}\text{Si}^{32}\text{S}$
Version:	1		silicon monosulfide
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		Q(300.)	=	1031.5737
Max. Frequency	=	3000	GHz	Q(225.)	=	773.9269
Max. J	=	99		Q(150.)	=	515.9410
LOGSTR	=	-6.4		Q(75.)	=	258.1666
LOGSTR1	=			Q(37.5)	=	129.2409
Isotope Correction	=	-1.977		Q(18.25)	=	64.7888
Minimum Energy	=	0.	cm ⁻¹	Q(9.375)	=	32.5612
Dipoles:		$\mu(a)$	= 0.715	A	=	
		$\mu(b)$	=	B	=	6061.924
		$\mu(c)$	=	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:	61002	Species Name:	$^{29}\text{Si}^{32}\text{S}$
Version:	1		silicon monoxide
Date:	Dec 1979		^{29}Si isotopic species
Contributor:	R. L. Poynter		
Lines Listed	= 98	Q(300.) =	701.7784
Max. Frequency	= 3000 GHz	Q(225.) =	526.8662
Max. J	= 98	Q(150.) =	351.2369
LOGSTR	= -5	Q(75.) =	175.7521
LOGSTR1	=	Q(37.5) =	88.0239
Isotope Correction	= -1.349	Q(18.25) =	44.1774
Minimum Energy	= 0 cm^{-1}	Q(9.375) =	22.2587
Dipoles:	$\mu(a) = 1.730$	A =	
	$\mu(b) =$	B =	8910.66
	$\mu(c) =$	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:	62001	Species Name:	OC ³⁴ S
Version:	2		carbonyl sulfide
Date:	Jan 1981		³⁴ S isotopic species
Contributor:	R. L. Poynter		

Lines Listed	=	99	Q(300.) =	1053.9019
Max. Frequency	=	3000 GHz	Q(225.) =	777.6780
Max. J	=	99	Q(150.) =	527.2301
LOGSTR	=	-6.4	Q(75.) =	263.7545
LOGSTR1	=		Q(37.5) =	132.0383
Isotope Correction	=	-1.376	Q(18.25) =	66.1911
Minimum Energy	=	0. cm ⁻¹	Q(9.375) =	33.2583
Dipoles:			A =	
	$\mu(a)$	= 0.715	B =	5932.8338
	$\mu(b)$	=	C =	
	$\mu(c)$	=		

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:	62032	Species Name:	¹⁸ OCS,
Version:	2		carbonyl sulfide,
Date:	Jan 1981		¹⁸ O isotopic species
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
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: $^{30}\text{Si}^{32}\text{S}$,
silicon monosulfide,
 ^{30}Si isotopic species

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: $\mu(a)$	=	1.730	A	=	
$\mu(b)$	=		B	=	8755.33
$\mu(c)$	=		C	=	

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

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

Species Tag:	62004	Species Name:	$^{28}\text{Si}^{34}\text{S}$,
Version:	1		silicon monosulfide,
Date:	Dec 1979		^{34}S isotopic species
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: HNO₃,
 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 $J = 1 + 0$ 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 Σ _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. Spectry. 75, 53. The calculational method used is from T. Amano and E. Hirota, 1974, J. Mol. Spectry. 53, 346. For S₂, the parameter μ(l) 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 = ± (-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: SO₂,
sulfur dioxide

Lines Listed	=	9622	Q(300.)	=	5899.2969
Max. Frequency	=	10000 GHz	Q(225.)	=	3765.3037
Max. J	=	74	Q(150.)	=	2075.8706
LOGSTR	=	-10	Q(75.)	=	738.9240
LOGSTR1	=	-1)	Q(37.5)	=	261.6373
Isotope Correction	=	-0.022	Q(18.25)	=	92.8325
Minimum Energy	=	0 cm ⁻¹	Q(9.375)	=	33.0674
Dipoles:	$\mu(a)$	=	A	=	60778.558
	$\mu(b)$	=	B	=	10317.913
	$\mu(c)$	=	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
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: HC₅N ,
cyanodiacetylene

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: $\mu(a)$	=	4.330	A =	
$\mu(b)$	=		B =	1331.33
$\mu(c)$	=		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 measured by the same authors.

Species Tag:	76001	Species Name:	HCCCC ¹³ CN,
Version:	1		cyanodiacetylene,
Date:	Dec 1979		¹³ C isotope on
Contributor:	R. L. Poynter		atom 1
Lines Listed	= 99	Q(300.) =	4742.4238
Max. Frequency	= 300 GHz	Q(225.) =	3448.2642
Max. J	= 99	Q(150.) =	2336.6826
LOGSTR	= -6.6	Q(75.) =	1185.7676
LOGSTR1	=	Q(37.5) =	593.0616
Isotope Correction	= -1.933	Q(18.25) =	296.6880
Minimum Energy	= 0. cm ⁻¹	Q(9.375) =	148.5251
Dipoles:	$\mu(a)$ = 4.330	A =	
	$\mu(b)$ =	B =	1318.18
	$\mu(c)$ =	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:	76002	Species Name:	HCCC ¹³ CCN,
Version:	1		cyanodiacetylene,
Date:	Dec 1979		¹³ C isotope
Contributor:	R. L. Poynter		on atom 2
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	Species Name:	HCC ¹³ CCCN,
Version:	1		cyanodiacetylene,
Date:	Dec 1979		¹³ C isotope
Contributor:	R. L. Poynter		on atom 3
Lines Listed	= 99	Q(300.) =	4700.0195
Max. Frequency	= 300 GHz	Q(225.) =	3417.4316
Max. J	= 99	Q(150.) =	2317.3931
LOGSTR	= -6.6	Q(75.) =	1175.1672
LOGSTR1	=	Q(37.5) =	587.8950
Isotope Correction	= -1.955	Q(18.25) =	294.1033
Minimum Energy	= 0 cm ⁻¹	Q(9.375) =	147.2313
Dipoles:	$\mu(a)$ = 4.329	A =	
	$\mu(b)$ =	B =	1329.95
	$\mu(c)$ =	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:	76004	Species Name:	HC ¹³ CCCCN,
Version:	1		cyanodiacetylene,
Date:	Dec 1979		¹³ C isotope
Contributor:	R. L. Poynter		on atom 4

Lines Listed	=	99	Q(300.) =	4744.6045
Max. Frequency	=	300 GHz	Q(225.) =	3449.8496
Max. J	=	99	Q(150.) =	2337.2217
LOGSTR	=	-6.6	Q(75.) =	1186.0413
LOGSTR1	=		Q(37.5) =	593.3350
Isotope Correction	=	-1.955	Q(18.25) =	296.8244
Minimum Energy	=	0 cm ⁻¹	Q(9.375) =	148.5935
Dipoles:			A =	
	μ(a) =	4.329	B =	1317.689
	μ(b) =		C =	
	μ(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:	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
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: HC₅¹⁵N,
cyanodiacetylene,
¹⁵N isotopic
species

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:				A	=	
	μ (a)	=	4.329	B	=	1298.639
	μ (b)	=		C	=	
	μ (c)	=				

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

The dipole moment was measured by the same authors.

Species Tag:	76007	Species Name:	DC ₅ N,
Version:	1		cyanodiacetylene,
Date:	Dec 1979		D isotopic species
Contributor:	R. L. Poynter		
Lines Listed	= 99	Q(300.)	= 4918.1348
Max. Frequency	= 300 GHz	Q(225.)	= 3564.5166
Max. J	= 99	Q(150.)	= 2417.1284
LOGSTR	= -6.6	Q(75.)	= 1229.4199
LOGSTR1	=	Q(37.5)	= 615.0352
Isotope Correction	= -3.824	Q(18.25)	= 307.6805
Minimum Energy	= 0 cm ⁻¹	Q(9.375)	= 153.9927
Dipoles:	μ(a) = 4.329	A =	
	μ(b) =	B =	1271.056
	μ(c) =	C =	

The experimental measurements were taken from A. J. Alexander, H. W. Kroto, and D. R. N. Walton, 1976, J. Mol. Spect. 62, 175.

The dipole moment was assumed to be the same as 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 ,
Version:	1		Hydrogen Bromide,
Date:	Feb 1980		⁸¹ Br isotopic
Contributor:	R. L. Poynter and H. M. Pickett		species

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:			A =	
	$\mu(a)$	= 0.828	B =	250250.2
	$\mu(b)$	=	C =	
	$\mu(c)$	=		

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
Version: 1
Date: Feb 1980
Contributor: H. M. Pickett

Species Name: ^{79}BrO ,
Bromine Monoxide,
 ^{79}Br isotopic species,
 $^2\Pi_{3/2}$ 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:				A	=	
	$\mu(a)$	=	1.765	B	=	12830.4
	$\mu(b)$	=		C	=	
	$\mu(c)$	=				

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 ,
Version:	1		Bromine Monoxide,
Date:	Feb 1980		^{81}Br isotopic species,
Contributor:	H. M. Pickett		$^2\Pi_{3/2}$ state
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(18.25) =	259.2984
Minimum Energy	= 0 cm^{-1}	Q(9.375) =	137.2459
Dipoles:	$\mu(a)$ = 1.794	A =	
	$\mu(b)$ =	B =	12777.08
	$\mu(c)$ =	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: $^{35}\text{ClNO}_3$
Chlorine nitrate

Lines Listed	=	4198		Q(300.)	=	100540.
Max. Frequency	=	3000	GHz	Q(225.)	=	65303.
Max. J	=	60		Q(150.)	=	35546.
LOGSTR	=	-6		Q(75.)	=	12567.
LOGSTR1	=	-6		Q(37.5)	=	4447.
Isotope Correction	=	-0.122		Q(18.25)	=	1574.
Minimum Energy	=	0	cm ⁻¹	Q(9.375)	=	557.
Dipoles:	$\mu(a)$	=	0.72	A	=	12105.8
	$\mu(b)$	=	0.28	B	=	2777.0
	$\mu(c)$	=	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: $^{37}\text{ClNO}_3$
 Chlorine nitrate

Lines Listed	=	4182		Q(300.)	=	103108.
Max. Frequency	=	3000	GHz	Q(225.)	=	66971.
Max. J	=	60		Q(150.)	=	36454.
LOGSTR	=	-6		Q(75.)	=	12888.
LOGSTR1	=	-6		Q(37.5)	=	4561.
Isotope Correction	=	-0.611		Q(18.25)	=	1614.
Minimum Energy	=	0	cm ⁻¹	Q(9.375)	=	572.
Dipoles:				A	=	12105.4
	$\mu(a)$	=	0.72	B	=	2707.6
	$\mu(b)$	=	0.28	C	=	2207.6
	$\mu(c)$	=	0			

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.