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# Submillimeter, Millimeter, and Microwave Spectral Line Catalogue

R. L. Poynter  
H. M. Pickett



June 1, 1981

National Aeronautics and  
Space Administration

Jet Propulsion Laboratory  
California Institute Of Technology  
Pasadena, California

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## ABSTRACT

This report describes a computer accessible catalogue of submillimeter, millimeter, and microwave spectral lines in the frequency range between 0 and 3000 GHz (i.e., wavelengths longer than 100  $\mu\text{m}$ ). 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 (133 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

Additions (9) and changes (24) have been made to the following molecular species:

### New Species (9)

NH<sub>2</sub>D  
H<sub>2</sub>O-V2  
H<sub>2</sub>O<sub>2</sub>  
CH<sub>3</sub>CHO-E  
O<sub>3</sub>-V2

O<sub>3</sub>-V13  
HOCL  
HOCL-37  
HNO<sub>3</sub>

### Revised Species (24)

NH<sub>3</sub>  
N-15-H<sub>3</sub>  
H<sub>2</sub>O  
CH<sub>2</sub>NH  
CH<sub>2</sub>ND  
O<sub>2</sub>  
O<sub>2</sub>-V1  
O-18-O  
CH<sub>3</sub>OH  
H<sub>2</sub>S  
PH<sub>3</sub>  
NH<sub>2</sub>CHO

CLO  
CL-37-0  
C<sub>2</sub>H<sub>5</sub>CN  
CH<sub>3</sub>CH<sub>2</sub>C-13-N  
CH<sub>3</sub>C-13-H<sub>2</sub>CN  
CH<sub>2</sub>DCH<sub>2</sub>CN-S  
CH<sub>2</sub>DCH<sub>2</sub>CN-A  
OCS  
OC-13-S  
OCS-34  
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 3000 GHz (i.e. wavelengths longer than 100 $\mu$ 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 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.



## 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  
(F13.4, F8.4 , F8.4 , I2 , F10.4 , I3 , I7 , I4 , I2I2, I1)

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  $\text{nm}^2 \text{ MHz}$  at 300K. (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  $\text{cm}^{-1}$ .

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.

QN: Quantum numbers for the upper and lower states coded according to QNFORM.

### 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  $2.9979 \times 10^{+18}$ .

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

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

where  $\nu_{ba}$  is the line frequency,  $xS_{ba}$  is the line strength,  $\mu_x$  is the dipole moment along the molecular axis  $x$ ,  $E''$  and  $E'$  are the lower and upper state energies respectively, and  $Q_{rs}$  is the rotation-spin partition function (using the same zero of energy as  $E'$  and  $E''$ ). Care must be taken to assure that  $xS_{ba}$  and  $Q_{rs}$  are determined with 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

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

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

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  $\alpha_{\max}$  is in units of  $\text{cm}^{-1}$ . The corresponding value of  $\alpha_{\max}$  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),  $\nu_{ba}$  is the line frequency in MHz.

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

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

The inverse of  $\sigma_{ba}$  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, and the value of  $Q_{rs}(300K)$  is listed in Section VI.

#### IV. General Comments on Precision

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

$$\epsilon_n^2 = \sum_{k,\ell} \frac{\partial v_n}{\partial p_k} \frac{\partial v_n}{\partial p_\ell} V_{k\ell} \quad (7)$$

in which  $\epsilon_n$  is the estimated error of frequency  $v_n$  and  $V_{k\ell}$  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

$$(V^{-1})_{k\ell} = \sum_m \frac{\partial v_m}{\partial p_k} \frac{\partial v_m}{\partial p_\ell} \epsilon_m^{-2} \quad (8)$$

in which the summation over  $m$  is over the experimental lines using experimental uncertainties,  $\epsilon_m$ . 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.

Experimental uncertainties in the literature vary from 1.6  $\sigma$  estimates to 3  $\sigma$  estimates and are more usually "guess-timates". Many times the statistical nature of the uncertainties are not stated. Therefore, the expected errors in predicted lines will usually reflect this ambiguity in laboratory uncertainties through Eq (6) and (7). 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 the 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 resonance.

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  $S_{ba}$  and errors in the rotation-spin partition function. (The vibration-electronic partition function does not enter directly because the catalogued 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.

## V. Format of Quantum Numbers

The quantum numbers of the catalogued lines are given in the field QN according to a format QNFORM, as discussed in Section II. In this section the identities of the quantum numbers will be described for each distinct format. The field QN will be regarded as being divided into 13 integers. The first 12 integers are two digits long and the last integer is a single digit (a FORTRAN 12I2, 1I format).

The spectroscopic nomenclature followed is the standard one in which upper state quantities are denoted by a single prime and lower state quantities are denoted by a double prime.

In addition,

L	electron orbital angular momentum
R	rotational angular momentum
$N = R+L$	
S	electron spin
$J = N+S$	total electron and rotational angular momentum
I	nuclear spin
$F_1 = I_1+J$	intermediate F value for two nuclear spins $I_1$ and $I_2$
$F = I_2 + F_1$	(for two non-zero nuclear spins)
$= I + J$	(for one non-zero nuclear spin)
$\Omega$	projection of J on the molecular axis of a linear molecule
K	projection of J on the symmetry axis of a symmetric rotor
p	parity under inversion (1 = gerade, -1 = ungerade)
v	vibrational quantum number
$K_{-1}$	prolate K quantum number for an asymmetric rotor
$K_{+1}$	oblate K quantum number for an asymmetric rotor

In all cases, half integer quantum numbers will be written into the QN field after rounding up to the next integer. For example,  $J = 1/2$  will be entered in the catalogue as a 1. The format specification QNFORM is designed so that the correct half-integer value can be recovered unambiguously.

The format integer QNFORM is allocated four digits. The most significant digit is zero for the standard formats described in Table V-1 and is non-zero for special-case formats which will be allocated as the need arises. Of the remaining three digits, the most significant is used to describe the type of species involved and the least significant digits are used to specify the nature of the integers in the field. The formats are shown in Tables V-1 and V-2.

Table V-1: Standard Quantum Number Formats

QNFOPM	ON	Remarks
<b>A. Atoms</b>		
010	$J' + \frac{1}{2}, J'' + \frac{1}{2}$	$I = 0, J$ half integer
020	$J', J''$	$I = 0, J$ integer
011	$J' + \frac{1}{2}, J'' + \frac{1}{2}, F' + \frac{1}{2}, F'' + \frac{1}{2}$	$J$ and $F$ half integer
012	$J' + \frac{1}{2}, J'' + \frac{1}{2}, F', F''$	$J$ half integer, $F$ integer
021	$J', J'', F' + \frac{1}{2}, F'' + \frac{1}{2}$	$J$ integer, $F$ half integer
022	$J', J'', F', F''$	$J$ and $F$ integer
<b>B. Linear molecules and Diatomic molecules</b>		
1XY	$J', J'', x', x'', y', y''$	$1\Sigma$ state
2XV	$J' + \frac{1}{2}, N', J'' + \frac{1}{2}, N'', x', x'', y', y''$	$2\Sigma$ state
3XY	$J', N', J'', N'', x', x'', y', y''$	$3\Sigma$ state
4XY	$J', p', J'', p'', x', x'', y', y''$	$1\Pi$ state
5XY	$J' + \frac{1}{2}, \Omega', J'' + \frac{1}{2}, p', J'' + \frac{1}{2}, \Omega'', x', x'', y', y''$	$2\Pi$ state
6XY	$J', \Omega', p', J'', \Omega'', p'', x', x'', y', y''$	$3\Pi$ state
7XY	$J', \Omega', p', J'', \Omega'', p'', x', x'', y', y''$	$1\Delta$ state
<b>C. Symmetric Rotors (3-fold symmetry or higher, <math>S = 0</math>)</b>		
8XY	$J', K', J'', K'', x', x'', y', y''$	
<b>D. Asymmetric Rotors</b>		
9XY	$J', K'_{-1}, K'_{+1}, J'', K''_{-1}, K''_{+1}, x', x'', y', y''$	closed shell molecule
95Y	$N', K'_{-1}, K'_{+1}, N'', K''_{-1}, K''_{+1}, J' + \frac{1}{2}, J'' + \frac{1}{2}, y', y''$	$S = \frac{1}{2}$ open shell radical
96Y	$N', K'_{-1}, K'_{+1}, N'', K''_{-1}, K''_{+1}, J', J'', y', y''$	$S = 1$ triplet state
$X = 0:$	$x = 0$	$Y = 0$
$X = 1:$	$x = F + \frac{1}{2}$ ( $F$ half integer)	$Y = F + \frac{1}{2}$ or $Y = F + \frac{1}{2}$ if $X = 4$
$X = 2:$	$x = F$ ( $F$ integer)	$Y = F$ or $Y = F$ if $X = 4$
$X = 4:$	$x = v$ vibrational state label (further specified in the species description)	
, signifies upper energy state, " signifies lower energy state		



Table V-2: Special-Case Quantum Number Formats

<u>QNFORM</u>	<u>QN</u>	<u>Remarks</u>
1300	J,N	$3\sum$ state "non-resonant" transition; frequency is $ g J$ where g is the molecular g factor i.e. the frequency is the Zeeman splitting for a $M = J$ level in a 0.78145 gauss magnetic field.

## VI. Documentation by Species

The documentation for each molecular or atomic species appears in order of "species tag." On the following page, immediately preceding the documentation, is an "Index of Species." This index lists all the species documentation contained in this publication, ordered by "species tag."

# INDEX OF SPECIES

1001	H-Atom	34001	O-18-0	51001	HCCCN
2001	D-Atom	34002	H2S	51002	C10
3001	HD	34003	PH3	52001	HCCC-13-N
12001	C-Atom	34004	H2O2	52002	HCC-13-CN
13001	C-13-Atom	35001	HDS	52003	HC-13-CCN
14001	N-Atom	36001	HC1	52004	HCCCN-15
14002	N-Atom-D-State	38001	HC1-37	52005	DCCCN
16001	O-Atom	40001	CH3CCH	52006	HOC1
17001	HO	41001	CH3CN	53001	C2H3CN
17002	NH3	41002	CH3CC-13-H	53002	C1-37-0
17003	CH3D	41003	CH3C-13-CH	54001	CH2CHC-13-N
18001	DO	41004	C-13 H3CCH	54002	CH2C-13-HCN
18002	N-15-H3	41005	CH3CCD	54003	C-13-H2CHCN
18003	H2O	41006	CH2DCCH	54004	CH2CDCN
18004	NH2D	42001	CH3CN-15	54005	HOC1-37
18005	H2O-v2	42002	CH2CO	55001	C2H5CN
19001	HO-18	43001	CHDCO	56001	CH3CH2C-13-N
19002	HDO	44001	CS	56002	CH3C-13-H2CN
27001	HCN	44002	SiO	56003	C-13-H3CH2CN
27002	HNC	44003	CH3CHO-A	56004	C2H5CN-15
28001	CO	44004	N2O	56005	CH2DCH2CN-S
28002	HC-13-N	44005	CH3CHO-E	56006	CH2DCH2CN-A
28003	HCN-15	45001	C-13-S	60001	OCs
28004	DCN	45002	Si-29-0	60002	SiS
28005	HNC-13	45003	NH2CHO	61001	OC-13-S
28006	HN-15-C	46001	CS-34	61002	O-18-CS
28007	DNC	46002	Si-30-0	62001	Si-29-S
29001	C-13-0	46003	H2CS	62002	O-18-CS
29002	HCO+	46004	C2H5OH	62003	Si-30-S
29003	CH2NH	46005	HC00H	62004	SiS-34
30001	CO-18	47001	H2C-13-S	63001	HN03
30002	HC-13-0+	47002	HC-13-00H	64001	S2
30003	DCO+	47003	DC00H	64002	S02
30004	H2CO	47004	HC00D	75001	HCCCCCN
30005	C-13-H2NH	48001	SO	76001	HCCCCC-13-N
30006	CH2N-15-H	48002	SO-v1	76002	HCCCC-13-CN
30007	CH2ND	48003	H2CS-34	76003	HCCC-13-CCN
30008	NO	48004	O3	76004	HCC-13-CCCN
31001	HCO-18+	48005	O3-v2	76005	HC-13-CCCN
31002	H2C-13-0	48006	O3-v1,3	76006	HCCCCCN-15
32001	O2	50001	S-34-0	76007	DCCCCCN
32002	O2-v1	50002	SO-18	80001	HBr-79
32003	CH3OH	50003	O3-SYM-0-18	82001	HBr-81
32004	H2CO-18	50004	O3-ASYM-0-18	95001	Br-79-0
				97001	Br-81-0

Species Tag: 1001	Page 1 of 1	Version: 1	Date: Oct, 1979
Species Name: Atomic Hydrogen  $2S_{1/2}$ ground state		Author: H. M. Pickett	
		Min. Int. = $8 \times 10^{-10}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 4.0		J Max. = ( $\frac{1}{2}$ )	Lines Listed = 1
Dipole Moments/Debye: $\mu_a =$ $\mu_b =$ magnetic $\mu_c =$			
Rot. Const./MHz: A = B = C =			

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

Species Tag: 2001	Page 1 of 1	Version: 1	Date: Oct. 1979
Species Name: Atomic Hydrogen Deuterium Isotope  $2S_{1/2}$ ground state		Author: H. M. Pickett	
		Min. Int. = $5 \times 10^{-11}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 6.0		J Max. = ( $\frac{1}{2}$ )	Lines Listed = 1
Dipole Moments/Debye: $\mu_a =$ $\mu_b =$ magnetic $\mu_c =$			
Rot. Const./MHz: A = B = 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  $4.695 \times 10^{-17}$  sec<sup>-1</sup>.

Species Tag: 3001	Page 1 of 1	Version: 1	Date: Oct. 1979
Species Name: HD Mono-deuterated molecular hydrogen		Author: H. M. Pickett	
		Min. Int. = $10^{-6}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 5.016		J Max. = (1)	Lines Listed = 1
Dipole Moments/Debye: $\mu_a = 5.85 \times 10^{-4}$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A = B = 1339100. C =			

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

# JPL SMM CATALOGUE

Species Tag: 12001	Page 1 of 1	Version: 1	Date: Oct. 1979
Species Name: Atomic Carbon  $^3P$ ground state		Author: H. M. Pickett	
		Min. Int. = $10^{-5}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T - 300K) = 7.8330		J Max. = (2)	Lines Listed = 2
Dipole Moments/Debye: $\mu_a =$ $\mu_b =$ magnetic $\mu_c =$			
Rot. Const./MHz: A = B = C =			

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

<u>J</u>	<u>Energy</u>	<u>Degeneracy</u>
0	0.0 cm <sup>-1</sup>	1
1	16.4168	3
2	43.4138	5

Species Tag: 13001	Page 1 of 1	Version: 1	Date: Oct. 1979
Species Name: Atomic Carbon $^{13}\text{C}$ isotope		Author: H. M. Pickett	
		Min. Int. = $10^{-16}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 15.666		J Max. = (2)	Lines Listed = 7
Dipole Moments/Debye: $\mu_a$ = $\mu_b$ = magnetic $\mu_c$ =			
Rot. Const./MHz: A =                      B =                      C =			

The fine structure intervals of  $^{12}\text{C}$  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, 1966 (Physics Letters A29, 461) were then used to compute the line frequencies. Intensities were calculated using the free electron g value.



Species Tag: 14001	Page 1 of 1	Version: 1	Date: Oct. 1979
Species Name: Atomic Nitrogen $^4S_{3/2}$ ground state		Author: H. M. Pickett	
		Min. Int. = $10^{-13}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 12.0		J Max. = (3/2)	Lines Listed = 2
Dipole Moments/Debye: $\mu_a$ = $\mu_b$ = magnetic $\mu_c$ =			
Rot. Const./MHz: A = B = C =			

The hyperfine transitions of atomic nitrogen at 15.6 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	Page 1 of 1	Version: 1	Date: Nov. 1979
Species Name: Atomic Nitrogen $^2D$ excited state		Author: H. M. Pickett	
		Min. Int. = $10^{-8}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 29.510		J Max. = (5/2)	Lines Listed = 6
Dipole Moments/Debye: $\mu_a$ = $\mu_b$ = magnetic $\mu_c$ =			
Rot. Const./MHz: A = B = C =			

The  $^2D_{5/2}$  state is 19223 cm<sup>-1</sup> above the ground  $^4S_{3/2}$  state. (C. E. Moore, 1949, Atomic Energy Levels I, U. S. N. Bureau of Stds.). The  $^2D_{3/2} - ^2D_{5/2}$  inverted fine structure transition at 260 GHz has a predicted uncertainty of  $\pm 600$  MHz, but the hyperfine structure intervals are uncertain by less than 1 MHz. (H. E. Radford and K. M. Evenson, 1968, Phys. Rev. 168, 70). The average spontaneous emission rate from the  $^2D$  states to the  $^4S$  states is  $1.06 \times 10^{-6}$  sec<sup>-1</sup>. In contrast, the spontaneous emission rate from  $^2D_{3/2}$  F = 5/2 to  $^2D_{5/2}$  F = 7/2 is  $3.15 \times 10^{-9}$  sec<sup>-1</sup>.

# JPL SPM CATALOGUE

Species Tag: 16001	Page 1 of 1	Version: 1	Date: Oct. 1979
Species Name: Atomic Oxygen $^3P$ ground state		Author: H. M. Pickett	
		Min. Int. = $10^{-4}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 7.4943		J Max. = (2)	Lines Listed = 1
Dipole Moments/Debye: $\mu_a$ = $\mu_b$ = magnetic $\mu_c$ =			
Rot. Const./MHz: A = B = C =			

The  $68\text{ cm}^{-1}$  J = 1-2 line of oxygen has 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. The partition function was calculated from the following table:

<u>J</u>	<u>Energy</u>	<u>Degeneracy</u>
0	227.0195	1
1	68.7165	3
2	0.0	5

Species Tag: 17001	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Hydroxyl Radical OH ground $^2\Pi_{3/2}$ and $^2\Pi_{1/2}$ states		Author: R. L. Poynter & H. M. Pickert	
		Min Int. = $10^{-13}$ cm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 83.328		J Max. = 19.5	Lines Listed = 125
Dipole Moments/Debye: $\mu_a$ = 1.667 $\mu_b$ = $\mu_c$ =			
Rot. Const./MHz: A =      B = 556140.9      C =			

The calculational method and microwave data are reported in R. A. Beaudet and R. L. Poynter, 1978, J. Phys. Chem. Ref. Data 7, 311. The partition function was calculated by a sum over states to J = 11.5. Other values are:

T	$Q_{sr}$
150K	40.230
70	21.800
30	16.354
10	15.696

Only the J = 5/2 - 3/2 and J = 3/2 - 1/2 submillimeter transitions are included in the catalogue.

Species Tag: 17002	Page 1 of 1	Version: 2	Date: Feb. 1981
Species Name: Ammonia, NH <sub>3</sub> , ground inversion states		Author: R.L. Poynter & H.M. Pickett	
		Min. Int. = 10 <sup>-17</sup> cm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 578.984		J Max. = 20	Lines Listed = 235
Dipole Moments/Debye: $\mu_a$ = $\mu_b$ = $\mu_c$ = 1.476			
Rot. Const./MHz: A = B = 298117.59 C = 186711.			

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.

Other values of the partition functions are:

<u>T</u>	<u>Q</u>
10	5.719
30	20.37
60	53.76
150	206.64
200	316.64

The rotational energy levels were computed from a fit of the far IR lines measured by J. Dowling, 1968, J. Mol. Spectrosc., 27, 527 and the J = 1 - 0, K = 0 transition reported by P. Helminger, F. DeLucia, and W. Gordy, 1971, J. Mol. Spectrosc. 39, 94. The C and D rotational constants which were not determined in the fit, were taken from D. Laughton, S. Freund and T. Oka, 1976, J. Mol. Spectrosc. 62, 263, and from S. Sundaram, F. Suzek, and F. Cleveland, 1960, J. C. P. 32, 251. The rotational constants were in good agreement with those of Laughton, et al.

Species Tag: 17003	Page 1 of 1	Version: 1	Date: Feb. 1980
Species Name: Deutero Methane  CH <sub>3</sub> D	Author: R. L. Poynter		
	Min. Int. = 10 <sup>-8</sup> nm <sup>2</sup> MHz		
Q (Spin-Rot., T - 300K) = 402.166	J Max. = 13	Lines Listed = 80	
Dipole Moments/Debye: $\mu_a = 5.6 \times 10^{-3}$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A = 157412. B = 116325.308 C = B			

The J = 0 1 line has been measured by H. M. Pickett, E. A. Cohen and T. G. Phillips, 1980, Ap. J. Letters, 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: 18001	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Deuterated hydroxyl  radical: OD $^2_{\Pi}$ ground states		Author: R.L. Poynter & H.M. Pickett	
		Min. Int. = $10^{-13}$ $\text{cm}^2\text{MHz}$	
Q (Spin-Rot., T = 300K) = 215.558		J Max. = 19.5	Lines Listed = 235
Dipole Moments/Debye: $\mu_a = 1.653$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A = B = 296312.0 C =			

The calculational method and microwave data are reported in R. A. Beaudet and R. L. Poynter, 1978, J. Phys. Chem. Ref. Data 7, 311. The partition function was calculated using the relation  $Q=6 Q_{\text{rot}} [1 + \exp(-188.112/T)]$ , in which  $Q_{\text{rot}}$  is the rotational partition function for a diatomic molecule. No submillimeter lines are currently listed in the catalogue for OD.

Species Tag: 18002	Page 1 of 1	Version: 2	Date: Jan 1981
Species Name: Ammonia, $^{15}\text{NH}_3$ ground inversion states		Author: R. Poynter	
		Min. Int. = $10^{-17}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 575.808		J Max. = 20	Lines Listed = 235
Dipole Moments/Debye: $\mu_a$ = $\mu_b$ = $\mu_c$ = 1.476			
Rot. Const./MHz. 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  $^{14}\text{NH}_3$ .

The partition function was determined by a sum over states to J = 20. Other values are:

<u>T</u>	<u>Q</u>
10	5.72
30	20.42
60	53.97
150	207.21



Species Tag: 18003	Page 1 of 1	Version: 2	Date: July 1980
Species Name: Water  H <sub>2</sub> O		Author: R.L. Poynter & H.M. Pickett	
		Min. Int. = 10 <sup>-9</sup> nm <sup>2</sup> MHz	
Q (Spin-Rot., T - 300K) = 178.037		J Max. = 15	Lines Listed = 151
Dipole Moments/Debye: $\mu_a = 0$ $\mu_b = 1.855$ $\mu_c = 0$			
Rot. Const./MHz: A = 835840.29      B = 435351.72      C = 278138.7			

The data set used in this new fit includes all the lines measured by F. C. De Lucia, P. Helminger, R. Cook, and W. Gordy (1972), Phys. Rev. A, 5, 487 as well as the interferometer lines below 10 THz measured by T. Kauppinen, T. Karkkainen, E. Kyro (1978), J. Mol. Spec. 71, 15. The dipole moment is from S. Clough, Y. Beers, G. P. Klein and L. Rothman (1973), J. Chem. Phys. 59, 3125. Other references are given in F. C. De Lucia, P. Helminger, and W. H. Kirchhoff, (1974), J. Phys. Chem. Ref. Data, 3, 211.

The partition function was determined by a sum over states to J = 15. Other values are:

<u>T</u>	<u>Q</u>
150	63.677
100	35.153
60	16.818
30	6.192
10	1.328

Species Tag: 18004	Page 1 of 1	Version: 1	Date: Jan. 1981
Species Name: Monodeutero Ammonia, NH <sub>2</sub> D, ground vibrational states		Author: H. M. Pickett	
		Min. Int. = 10 <sup>-10</sup> nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 1258.		J Max. = 14	Lines Listed = 5036
Dipole Moments/Debye: $\mu_a = -0.18$ $\mu_b = 0.$ $\mu_c = 1.463$			
Rot. Const./MHz: A = 290124.      B = 192194.      C = 140797.			

The experimental lines were measured by F. C. DeLucia and P. Helminger, 1975, J. Mol. Spec. 54, 200 and by E. A. Cohen and H. M. Pickett at JPL. The dipole moments and quadrupole splitting was 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	Page 1 of 1	Version: 1	Date: Jan. 1981
Species Name: Water excited bending state, $\nu_2$ or (010) $H_2O$		Author: H. M. Pickett	
		Min. Int. = $10^{-10}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T - 300K) = 169.226		J Max. = 12	Lines Listed = 122
Dipole Moments/Debye: $\mu_a = 0$ $\mu_b = 1.855$ $\mu_c = 0$			
Rot. Const./MHz: A = 933052. B = 440318. C = 273710.			

The rotational lines were determined by M. Herman, J. W. C. Johns, and A. R. W. McKellar, 1979, Can. J. Phys. 57, 397 and H. Kuze, 1980, Ap. J. 239, 1131. These lines were fit to the Hamiltonian of C. Camy-Peyret and J. M. Flaud, 1976, Molec. Phys. 32, 523 in such a way that the parameters of Camy-Peyret and Flaud were modified in a least squares sense to accomodate the rotational lines. The partition function was determined by a sum over states. Additional values are:

<u>T</u>	<u>Q</u>
10	1.325
30	5.983
60	15.964
100	33.350
150	60.446

The zero of energy is  $1594.75 \text{ cm}^{-1}$  above the zero of energy for the ground state species.

Species Tag: 19001	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Hydroxyl radical Oxygen - 18 isotope $^{18}\text{OH}$		Author: R. L. Poynter & H. M. Pickett	
		Min. Int. = $10^{-13}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 83.882		J Max. = 20	Lines Listed = 113
Dipole Moments/Debye: $\mu_a$ = 1.667 $\mu_b$ = $\mu_c$ =			
Rot. Const./MHz: A =      B = 552470.      C =			

The calculational method and microwave data are reported in R. A. Beaudet and R. L. Poynter, 1978, J. Phys. Chem. Ref. Data 7, 311. The partition function was calculated using the  $^{16}\text{OH}$  value and the ratio of the B values. No pure rotational lines are currently listed in the catalogue.

Species Tag: 19002	Page 1 of 1	Version: 1	Date: Feb. 1980
Species Name: Water Single Deuterium Isotope HDO		Author: R. L. Poynter	
		Min. Int. = $10^{-13}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 146.05	J Max. = 13	Lines Listed = 221	
Dipole Moments/Debye: $\mu_a = 0.657$ $\mu_b = 1.732$ $\mu_c = 0.$			
Rot. Const./MHz: A = 701931.5 B = 272912.6 C = 192055.2			

The observed lines are from F. C. De Lucia, R. L. Cook, P. Helminger, and W. Gordy (1971), J. Chem. Phys. 55, 5334, and J. W. Fleming and M. J. Gibson, (1976), J. Mol. Spect. 62, 326. 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. De Lucia, P. Helminger, and W. H. Kirchhoff, (1974), J. Phys. and Chem. Ref. Data 3, 211.

Due to model problems and an incomplete least squares fitting program for this special case, no least squares fit was done for this molecule. Rather, the line frequencies were calculated in double precision using the set of rotational constants determined by De Lucia, et al. (1971, 1974) with a Hamiltonian that included up through tenth order distortion terms. The lower frequency lines that are computed from this Hamiltonian are in reasonable agreement with De Lucia, et al., but the higher frequency, higher J lines show deviations, possibly due to round off problems. The error estimates were set to a fixed 160 MHz for all the calculated lines, since our present program does not give the information necessary to evaluate the predicted errors.

Further work will be done on this problem. The present list is therefore an interim set of results.

Species Tag: 27001	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Hydrogen Cyanide HCN		Author: R. L. Poynter	
		Min. Int. = $10^{-4}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 424.154		J Max. = 34	Lines Listed = 45
Dipole Moments/Debye: $\mu_a$ = 2.984 $\mu_b$ = $\mu_c$			
Rot. Const./MHz: A = B = 44315.975 C =			

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

Species Tag: 27002	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Hydrogen Isocyanide HNC		Author: R. L. Poynter	
		Min. Int. = $10^{-3}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 138.223		J Max. = (34)	Lines Listed = 34
Dipole Moments/Debye: $\mu_a = 2.699$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A = B = 45332.00 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	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Carbon Monoxide  CO	Author: R. L. Poynter		
	Min. Int. = 10 <sup>-5</sup> nm <sup>2</sup> MHz		
Q (Spin-Rot., T = 300K) = 108.787	J Max. = (26)	Lines Listed = 26	
Dipole Moments/Debye: $\mu_a$ = 0.1098 $\mu_b$ = $\mu_c$ =			
Rot. Const./MHz: A =      B = 57635.97      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. Muentner, 1975, J. Mol. Spect. 55, 490.



Species Tag: 28002	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Hydrogen Cyanide Carbon - 13 isotope $\text{H } ^{13}\text{CN}$		Author: R. L. Poynter	
		Min. Int. = $10^{-4}$ $\text{nm}^2\text{MHz}$	
Q (Spin-Rot., T = 300K) = 435.385		J Max. = 34	Lines Listed = 45
Dipole Moments/Debye: $\mu_a = 2.984$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A = B = 43170.137 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	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Hydrogen Cyanide Nitrogen - 15 isotope $\text{hC } ^{15}\text{N}$		Author: R. L. Poynter	
		Min. Int. = $3 \times 10^{-3}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 435.204		J Max. = 35	Lines Listed = 35
Dipole Moments/Debye: $\mu_a = 2.984$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A =      B = 43027.69      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: 28004	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Hydrogen Cyanide Deuterium isotope DCN		Author: R. L. Poynter	
		Min. Int. = $7 \times 10^{-5}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 518.916		J Max. = 41	Lines Listed = 54
Dipole Moments/Debye: $\mu_a$ = 2.984 $\mu_b$ = $\mu_c$ =			
Rot. Const./MHz: A = B = 36207.46 C =			

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

Species Tag: 28005	Page 1 of 1	Version: 1	Date: Dec, 1979
Species Name: Hydrogen Isocyanide Carbon - 13 isotope HN <sup>13</sup> C		Author: R. L. Poynter	
		Min. Int. = $2 \times 10^{-3}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 143.880		J Max. = (35)	Lines Listed = 35
Dipole Moments/Debye: $\mu_a = 2.699$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A =      B = 43545.61      C =			

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

Species Tag: 28006	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Hydrogen Isocyanide Nitrogen - 15 isotope $\text{H } ^{15}\text{NC}$		Author: R. L. Poynter	
		Min. Int. = $2 \times 10^{-3}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 141.013		J Max. = (33)	Lines Listed = 33
Dipole Moments/Debye: $\mu_a = 2.699$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A = B = 44433.04 C =			

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

Species Tag: 28007	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Hydrogen Isocyanide Deuterium isotope DNC		Author: R. L. Poynter	
		Min. Int. = $10^{-3}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 164.169		J Max. = (39)	Lines Listed = 39
Dipole Moments/Debye: $\mu_a$ = 2.699 $\mu_b$ = $\mu_c$ =			
Rot. Const./ MHz: A =      B = 38152.995      C =			

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

Species Tag: 29001	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Carbon monoxide Carbon - 13 isotope $^{13}\text{CO}$		Author: R. L. Poynter	
		Min. Int. = $8 \times 10^{-6}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 113.776		J Max. = (27)	Lines Listed = 27
Dipole Moments/Debye: $\mu_a = 0.110$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A = B = 55101.02 C =			

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

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

Species Tag: 29002	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Formyl radical cation  HCO <sup>+</sup>	Author: R. L. Poynter		
	Min. Int. = 10 <sup>-3</sup> nm <sup>2</sup> MHz		
Q (Spin-Rot., T = 300K) = 140.504	J Max. = (33)	Lines Listed = 33	
Dipole Moments/Debye: $\mu_a$ = 3.30 $\mu_b$ = $\mu_c$ =			
Rot. Const./MHz: A = B = 44594.46 C =			

Only one line has been observed in the laboratory, by R. C. Woods, T. A. Dixon, R. J. Saykally, and P. G. Szanto, (1975), Phys. Rev. Lett. 35, 1269.

The dipole moment was estimated theoretically in the same paper.



Species Tag: 29003	Page 1 of 1	Version: 2	Date: Jan 1981
Species Name: Methyleneimine CH <sub>2</sub> NH		Author: R. Poynter	
		$10^{-8}$ Min. Int. = below 120 GHz nm <sup>2</sup> MHz $10^{-5}$ above 120 GHz	
Q (Spin-Rot., T = 300K) = 5892.86		J Max. = 33	Lines Listed = 2834
Dipole Moments/Debye: $\mu_a$ = 1.325 $\mu_b$ = 1.530 $\mu_c$ =			
Rot. Const./MHz: A = 196211.045      B = 34532.395      C = 29352.232			

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

Additional values of the partition function are:

<u>T</u>	<u>Q</u>
10	37.62
30	189.12
60	530.52
150	2086.92
200	3210.36

Species Tag: 30001	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Carbon Monoxide oxygen - 18 isotope $C^{18}O$		Author: R. L. Poynter	
		Min. Int. = $8 \times 10^{-6}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 114.2096		J Max. = (27)	Lines Listed = 27
Dipole Moments/Debye: $\mu_a = 0.110$ $\mu_b =$ $\mu_c = 28$			
Rot. Const./MHz: A = B = 54891.425 C =			

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

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

Species Tag: 30002	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Formyl radical cation carbon - 13 isotope $\text{H}^{13}\text{CO}^+$		Author: R. L. Poynter	
		Min. Int. = $3 \times 10^{-3}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 144.437		J Max. = (34)	Lines Listed = 34
Dipole Moments/Debye: $\mu_a = 3.30$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A =      B = 43377.36      C =			

Only one line has been observed in the laboratory, by R. C. Woods, R. J. Saykally, T. A. Dixon, P. G. Szanto, and T. Anderson, (1976) 31st Symposium on Molecular Spectroscopy, Columbus, Ohio.

Species Tag: 30003	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Formyl radical cation Deuterium isotope $\text{DCO}^+$		Author: R. L. Poynter	
		Min. Int. = $2 \times 10^{-3}$ $\text{cm}^2\text{MHz}$	
Q (Spin-Rot., T = 300K) = 173.872		J Max. = (42)	Lines Listed = 41
Dipole Moments/Debye: $\mu_a = 3.30$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A = B = 36019.76 C =			

Only one line has been observed in the laboratory, by R. C. Woods, R. J. Saykally, T. A. Dixon, P. G. Szanto, and T. Anderson, (1976) 31st Symposium on Molecular Spectroscopy, Columbus, Ohio.

Species Tag: 30004	Page 1 of 1	Version: 1	Date: Jan. 1980
Species Name: Formaldehyde $H_2CO$		Author: R. L. Poynter	
		Min. Int. = $10^{-20}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 2876.7		J Max. = 40	Lines Listed = 611
Dipole Moments/Debye: $\mu_a = 2.331$ $\mu_b = 0.$ $\mu_c = 0.$			
Rot. Const./MHz: A = 281925.97      B = 38836.582      C = 34001.6729			

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; 1973, 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, R. 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	Page 1 of 1	Version: 1	Date: Jan. 1980
Species Name: Methylenimine Carbon - 13 isotope $^{13}\text{CH}_2\text{NH}$		Author: R. L. Poynter	
		Min. Int. = $10^{-8}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 2012.45		J Max. = 10	Lines Listed = 439
Dipole Moments/Debye: $\mu_a = 1.325$ $\mu_b = 1.530$ $\mu_c = 0.$			
Rot. Const./MHz: A = 196195.217 B = 33747.872 C = 28707.047			

The computational method is the same as that used on the parent species,  $\text{CH}_2\text{NH}$ . 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	Page 1 of 1	Version: 1	Date: Jan. 1980
Species Name: Methylenimine		Author: R. L. Poynter	
Nitrogen - 15 isotope			
$\text{CH}_2 \text{ } ^{15}\text{NH}$		Min. Int. = $10^{-8}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 2015.792		J Max. = 10	Lines Listed = 440
Dipole Moments/Debye: $\mu_a$ = 1.325 $\mu_b$ = 1.530 $\mu_c$ = 0.			
Rot. Const./MHz: A = 195738.07      B = 33736.100      C = 28688.614			

The computational method is the same as that used on the parent species,  $\text{CH}_2\text{NH}$ . 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	Page 1 of 1	Version: 2	Date: Feb 1981
Species Name: Methylenimine Deuterium on nitrogen atom $\text{CH}_2\text{ND}$		Author: R. L. Poynter	
		Min. Int. = $10^{-8}$ below 120 GHz, $2 \times 10^{-5}$ above 120 GHz	
Q (Spin-Rot., T = 300K) = 2393.69		J Max. = 14	Lines Listed = 1834
Dipole Moments/Debye: $\mu_a = 1.325$ $\mu_b = 1.530$ $\mu_c =$			
Rot. Const./MHz: A = 157673.877      B = 32069.366      C = 26563.849			

The computational method is the same as that used for the parent species,  $\text{CH}_2\text{NH}$ . 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.

Additional values of the partition function are:

<u>T</u>	<u>Q</u>
10	15.21
30	76.71
60	215.37
150	847.55
200	1303.93



Species Tag: 30008	Page 1 of 1	Version: 1	Date: Feb. 1980
Species Name: Nitric Oxide ground $2\Pi$ states NO		Author: H. M. Pickett	
		Min. Int. = $10^{-20}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 1159.464		J Max. = 35.5	Lines Listed = 1909
Dipole Moments/Debye: $\mu_a = 0.15872$ $\mu_b = 0.$ $\mu_c = 0.$			
Rot. Const./MHz: A = B = 50849.06 C =			

The spectrum of NO was fit to the fine structure Hamiltonian described by C. Amiot, R. Bacis and G. Guelachvili, 1978, Can. J. Phys. 56, 251, along with the hyperfine Hamiltonian described by W. L. Meerts, 1976, Chem. Phys. 14, 421. The radio frequency lines are from W. L. Meerts and A. Dymanus, 1972, J. Mol. Spectroscopy. 44, 320. The millimeter lines were measured at JPL by H. M. Pickett and E. A. Cohen. The partition function was determined by a sum over states to  $J=71/2$ . Other values are:

<u>T</u>	<u>Q</u>
10	30.394
30	80.168
60	162.551
100	296.509
150	492.323

Species Tag: 31001	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Formyl radical cation Oxygen - 18 isotope $\text{HC } ^{18}\text{O}^+$		Author: R. L. Poynter	
		Min. Int. = $3 \times 10^{-3}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 145.427		J Max. = (34)	Lines Listed = 34
Dipole Moments/Debye: $\mu_a =$ $\mu_b = 3.30$ $\mu_c =$			
Rot. Const./MHz: A = B = 43081.217 C =			

Only one line has been observed in the laboratory, by R. C. Woods, R. J. Saykally, T. A. Dixon, P. G. Szanto, and T. Anderson, (1976) 31st Symposium on Molecular Spectroscopy, Columbus, Ohio.

Species Tag: 31002	Page 1 of 1	Version: 1	Date: Jan. 1980
Species Name: Formaldehyde Carbon - 13 isotope $H_2^{13}CO$		Author: R. L. Poynter Min. Int. = $5 \times 10^{-10}$ $nm^2 MHz$	
Q (Spin-Rot., T = 300K) = 2949.7		J Max. = 40	Lines Listed = 601
Dipole Moments/Debye: $\mu_a = 2.331$ $\mu_b = 0.$ $\mu_c = 0.$			
Rot. Const./MHz: A = 281930.85 B = 37811.92 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. 169, 429.

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

Species Tag: 32001	Page 1 of 1	Version: 2	Date: June 1980
Species Name: Molecular Oxygen $^{16}\text{O}_2$ $v = 0$ state of ground $^3\Sigma_g^-$ electronic state		Author: H. M. Pickett	
		Min. Int. = $10^{-32}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T - 300K) = 218.529		J Max. = 60	Lines Listed = 174
Dipole Moments/Debye: $\mu_a =$ $\mu_b =$ magnetic $\mu_c =$			
Rot. Const./MHz: A = B = 43099.795 C =			

The measurements and calculational method are from T. Amano and E. Hirota, 1974, J. Mol. Spectroscopy 53, 346. The Raman lines of  $\text{O}_2$  (M. Loete and H. Berger, 1977, J. Mol. Spectroscopy 63, 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.

The value of Q is determined by a sum over states to  $J = 60$ . Other values are:

<u>T</u>	<u>Q</u>
10	8.306
30	22.615
60	44.326
100	73.327
150	109.605

Species Tag: 32002	Page 1 of 1	Version: 2	Date: Oct. 1979
Species Name: Molecular Oxygen $^{16}\text{O}_2$ v = 1 state of the ground $^3\Sigma_g^-$ state		Author: H. M. Pickett	
		Min. Int. = $10^{-10}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 220.918		J Max. = (40)	Lines Listed = 63
Dipole Moments/Debye: $\mu_a$ = $\mu_b$ = magnetic $\mu_c$ =			
Rot. Const./MHz: A = B = 42626.9 C =			

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

The value of Q was determined by a sum over states to J = 60. Other values are:

<u>T</u>	<u>Q</u>
10	8.348
30	22.819
60	44.772
100	74.097
150	110.779

Species Tag: 32003	Page 1 of 1	Version: 2	Date: Nov. 1980
Species Name: Methyl Alcohol (Methanol)		Author: H. M. Pickett	
CH <sub>3</sub> OH lowest A, E <sub>1</sub> , and E <sub>2</sub> vibrational states		Min. Int. = 10 <sup>-10</sup> nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 6414.2516		J Max. = 12	Lines Listed = 709
Dipole Moments/Debye: $\mu_a$ = 0.885 $\mu_b$ = 1.440 $\mu_c$ = 0			
Rot. Const./MHz: A = 127,484.      B = 24,679.98      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 partition function is twice the value for a rigid rotor with the rotational constants given above. The quantum numbers for methanol are listed in the 840 format even though methanol is not a symmetric rotor. The y 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 <sub>1</sub>	no direct correspondence
4	E <sub>2</sub>	no direct correspondence

Species Tag: 32004	Page 1 of 1	Version: 1	Date: Feb. 1980
Species Name: Formaldehyde Oxygen - 18 isotope $\text{H}_2\text{C}^{18}\text{O}$		Author: R. L. Poynter	
		Min. Int. = $10^{-9}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 3017.226		J Max. = 20	Lines Listed = 449
Dipole Moments/Debye: $\mu_a = 2.331$ $\mu_b = 0.$ $\mu_c = 0.$			
Rot. Const./MHz: A = 281993.0      B = 36903.573      C = 32514.740			

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. K. 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.  
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 species.

Species Tag: 34001	Page 1 of 1	Version: 2	Date: Oct. 1980
Species Name: $18_0 16_0$ Molecular Oxygen - $O^{18}$ species ground state		Author: H. M. Pickett	
		Min. Int. = $2.5 \times 10^{-11}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 462.32		J Max. = (42)	Lines Listed = 132
Dipole Moments/Debye: $\mu_a =$ $\mu_b =$ magnetic $\mu_c =$			
Rot. Const./MHz: A = B = 40708. C =			

The measurements and calculational method are from T. Amano and E. Hirota, 1974, J. Mol. Spectroscopy 53, 346. Intensities of magnetic dipole transitions have been calculated using the g values obtained from magnetic resonance by K. D. Bowers, R. A. Kamper and C. D. Lustig, 1959, Proc. Roy. Soc. (Lond.) A251, 565. The zero-frequency absorption is included but the frequency is set to a synthetic frequency of  $|g|J$  for the given level.

The value of Q is determined by a sum over states to J = 60. Other values are:

<u>T</u>	<u>Q</u>
10K	17.13
30	47.46
60	93.44
100	154.85
150	231.67



Species Tag: 34002	Page 1 of 1	Version: 2	Date: July 1980
Species Name: Hydrogen Sulfide  $H_2S$		Author: R.L. Poynter & H.M. Pickett	
		Min. Int. = $10^{-8}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T - 300K) = 514.197		J Max. = 15	Lines Listed = 311
Dipole Moments/Debye: $\mu_a = 0.$ $\mu_b = 0.974$ $\mu_c = 0.$			
Rot. Const./MHz: A = 310182.24      B = 270884.05      C = 141705.880			

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. De Lucia, 1972, J. Chem. Phys. 56, 4581.  
P. Helminger, F. C. De Lucia, and W. H. Kirchhoff, 1973, J. Phys. Chem. Ref. Data, 2, 213.

The dipole moment was reported by C. Huiszoon and A. Dymanus, 1965, Physica, 31, 1049.

The partition function was calculated by a sum over states to J = 15. Other values are:

<u>T</u>	<u>Q</u>
150	182.783
100	100.157
60	47.239
30	17.296
10	3.234

Species Tag: 34003	Page 1 of 1	Version: 2	Date: Feb. 1981
Species Name: Phosphine $\text{PH}_3$		Author: R. L. Poynter	
		Min. Int. = $10^{-17}$ $\text{nm}^2\text{MHz}$	
Q (Spin-Rot., T = 300K) = 608.55		J Max. = (19)	Lines Listed = 142
Dipole Moments/Debye: $\mu_a = 7.2 \times 10^{-5}$ $\mu_b =$ $\mu_c = 0.574$			
Rot. Const./MHz: A = <sup>*centrifugally induced</sup> B = 133480.22 C = 117488.39			

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, J. Quant. Spectrosc. and Radiat. Transfer, in press, 1981.

The dipole moment measured by P. B. Davies, et al., above, is  $0.57395 \pm 0.0003\text{D}$ .

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.

Other values of the partition function are:

<u>T</u>	<u>Q</u>
10	4.29
30	20.16
60	55.56
150	216.24
200	332.10

Species Tag: 34004	Page 1 of 1	Version: 2	Date: Oct 1980
Species Name: Hydrogen Peroxide ground torsional states H <sub>2</sub> O <sub>2</sub>		Author: H. M. Pickett	
		Min. Int. = 10 <sup>-8</sup> nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 7651.8		J Max. = 24	Lines Listed = 883
Dipole Moments/Debye: $\mu_a$ = $\mu_b$ = $\mu_c$ = 1.5728			
Rot. Const./MHz: A = 301878. B = 26211.9 C = 25099.14			

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

Species Tag: 35001	Page 1 of 1	Version: 1	Date: 1980
Species Name: Hydrogen Sulfide Deuterium Isotope  HDS	Author: R. L. Poynter		
	Min. Int. = $4 \times 10^{-12}$ nm <sup>2</sup> /MHz		
Q (Spin-Rot., T - 300K) = 430.900	J Max. = 20	Lines Listed = 1138	
Dipole Moments/Debye: $\mu_a = 0.470$ $\mu_b = 0.974$ $\mu_c = 0.$			
Rot. Const./MHz: A = 292351.302      B = 147861.801      C = 96704.120			

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 40, 125. G. Steenbeckliars, 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	Page 1 of 1	Version: 1	Date: Feb. 1980
Species Name: Hydrogen Chloride H <sup>35</sup> Cl		Author: R. L. Foynter & H. M. Pickett	
		Min. Int. = $5 \times 10^{-2}$ cm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 81.232		J Max. = 4	Lines Listed = 17
Dipole Moments/Debye: $\mu_a = 1.109$ $\mu_b = 0$ $\mu_c = 0$			
Rot. Const./MHz: A =                      B = 312989.3      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: 38001	Page 1 of 1	Version: 1	Date: Feb. 1980
Species Name: Hydrogen Chloride  Chlorine - 37 isotope $\text{H}^{37}\text{Cl}$		Author: R. L. Poynter & H. L. Pickett	
		Min. Int. = $5 \times 10^{-2}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 81.352		J Max. = 4	Lines Listed = 17
Dipole Moments/Debye: $\mu_a = 1.109$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A = B = 312519.12 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	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Propyne  CH <sub>3</sub> CCH		Author: R. L. Poynter	
		Min. Int. = $3 \times 10^{-5}$ nm <sup>2</sup> MHz for J > 14	
Q (Spin-Rot., T = 300K) = 5428.80		J Max. = 80	Lines Listed = 813
Dipole Moments/Debye: $\mu_a = 0.750$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A = 158590.      B = 8545.860      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. Muentner and V. W. Laurie, 1966, J. Chem. Phys. 45, 855.

Species Tag: 41001	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Acetonitrile  CH <sub>3</sub> CN  ground state		Author: R. L. Poynter  Min. Int. = $3 \times 10^{-5}$ nm <sup>2</sup> MHz for J > 14	
Q (Spin-Rot., T = 300K) = 15145.		J Max. = 82	Lines Listed = 1441
Dipole Moments/Debye: $\mu_a$ = 3.919 $\mu_b$ = $\mu_c$ =			
Rot. Const./MHz: A = 158290.      B = 9198.8993      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. Kukoiich, 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	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Propyne, Carbon - 13 isotope on atom 1 $\text{CH}_3 \text{C}^{13}\text{CH}$		Author: R. L. Poynter Min. Int. = $3 \times 10^{-5}$ nm <sup>2</sup> MHz for J > 14	
Q (Spin-Rot., T = 300K) = 5596.11		J. Max. = 80	Lines Listed = 822
Dipole Moments/Debye: $\mu_a = 0.750$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A = 158590. B = 8290.259 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: 41003	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Propyne, Carbon - 13 isotope on atom 2 $\text{CH}_3^{13}\text{CCH}$		Author: R. L. Poynter	
		Min. Int. = $3 \times 10^{-5}$ nm <sup>2</sup> MHz for J > 14	
Q (Spin-Rot., T = 300K) = 5431.06		J Max. = 79	Lines Listed = 813
Dipole Moments/Debye: $\mu_a = 0.750$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A = 158590. B = 8542.304 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	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Propyne, carbon - 13 isotope on atom 3 $H_3^{13}CCCH$		Author: R. L. Poynter	
		Min. Int. = $3 \times 10^{-5}$ nm <sup>2</sup> MHz for J > 14	
Q (Spin-Rot., T = 300K) = 5580.65		J Max. = 80	Lines Listed = 821
Dipole Moments/Debye: $\mu_a = 0.750$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A = 158590.      B = 81313.24      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	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Propyne, Deuterium isotope on carbon atom 1 CH <sub>3</sub> CCD		Author: R. L. Poynter	
		Min. Int. = $3 \times 10^{-5}$ nm <sup>2</sup> MHz for J > 14	
Q (Spin-Rot., T = 300K) = 5956.732		J Max. = 82	Lines Listed = 800
Dipole Moments/Debye: $\mu_a$ = 0.750 $\mu_b$ = $\mu_c$ =			
Rot. Const./MHz: A = 158590.0 B = 7788.158 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.

The dipole moment was assumed to be the same as the parent species for this calculation. An experimental value, 0.770D (avg.) corrected for the new OCS standard, has been reported by Muentner and Laurie (above). This result came to our attention too late to include in this version.

Species Tag: 41006	Page 1 of 1	Version: 1	Date: Jan. 1980
Species Name: Propyne Deuterium isotope on methyl carbon atom $\text{CH}_2\text{D CCH}$		Author: R. L. Poynter	
		Min. Int. = $2 \times 10^{-10}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 9982.44		J Max. = 15	Lines Listed = 223
Dipole Moments/Debye: $\mu_a = 0.750$ $\mu_b = 0.$ $\mu_c = 0.$			
Rot. Const./MHz: A = 117744.370      B = 8155.784      C = 8025.577			

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

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

Species Tag: 42001	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Acetonitrile Nitrogen - 15 isotope $\text{CH}_3 \text{C}^{15}\text{N}$		Author: R. L. Poynter	
		Min. Int. = $2 \times 10^{-5}$ nm <sup>2</sup> MHz for J > 14	
Q (Spin-Rot., T = 300K) = 15145		J Max. = 90	Lines Listed = 2755
Dipole Moments/Debye: $\mu_a = 3.919$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A = 158290. B = 9198.8993 C = B			

The experimental measurements were obtained from A. Bauer and S. Maes, 1969, J. de Phys. 30, 169; J. Demaison, A. Dubrulle, D. Boucher, J. Burie, 1969, J. Mol. Spect. 76, 1.

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

Species Tag: 42002	Page 1 of 1	Version: 1	Date: Jan. 1980
Species Name: Ketene $H_2CCO$		Author: R. L. Poynter	
		Min. Int. = $3 \times 10^{-15}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 10322.9		J Max. = 29	Lines Listed = 835
Dipole Moments/Debye: $\mu_a = 1.422$ $\mu_b = 0$ $\mu_c = 0$			
Rot. Const./MHz: A = 282473      B = 10293.80      C = 9916.38			

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

- B. Fabricant, D. Krieger, and J. S. Muentzer, 1977, J. Chem. Phys. 67, 1576.  
J. W. C. Johns, J. M. R. Stone, and G. Winnewisser, 1972, J. Mol. Spect. 42, 523.  
H. R. Johnson and M. W. P. Strandberg, 1952, J. Chem. Phys. 20, 687.

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

Species Tag: 43001	Page 1 of 1	Version: 1	Date: Jan. 1980
Species Name: Ketene		Author: R. L. Poynter	
Deuterium isotope HDCCO		Min. Int. = $10^{-23}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 6682.68		J Max. = 29	Lines Listed = 886
Dipole Moments/Debye: $\mu_a = 1.422$ $\mu_b = 0.$ $\mu_c = 0.$			
Rot. Const./MHz: A = 194313.0      B = 9647.396      C = 9174.975			

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

L. Nemes and M. Winnewisser, 1976, Z. Naturforsch. 31a, 272.

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



Species Tag: 44001	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Carbon Monosulfide ground state CS	Author: R. L. Poynter		
	Min. Int. = $4 \times 10^{-5}$ nm <sup>2</sup> MHz		
Q (Spin-Rot., T = 300K) = 255.515	J Max. = (60)	Lines Listed = 60	
Dipole Moments/Debye: $\mu_a$ = 1.957 $\mu_b$ = $\mu_c$ =			
Rot. Const./MHz: A = B = 24495.554 C =			

The experimental data were taken from the following papers:

R. Kewley, K. V. L. N. Sastry, M. Winnewisser, and W. Gordy, 1962, J. Chem. Phys. 39, 2856.

R. C. Mockler and G. R. Bird, 1955, Phys. Rev. 98, 1837.

The dipole moment is from G. Winnewisser and R. L. Cook, 1968, J. Mol. Spect. 28, 266.

Species Tag: 44002	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Silicon Monoxide $^{28}\text{Si O}$		Author: R. L. Poynter	
		Min. Int. = $3 \times 10^{-5}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 287.232		J Max. = 66	Lines Listed = 66
Dipole Moments/Debye: $\mu_a = 3.098$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A = B = 21787.46 C =			

The experimental data were taken from the following papers:

E. Tiemann, 1974, J. Phys. Chem. Ref. Data, T. Törring, 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.

A more recent set of measurements, discovered too late to include in this edition, has been given by E. L. Manson, W. W. Clark, F. C. De Lucia, and W. Gordy, 1977, Phys. Rev. A15, 223. The catalogue predictions are within three standard deviations of their measurements.

Species Tag: 44003	Page 1 of 1	Version: 1	Date: Jan. 1980
Species Name: Acetaldehyde ground vibrational A state  CH <sub>3</sub> CHO		Author: R. L. Poynter  Min. Int. = $6 \times 10^{-9}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 12112.28		J Max. = 20	Lines Listed = 1347
Dipole Moments/Debye: $\mu_a$ = 2.550 $\mu_b$ = 0.870 $\mu_c$ = 0.			
Rot. Const./MHz: A = 56609.474    B = 10162.766    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	Page 1 of 1	Version: 1	Date: Jan. 1980
Species Name: Nitrous Oxide $N_2O$		Author: R. L. Poynter & H. M. Pickett	
		Min. Int. = $2 \times 10^{-7}$ cm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) =		J Max. = 61	Lines Listed = 61
Dipole Moments/Debye: $\mu_a$ = .1608 $\mu_b$ = $\mu_c$ =			
Rot. Const./MHz: A =      B = 12561.637      C =			

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

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

Species Tag: 44005	Page 1 of 1	Version: 1	Date: Dec. 1980
Species Name: Acetaldehyde E state  CH <sub>3</sub> CHO	Author: H. M. Pickett		
	Min. Int. = 10 <sup>-10</sup> nm <sup>2</sup> MHz		
Q (Spin-Rot., T - 300K) = 12112.3	J Max. = 15	Lines Listed = 691	
Dipole Moments/Debye: μ <sub>a</sub> = 2.55      μ <sub>b</sub> = 0.870      μ <sub>c</sub> = 0			
Rot. Const./MHz: A = 56448.5	B = 10160.1	C = 9101.3	

The experimental lines of the lowest torsional state of E symmetry are listed in A. Bander, 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  $P_a$ ,  $P_a^2$ ,  $P_a^4$ ,  $P_a^3$ ,  $P_a^3P^2$ , and  $P_a^5$  terms. The fit produced observed - calculated frequencies which were 3.5 times the experimental uncertainties in an rms sense. Calculated values of  $\mu^2$  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	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Carbon Monosulfide  Carbon - 13 isotope $^{13}\text{CS}$		Author: R. L. Poynter	
		Min. Int. = $3 \times 10^{-5}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 270.652		J Max. = (62)	Lines Listed = 62
Dipole Moments/Debye: $\mu_a = 1.957$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A = B = 23123.807 C =			

The experimental measurement was reported by R. C. Mockler and G. R. Bird, 1955, Phys. Rev. 98, 1837.

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

Species Tag: 45002	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Silicon Monoxide silicon - 29 isotope $^{29}\text{Si O}$		Author: R. L. Poynter	
		Min. Int. = $4 \times 10^{-5}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 290.878		J Max. = 66	Lines Listed = 66
Dipole Moment /Debye: $\mu_a = 3.098$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A = B = 21514.07 C =			

The experimental data were taken from the following papers:

E. Tiemann, 1974, J. Phys. Chem. Ref. Data, T. Törring, 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.

A more recent set of measurements, discovered too late to include in this edition, has been given by E. L. Manson, W. W. Clark, F. C. De Lucia, and W. Gordy, 1977, Phys. Rev. A15, 223. The catalogue predictions are within three standard deviations of their measurements.

Species Tag: 45003	Page 1 of 1	Version: 2	Date: Jan. 1981
Species Name: Formamide, NH <sub>2</sub> CHO		Author: R. Poynter	
		Min. Int. = $10^{-8}$ below 120 GHz $\text{cm}^2\text{MHz}$ $10^{-5}$ above 120 GHz	
Q (Spin-Rot., T = 300K) = 29155.55		J Max. = 30	Lines Listed = 3476
Dipole Moments/Debye: $\mu_a = 316.6$ $\mu_b = 0.852$ $\mu_c =$			
Rot. Const./MHz: A = 72716.945      B = 11373.453      C = 9833.903			

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

- C. C. Costair 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.

Additional values of the partition function are:

<u>T</u>	<u>Q</u>
10	180.24
30	926.52
60	2613.45
150	10313.73
200	15874.68



Species Tag: 46001	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Carbon Monosulfide  Sulfur - 34 isotope  C <sup>34</sup> S		Author: R. L. Poynter	
		Min. Int. = $3 \times 10^{-5}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 259.665		J Max. = (61)	Lines Listed = 61
Dipole Moments/Debye: $\mu_a$ = 1.957 $\mu_b$ = $\mu_c$ =			
Rot. Const./MHz: A = B = 24103.550 C =			

The experimental measurement was reported by R. C. Mockler and G. R. Bird, 1955, Phys. Rev. 98, 1837.

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

Species Tag: 46002	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Silicon Monoxide Silicon - 30 isotope $^{30}\text{Si O}$		Author: R. L. Poynter	
		Min. Int. = $3 \times 10^{-5}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 294.358		J Max. = 67	Lines Listed = 67
Dipole Moments/Debye: $\mu_a = 3.098$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A =      B = 21259.48      C =			

The experimental data were taken from the following papers:

E. Tiemann, 1974, J. Phys. Chem. Ref. Data, T. Törring, 1968, Z. Naturforsch. 23a, 777.

The dipole moment was reported by J. W. Raymonda, J. S. Muentner, and W. A. Klemperer, 1970, J. Chem. Ref. Data, T. Törring, 1968, Z. Naturforsch.

A more recent set of measurements, discovered too late to include in this edition, has been given by E. L. Manson, W. W. Clark, F. C. De Lucia, and W. Gordy, 1977, Phys. Rev. A15, 223. The catalogue predictions are within three standard deviations of their measurements.

Species Tag: 46003	Page 1 of 1	Version: 1	Date: Jan. 1980
Species Name: Thioformaldehyde $H_2CS$		Author: R. L. Poynter	
		Min. Int. = $8 \times 10^{-10}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 5984.646		J Max. = 27	Lines Listed = 517
Dipole Moments/Debye: $\mu_a = 1.649$ $\mu_b = 0.$ $\mu_c = 0.$			
Rot. Const./MHz: A = 291291.641      B = 17699.628      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 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 taken from B. Fabricant, D. Krieger, and J. S. Muentert, 1977, J. Chem. Phys. 67, 1576.

Species Tag: 46004	Page 1 of 1	Version: 1	Date: Jan 1980
Species Name: Ethyl Alcohol ground trans state $C_2H_5OH$		Author: R. L. Poynter	
		Min. Int. = $3 \times 10^{-10}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 17010.5		J Max. = 20	Lines Listed = 1236
Dipole Moments/Debye: $\mu_a$ = 0.046 $\mu_b$ = 1.438 $\mu_c$ = 0.			
Rot. Const./MHz: A = 34891.75      B = 9350.635      C = 8135.236			

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

M. 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	Page 1 of 1	Version: 1	Date: Jan, 1980
Species Name: Formic Acid  ground trans state  HCOOH		Author: R. L. Poynter	
		Min. Int. = $6 \times 10^{-10}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 8884.2		J Max. = 20	Lines Listed = 1888
Dipole Moments/Debye: $\mu_a$ = 1.396 $\mu_b$ = 0.260 $\mu_c$ = 0.			
Rot. Const./MHz: A = 77512.25      B = 12055.11      C = 10416.12			

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

J. Bellet, C. Samson, G. Steenbeckeliers, and R. Wertheimer, 1971, J. Mol. Structure 9, 49.

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

R. Trambarulo, A. Clark, and C. Hearn, 1958, J. Chem. Phys. 28, 736.

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

Species Tag: 47001	Page 1 of 1	Version: 1	Date: Jan. 1980
Species Name: Thioformaldehyde		Author: R. L. Poynter	
Carbon - 13 isotope $\text{H}_2^{13}\text{CS}$		Min. Int. = $2 \times 10^{-9}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 6219.87		J Max. = 10	Lines Listed = 110
Dipole Moments/Debye: $\mu_a = 1.649$ $\mu_b = 0.$ $\mu_c = 0.$			
Rot. Const./MHz: A = 291660.0      B = 16998.342      C = 16030.791			

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 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	Page 1 of 1	Version: 1	Date: Jan. 1980
Species Name: Formic Acid trans state Carbon - 13 isotope H <sup>13</sup> COOH		Author: R. L. Poynter	
		Min. Int. = 10 <sup>-10</sup> nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 8896.76		J Max. = 20	Lines Listed = 1194
Dipole Moments/Debye: $\mu_a$ = 1.396 $\mu_b$ = 0.260 $\mu_c$ = 0.			
Rot. Const./MHz: A = 77580.494    B = 12053.567    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	Page 1 of 1	Version: 1	Date: Jan. 1980
Species Name: Formic Acid Deuterium isotope on C-atom DCOOH		Author: R. L. Poynter	
		Min. Int. = $2 \times 10^{-9}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 10531.19		J Max. = 20	Lines Listed = 628
Dipole Moments/Debye: $\mu_a$ = 1.396 $\mu_b$ = 0.260 $\mu_c$ = 0.			
Rot. Const./MHz: A = 57709.33      B = 12055.971      C = 9955.609			

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

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

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

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



Species Tag: 47004	Page 1 of 1	Version: 1	Date: Jan. 1980
Species Name: Formic Acid Deuterium isotope on O-atom HCOOD		Author: R. L. Poynter	
		Min. Int. = $10^{-9}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 9954.87		J Max. = 20	Lines Listed = 612
Dipole Moments/Debye: $\mu_a$ = 1.396 $\mu_b$ = 0.260 $\mu_c$ = 1.			
Rot. Const./MHz: A = 66100.14 B = 11762.577 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 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: 48001	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Sulfur monoxide SO <sup>3</sup> Σ ground state		Author: H. M. Pickett	
		Min. Int. = 10 <sup>-6</sup> nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 850.099		J Max. = 50	Lines Listed = 330
Dipole Moments/Debye: μ <sub>a</sub> = 1.55      μ <sub>b</sub> =      μ <sub>c</sub> =			
Rot. Const./MHz: A =      B = 21523.02      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.

The partition function was obtained by a sum over states to J=50. Other values are

<u>T</u>	<u>Q</u>
10K	17.284
30	69.382
60	154.400
100	269.677
150	414.502

Species Tag: 48002	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Sulfur Monoxide $v = 1$ vibrationally excited state of the ground $^3\Sigma$ electronic state		Author: H. M. Pickett	
		Min. Int. = $4 \times 10^{-6}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 856.726		J Max. = 50	Lines Listed = 261
Dipole Moments/Debye: $\mu_a = 1.55$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A =      B = 21351.0      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  $1111.5 \text{ cm}^{-1}$  above  $v=0$  (G. Herzberg, 1950, Spectra of Diatomic Molecules, Van Nostrand, New York). The partition function is determined by a sum over states to  $J = 50$ . Other values are:

<u>T</u>	<u>Q</u>
10K	17.341
30	69.781
60	155.452
100	271.644
150	417.628

C-2

Species Tag: 48003	Page 1 of 1	Version: 1	Date: Jan. 1980
Species Name: Thioformaldehyde  Sulfur - 34 isotope $\text{H}_2\text{C}^{34}\text{S}$		Author: R. L. Poynter	
		Min. Int. = $3 \times 10^{-9}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 6084.57		J Max. = 10	Lines Listed = 111
Dipole Moments/Debye: $\mu_a = 1.647$ $\mu_b = 0.$ $\mu_c = 0.$			
Rot. Const./MHz: A = 291660.    B = 17387.949    C = 16376.922			

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333. The measurements were taken from 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: 48004	Page 1 of 1	Version: 1	Date: Jan. 1980
Species Name: Ozone ground state  $^{16}\text{O}_3$	Author: R. L. Poynter and H. M. Pickett		
	Min. Int. = $3 \times 10^{-10}$ nm <sup>2</sup> MHz		
Q (Spin-Rot., T = 300K) = 3378.28	J Max. = 40	Lines Listed = 1465	
Dipole Moments/Debye: $\mu_a = 0.$ $\mu_b = 0.5324$ $\mu_c = 0.$			
Rot. Const./MHz: A = 106535.234 B = 13349.0901 C = 11834.5235			

The catalog of the ozone lines is based on the work of M.J.C. Depannemaecker, B. Dutelage, 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.

Species Tag: 48005	Page 1 of 1	Version: 1	Date: Jan. 1981
Species Name: Ozone, $\nu_2$ vib. state  $^{16}\text{O}_3$ , (010) state		Author: R. Poynter	
		Min. Int. = $10^{-8}$ below 120 GHz $\text{nm}^2\text{MHz}$ $10^{-5}$ above 120 GHz	
Q (Spin-Rot., T = 300K) = 3367.8162		J Max. = 30	Lines Listed = 734
Dipole Moments/Debye: $\mu_a$ = $\mu_b$ = 0.5324 $\mu_c$ =			
Rot. Const./MHz: A = 108137.979 B = 13311.143 C = 11765.222			

The  $\nu_2$  ozone lines were derived from a fit of the data given by M. J. C. Depannemaecker, B. Duterage, and M. J. Bellet, 1977, J. Quant. Spect. and Radiat. Transfer 17, 519. Additional lines are listed in F. J. Lovas, 1978, J. Phys. Chem. Ref. Data., 7, 1445.

Additional values of the partition function are:

<u>T</u>	<u>Q</u>
10	20.88
30	107.12
60	302.01
150	1191.47
200	1833.80

The energy origin of this vibrational species is  $701 \text{ cm}^{-1}$  above the ground state energy origin.



Species Tag: 50001	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Sulfur Monoxide Sulfur 34 isotope $^3\Sigma$ ground state $^{34}\text{SO}$		Author: H. M. Pickett	
		Min. Int. = $10^{-6}$ cm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 866.870		J Max. = 50	Lines Listed = 280
Dipole Moments/Debye: $\mu_a = 1.55$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A =      B = 21102.72      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.

The partition function was determined by a sum over states. Other values are:

<u>T</u>	<u>Q</u>
10K	17.554
30	70.654
60	157.354
100	274.922
150	422.629



Species Tag: 50002	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Sulfur Monoxide Oxygen 18 isotope		Author: H. M. Pickett	
		Min. Int. = $10^{-5}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 917.393		J Max. = 50	Lines Listed = 179
Dipole Moments/Debye: $\mu_a$ = 1.55 $\mu_b$ = $\mu_c$ =			
Rot. Const./MHz: A =      B = 19929.      C =			

The calculational method is described in T. Amano and E. Hirota, 1974, J. Molec. Spectroscopy 53, 346. The value of  $\mu$  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.

The partition function was determined by a sum over states. Other values are:

<u>T</u>	<u>Q</u>
10K	18.370
30	74.493
60	166.257
100	290.728
150	447.118

Species Tag: 50003	Page 1 of 1	Version: 1	Date: Feb. 1980
Species Name: Symmetric $^{18}\text{O}$ Ozone ground state $^{16}\text{O}-^{18}\text{O}-^{16}\text{O}$		Author: H. M. Pickett & R. L. Poynter	
		Min. Int. = $10^{-9}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 3525.63		J Max. = 40	Lines Listed = 1568
Dipole Moments/Debye: $\mu_a = 0.$ $\mu_b = 0.5324$ $\mu_c = 0.$			
Rot. Const./MHz: A = 98646.687      B = 13352.732      C = 11731.767			

The catalog of symmetric  $^{18}\text{O}$  ozone is based on the work of J. Depannemaecker and J. Bellet (1977, J. Molo Specty. 66, 106). The dipole moment used is the  $^{16}\text{O}_3$  value.

Species Tag: 50004	Page 1 of 1	Version: 1	Date: Feb. 1980
Species Name: Asymmetric $^{18}\text{O}$  Ozone $^{18}\text{O}-^{16}\text{O}-^{16}\text{O}$		Author: H. M. Pickett & R. L. Poynter	
		Min. Int. = $10^{-9}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 7213.74		J Max. = 40	Lines Listed = 4036
Dipole Moments/Debye: $\mu_a = 0.0068$ $\mu_b = 0.5324$ $\mu_c = 0.$			
Rot. Const./MHz: A = 104573.161      B = 12591.533      C = 11212.5057			

The catalog of asymmetric  $^{18}\text{O}$  ozone is based on the work of J. Depannemaecker and J. Bellet (1977, J. Mol. Spectry. 66, 106). The dipole moment used is the  $^{16}\text{O}_3$  value rotated to the inertial axes of asymmetric  $^{18}\text{O}$  ozone (based on the equilibrium structure).

Species Tag: 51001	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Cyanoacetylene HCCCN		Author: R. L. Poynter	
		Min. Int. = $2 \times 10^{-7}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 4123.26		J Max. = 99	Lines Listed = 154
Dipole Moments/Debye: $\mu_a$ = 3.599 $\mu_b$ = $\mu_c$ =			
Rot. Const./MHz: A =      B = 4549.059      C =			

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

The dipole moment was remeasured by the above authors as 3.72<sup>d</sup>D. An old value, 3.599D, was used in the present calculations, so the intensities should be multiplied by a factor of 1.071.

Species Tag: 51002	Page 1 of 1	Version: 2	Date: Oct. 1980
Species Name: Chlorine Monoxide		Author: H. M. Pickett	
$2\pi$ states $^{35}\text{ClO}$ $v = 0$		Min. Int. = $10^{-10}$ $\text{cm}^2\text{MHz}$	
Q (Spin-Rot., T = 300K) = 3291.80		J Max. = 87.5	Lines Listed = 2610
Dipole Moments/Debye: $\mu_a = 1.239$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A = B = 18602.86 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,  $\eta_1$ ,  $\eta_2$ , and  $\eta_3$ . The partition function was determined by a sum over states to F = 86 for both the  $\Omega = 1/2$  and  $\Omega = 3/2$  states. Other values are:

<u>T</u>	<u>Q</u>
150	1424.28
100	921.36
60	553.46
30	284.09
10	105.25

Species Tag: 52001	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Cyanoacetylene carbon - 13 isotope on atom 1 $\text{H}^{13}\text{CCN}$		Author: R. L. Poynter	
		Min. Int. = $2 \times 10^{-7}$ $\text{cm}^2/\text{MHz}$	
Q (Spin-Rot., T = 300K) = 4140.42		J Max. = 99	Lines Listed = 152
Dipole Moments/Debye: $\mu_a = 3.599$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A =      B = 4530.198      C =			

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

The dipole moment was remeasured by the above authors as 3.724D. An old value, 3.599D, was used in the present calculations, so the intensities should be multiplied by a factor of 1.071.

Species Tag: 52002	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Cyanoacetylene Carbon - 13 isotope on atom 2 HC <sup>13</sup> CCN		Author: R. L. Poynter	
		Min. Int. ~ 2 x 10 <sup>-7</sup> nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 4140.82		J Max. = 99	Lines Listed = 146
Dipole Moments/Debye: $\mu_a$ = 3.599 $\mu_b$ = $\mu_c$ =			
Rot. Const./ MHz: A =      B = 4529.76      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. An old value, 3.599D, was used in the present calculations, so the intensities should be multiplied by a factor of 1.071.

Species Tag: 52003	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Cyanoacetylene Carbon - 13 isotope on atom 3 H <sup>13</sup> CCCN		Author: R. L. Poynter	
		Min. Int. = $2 \times 10^{-7}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 4254.5		J Max. = 99	Lines Listed = 144
Dipole Moments/Debye: $\mu_a$ = 3.599 $\mu_b$ = $\mu_c$ =			
Rot. Const./MHz: A = B = 4408.44 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. An old value, 3.599D, was used in the present calculations, so the intensities should be multiplied by a factor of 1.071.



Species Tag: 52004	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Cyanoacetylene  Nitrogen - 15 isotope, HCCC <sup>15</sup> N		Author: R. L. Poynter	
		Min. Int. = $4 \times 10^{-6}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 1415.581		J Max. = 99	Lines listed = 99
Dipole Moments/Debye: $\mu_a$ = 3.599 $\mu_b$ = $\mu_c$ =			
Rot. Const./MHz: A = B = 4416.75 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. An old value, 3.599D, was used in the present calculations, so the intensities should be multiplied by a factor of 1.071.

Species Tag: 52005	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Cyanoacetylene Deuterium Isotope DCCCN		Author: R. L. Poynter	
		Min. Int. = $10^{-7}$ cm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 4443.03		J Max. = 99	Lines Listed = 156
Dipole Moments/Debye: $\mu_a = 3.724$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A =      B = 4221.58      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	Page 1 of 1	Version: 1	Date: Jan. 1981
Species Name: Hypochlorous acid, HO <sup>35</sup> Cl		Author: R. Poynter	
		Min. Int. = $1.0 \times 10^{-8}$ below 120 GHz, $\text{nm}^2 \text{MHz}$ $10^{-5} \text{nm}^2 \text{MHz}$ above this frequency	
Q (Spin-Rot., T = 300K) = 9481.708		J Max. = 20	Lines Listed = 671
Dipole Moments/Debye: $\mu_a = 1.3$ $\mu_b = 0.367$ $\mu_c =$			
Rot. Const./MHz: A = 613481.8      B = 15118.415      C = 14724.188			

Because experimental data reported by M. Suzuki and A. Guarnieri, 1975, Z. Naturforsch. 30a, 497, and A. Mirri, F. Scappini, and G. Cazzoli, 1971, J. Mol. Spect. 38, 218, were not adequate to determine the A constant the spectral lines of this molecule were computed from ground state constants and covariance reported in the IR study of J. S. Wells, R. L. Sams, and W. J. Lafferty, 1979, J. Mol. Spect. 77, 349. The dipole moment was reported by D. G. Lister and D. J. Millen, 1971, Trans. Far. Soc. 67, 601. The quadrupole coupling constants were from Mirri, et.al. Quadrupole splittings were only calculated through J = 5, to reduce the total number of lines generated.

Other values of the partition function are:

<u>T</u>	<u>Q</u>
10	59.08
30	302.20
60	851.44
150	3357.56
200	5167.28

Species Tag: 53001	Page 1 of 1	Version: 1	Date: Jan, 1980
Species Name: Acrylonitrile $C_2 H_3 CN$		Author: R. L. Poynter	
		Min. Int. = $10^{-9}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 26198.1		J Max. = 40	Lines Listed = 3697
Dipole Moments/Debye: $\mu_a = 3.68$ $\mu_b = 1.25$ $\mu_c = 0.$			
Rot. Const./MHz: A = 49850.712      B = 4971.0849      C = 4513.8005			

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

- C. C. Costain and B. P. Stoicheff, 1959, J. Chem. Phys. 30, 777.  
M. C. L. Gerry and G. Winnewisser, 1973, J. Mol. Spect. 48, 1.  
M. C. L. Gerry, K. Yamada, and G. Winnewisser, 1979, J. Phys. Chem. Ref. Data 8, 107.

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

Species Tag: 53002	Page 1 of 1	Version: 2	Date: Oct. 1980
Species Name: Chlorine Monoxide		Author: H. M. Pickett	
$^2\Pi$ states Chlorine - 37 isotope $^{37}\text{ClO}$ $v = 0$		Min. Int. = $10^{-10}$ $\text{nm}^2\text{MHz}$	
Q (Spin-Rot., T = 300K) = 3348.0		J Max. = 83	Lines Listed = 2645
Dipole Moments/Debye: $\mu_a = 1.239$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A = B = 1828.70 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,  $\eta_1$ ,  $\eta_2$ , and  $\eta_3$ . The partition function was determined by a sum over states to F = 86 for both the  $\Omega = 1/2$  and  $\Omega = 3/2$  states. Other values are:

<u>T</u>	<u>Q</u>
150	1448.48
100	936.93
60	562.72
30	288.72
10	106.79

Species Tag: 54001	Page 1 of 1	Version: 1	Date: Jan. 1980
Species Name: Acrylonitrile Carbon - 13 isotope on atom 1 $\text{CH}_2 \text{CH}^{13}\text{CN}$		Author: R. L. Poynter	
		Min. Int. = $4 \times 10^{-9}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 26333.		J Max. = 10	Lines Listed = 118
Dipole Moments/Debye: $\mu_a = 3.68$ $\mu_b = 1.25$ $\mu_c = 0$			
Rot. Const./MHz: A = 49781.      B = 4948.153      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	Page 1 of 1	Version: 1	Date: Jan. 1980
Species Name: Acrylonitrile carbon - 13 isotope on atom 2 $\text{CH}_2^{13}\text{CHCN}$		Author: R. L. Poynter	
		Min. Int. = $3 \times 10^{-9}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 26665.		J Max. = 10	Lines Listed = 117
Dipole Moments/Debye: $\mu_a = 3.68$ $\mu_b = 1.25$ $\mu_c = 0$			
Rot. Const./MHz: A = 48645.      B = 4948.700      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	Page 1 of 1	Version: 1	Date: Jan. 1980
Species Name: Acrylonitrile  Carbon - 13 isotope on atom 3  $^{13}\text{CH}_2\text{CHCN}$	Author: R. L. Poynter		
	Min. Int. = $3 \times 10^{-9}$ nm <sup>2</sup> MHz		
Q (Spin-Rot., T = 300K) = 27087.5	J Max. = 10	Lines listed =	
Dipole Moments/Debye: $\mu_a$ = 3.68 $\mu_b$ = 1.25 $\mu_c$ = 0			
Rot. Const./MHz: A = 49180. B = 4837.34 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	Page 1 of 1	Version: 1	Date: Jan. 1980
Species Name: Acrylonitrile Deuterium isotope on atom 2 CH <sub>2</sub> CDCN		Author: R. L. Poynter	
		Min. Int. = $9 \times 10^{-10}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., 1 - 300K) = 29697.8		J Max. = 10	Lines Listed = 322
Dipole Moments/Debye: $\mu_a = 3.68$ $\mu_b = 1.25$ $\mu_c = 0$			
Rot. Const./MHz: A = 40198.6      B = 4934.35      C = 4388.41			

The methods used on this species were the same as for the parent species, given in tag #53001. The measurements were taken from C. C. Costain and B. P. Stoicheff, 1959, J. Chem. Phys. 30, 77.

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

Species Tag: 54005	Page 1 of 1	Version: 1	Date: Jan. 1981
Species Name: Hypochlorous acid, HO <sup>37</sup> Cl		Author: R. Poynter	
		Min. Int. = $10^{-8}$ below 120 GHz; $\text{nm}^2\text{MHz}$ $10^{-5}$ $\text{nm}^2\text{MHz}$ above this frequency	
Q (Spin-Rot., T = 300K) = 9657.239		J Max. = 20	Lines Listed = 673
Dipole Moments/Debye: $\mu_a = 1.3$ $\mu_b = .367$ $\mu_c =$			
Rot. Const./MHz: A = 613455.020      B = 14851.929      C = 14471.418			

The comments made for HO<sup>35</sup>Cl (Tag 52006) also apply here, except as follows: The quadrupole coupling constants were refitted, using rotational constants and covariance frozen to those determined by Wells, et. al., 1979, J. Mol. Spect. 77, 349. The dipole moment was assumed the same as in HO<sup>35</sup>Cl. Quadrupole splittings were only computed up through J = 5, as for HO<sup>35</sup>Cl.

Other values of the partition function are:

<u>T</u>	<u>Q</u>
10	60.16
30	307.52
60	866.44
150	3417.00
200	5258.76

Species Tag: 55001	Page 1 of 1	Version: 2	Date: Jan. 1981
Species Name: Ethyl Cyanide $C_2H_5CN$		Author: R. L. Poynter	
		Min. Int. = $10^{-9}$ nm <sup>2</sup> /MHz below 160 GHz, $10^{-5}$ above 160 GHz	
Q (Spin-Rot., T = 300K) = 11848.1		J Max. = 21	Lines Listed = 3684
Dipole Moments/Debye: $\mu_a = 3.850$ $\mu_b = 1.23$ $\mu_c = 0.$			
Rot. Const./MHz: A = 27663.66      B = 4714.144      C = 4235.041			

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333, and W. H. Kirchhoff and D. R. Johnson, 1973, J. Mol. Spect. 45, 159. The measurements were taken from the following papers:

J. Burie, J. Demaison, A. Dubrille, and D. Boucher, 1978, J. Mol. Spect. 72, 275.

D. R. Johnson, F. J. Lovas, C. A. Gottlieb, E. W. Gottlieb, M. M. Litvak, M. Guelin, and P. Thaddeus, 1977, Ap. J. 218, 370.

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

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

Additional values of the partition function are:

<u>I</u>	<u>Q</u>
10	685.2
30	3544.2
60	10013.2
150	39553.3
200	60889.3

Species Tag: 56001	Page 1 of 1	Version: 2	Date: Jan. 1981
Species Name: Ethyl Cyanide carbon - 13 isotope on atom 1 $\text{CH}_3\text{CH}_2^{13}\text{CN}$		Author: R. L. Poynter	
		Min. Int. = $10^{-9}$ below 160 GHz $10^{-5}$ above 160 GHz $\text{cm}^2/\text{MHz}$	
Q (Spin-Rot., T = 300K) = 112465.7		J Max. = 10	Lines Listed = 1183
Dipole Moments/Debye: $\mu_a = 3.840$ $\mu_b = 1.370$ $\mu_c = 0$			
Rot. Const./MHz: A = 27634.94      B = 4689.805      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 the following papers:

H. M. Heise, H. Lutz, and H. Driezler, 1973, Z. Naturforsch. 29a, 1345.

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

Additional values of the partition function are:

<u>T</u>	<u>Q</u>
10	688.98
30	3563.76
60	10068.39
150	39771.69
200	61225.53

Species Tag: 56002	Page 1 of 1	Version: 2	Date: Jan. 1981
Species Name: Ethyl Cyanide Carbon - 13 isotope on atom 2 $\text{CH}_3^{13}\text{CH}_2\text{CN}$		Author: R. L. Poynter	
		Min. Int. = $10^{-9}$ below 160 GHz $10^{-5}$ above 160 GHz $\text{nm}^2\text{MHz}$	
Q (Spin-Rot., T = 300K) = 113691.5		J Max. = 10	Lines Listed = 1252
Dipole Moments/Debye: $\mu_a = 3.840$ $\mu_b = 1.370$ $\mu_c = 0.$			
Rot. Const./MHz: A = 27045.40 B = 4697.866 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 the following papers:

H. M. Heise, H. Lutz, and H. Driezler, 1973, Z. Naturforsch. 29a, 1345.

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

Additional values of the partition function are:

<u>T</u>	<u>Q</u>
10	696.5
30	3602.6
60	10178.1
150	40205.2
200	61892.8

Species Tag: 56003	Page 1 of 1	Version: 2	Date: Jan. 1981
Species Name: Ethyl Cyanide Carbon - 13 isotope on atom 3 $^{13}\text{CH}_3\text{CH}_2\text{CN}$		Author: R. L. Poynter	
		Min. Int. = $10^{-9}$ below 160 GHz $2 \text{ nm}^2 \text{ MHz}$ $10^{-5}$ above 160 GHz	
Q (Spin-Rot., T = 300K) = 115303.9		J Max. = 10	Lines Listed = 1183
Dipole Moments/Debye: $\mu_a = 3.840$ $\mu_b = 1.370$ $\mu_c =$			
Rot. Const./MHz: A = 27342.174      B = 4597.939      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 the following papers:

H. M. Heise, H. Lutz, and H. Driezler, 1973, Z. Naturforsch. 29a, 1345.

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

Additional values of the partition function are:

<u>T</u>	<u>Q</u>
10	706.3
30	3653.6
60	10322.3
150	40775.2
200	62770.5

Species Tag: 56004	Page 1 of 1	Version: 1	Date: Jan. 1980
Species Name: Ethyl Cyanide Nitrogen - 15 - isotope $\text{CH}_3\text{CH}_2\text{C}^{15}\text{N}$		Author: R. L. Poynter Min. Int. = $2 \times 10^{-9}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 38458.		J Max. = 20	Lines Listed = 1621
Dipole Moments/Debye: $\mu_a = 3.840$ $\mu_b = 1.370$ $\mu_c = 0.$			
Rot. Const./MHz: A = 27541.953    B = 4574.771    C = 4119.4300			

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:

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.

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Species Tag: 56005	Page 1 of 1	Version: 2	Date: Jan. 1981
Species Name: Ethyl Cyanide Deuterium isotope on methyl carbon atom trans to CN group $\text{CH}_2\text{D CH}_2\text{CN} - \text{S}$		Author: R. L. Poynter	
		Min. Int. = $10^{-9}$ below 160 GHz $10^{-5}$ above 160 GHz $\text{nm}^2\text{MHz}$	
Q (Spin-Rot., T = 300K) = 118802.0		J Max. = 10	Lines Listed = 1166
Dipole Moments/Debye: $\mu_a = 3.840$ $\mu_b = 1.370$ $\mu_c = 0$			
Rot. Const./MHz: A = 27650.795      B = 4425.061      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 the following papers:

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.

Additional values of the partition function are:

<u>T</u>	<u>Q</u>
10	727.56
30	3765.16
60	10635.15
150	42011.94
200	64674.63



Species Tag: 56006	Page 1 of 1	Version: 2	Date: Jan. 1981
Species Name: Ethyl Cyanide Deuterium Isotope on methyl carbon gauche to CN group $\text{CH}_2\text{DCH}_2\text{CN-a}$		Author: R. L. Poynter	
		Min. Int. $10^{-9}$ below 160 GHz $10^{-5}$ above 160 GHz $\text{nm}^2\text{MHz}$	
Q (Spin-Rot., T = 300K) = 121064.4		J Max. = 10	Lines Listed = 1286
Dipole Moments/Debye: $\mu_a = 3.840$ $\mu_b = 1.370$ $\mu_c = 0$			
Rot. Const./MHz: A = 25022.568 B = 4583.422 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 the following papers:

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.

Additional values of the partition function are:

<u>T</u>	<u>Q</u>
10	741.5
30	3836.0
60	10837.9
150	42812.2
200	65906.4

Species Tag: 60001	Page 1 of 1	Version: 2	Date: Jan. 1981
Species Name: OCS Carbonyl sulfide		Author: R. L. Poynter	
		Min. Int. = $4 \times 10^{-7}$ cm <sup>2</sup> /MHz	
Q (Spin-Rot., T = 300K) = 1028.17		J Max. = 99	Lines Listed = 99
Dipole Moments/Debye: $\mu_a$ = $\mu_b$ = .715 $\mu_c$ =			
Rot. Const./MHz: A =                      B = 6081.4921                      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.

Other values of the partition function are:

<u>T</u>	<u>Q</u>
10	34.60
30	103.12
60	205.90
150	514.25
200	685.56

Species Tag: 60002	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Silicon Monosulfide $^{28}\text{Si } ^{32}\text{S}$		Author: R. L. Poynter	
		Min. Int. = $9 \times 10^{-6}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 688.940		J Max. = 97	Lines Listed = 97
Dipole Moments/Debye: $\mu_a = 1.730$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A =      B = 9077.45      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	Page 1 of 1	Version: 2	Date: Jan. 1981
Species Name: $O^{13}CS$ Carbonyl sulfide, Carbon $^{-13}$ isotopic species		Author: R. L. Poynter	
		Min. Int. = $4 \times 10^{-7}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 1031.491		J Max. = 99	Lines Listed = 99
Dipole Moments/Debye: $\mu_a$ = $\mu_b$ = 0.715 $\mu_c$ =			
Rot. Const./MHz: A = B = 6061.9240 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.

Other values of the partition function are:

<u>T</u>	<u>Q</u>
10	34.71
30	103.45
60	206.57
150	515.91
200	687.91

Species Tag: 61002	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Silicon Monosulfide  Silicon - 29 isotope  $^{29}_{\text{Si}} \ ^{32}_{\text{S}}$		Author: R. L. Poynter	
		Min. Int. = $9 \times 10^{-6}$ $\text{cm}^2\text{MHz}$	
Q (Spin-Rot., T = 300K) = 701.830		J Max. = 98	Lines Listed = 98
Dipole Moments/Debye: $\mu_a = 1.730$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A = B = 8910.66 C =			

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

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

Species Tag: 62001	Page 1 of 1	Version: 2	Date: Jan. 1981
Species Name: OC <sup>34</sup> S, Carbonyl Sulfide  <sup>34</sup> S isotope species		Author: R. L. Poynter	
		Min. Int. = $4 \times 10^{-7}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 1053.928		J Max. = 99	Lines Listed = 99
Dipole Moments/Debye: $\mu_a$ = $\mu_b$ = .715 $\mu_c$ =			
Rot. Const./MHz: A =                      B = 5932.8338                      C =			

The measurements were taken from the data sets given in A. Dubrulle, J. Demaison, J. Burie, and D. Boucher, 1980, Z. Naturforsch, 35a, 471, and F. J. Lovas, 1978, J. Phys. Chem. Ref. Data, 7, 1445.

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

Other values of the partition function are:

<u>T</u>	<u>Q</u>
10	35.46
30	105.69
60	211.05
150	527.13
200	702.73

Species Tag: 62002	Page 1 of 1	Version: 2	Date: Jan. 1981
Species Name: <sup>18</sup> OCS, Carbonyl Sulfide		Author: R. L. Poynter	
<sup>18</sup> O isotopic modification		Min. Int. = $4 \times 10^{-7}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 1096.031		J Max. = 99	Lines Listed = 99
Dipole Moments/Debye: $\mu_a$ = $\mu_b$ = .715 $\mu_c$ =			
Rot. Const./MHz: A = B = 5704.8574 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.

Other values of the partition function are:

<u>T</u>	<u>Q</u>
10	36.86
30	109.90
60	219.47
150	548.18
200	730.80

Species Tag: 62003	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Silicon Monosulfide		Author: R. L. Poynter	
Silicon - 30 isotope $^{30}\text{Si} \ ^{32}\text{S}$		Min. Int. = $8 \times 10^{-6}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 714.275		J Max. = 99	Lines Listed = 99
Dipole Moments/Debye: $\mu_a = 1.730$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A =      B = 8755.33      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	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Silicon Monosulfide Sulfur - 34 - isotope $^{28}\text{Si} \ ^{34}\text{S}$		Author: R. L. Poynter	
		Min. Int. = $9 \times 10^{-6}$ $\text{cm}^2/\text{MHz}$	
Q (Spin-Rot., T = 300K) = 708.329		J Max. = 99	Lines Listed = 99
Dipole Moments/Debye: $\mu_a = 1.730$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A = B = 8828.86 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	Page 1 of 1	Version: 1	Date: Sept, 1980
Species Name: Nitric acid $\text{HNO}_3$		Author: R. Poynter	
		Min. Int. = $10^{-8}$ $\text{nm}^2\text{MHz}$	
Q (Spin-Rot., T - 300K) = 27912.921		J Max. = 40	Lines Listed = 7259
Dipole Moments/Debye: $\mu_a = 1.986$ $\mu_b = .882$ $\mu_c = 0$			
Rot. Const./MHz: A = 13010.9867 B = 12099.9025 C = 6260.6680			

The data set used in this fit includes all lines with  $J \leq 40$  as reported by G. Cazzoli and F. C. DeLucia, (1979), J. Mol. Spectrosc. 76, 131. (We omit 8 out of 132 observed lines with  $J > 40$ ). The dipole moment was taken from the remeasurements reported by A. P. Cox and J. M. Riveros, (1965), J. Chem. Phys. 42, 3106. Very small quadrupole splittings were resolvable for only the  $J = 1 \leftarrow 0$  transitions at dry ice temperatures. Because of the extremely large number of lines for this molecule, these splittings were not included. Information on these quadrupole splittings can be found in D. J. Millen and J. R. Morton, (1960), J. Chem. Soc., 1523.

The partition function was determined by a sum over states to  $J = 40$ . Other values are:

T	Q
10	171.79
30	885.76
60	2500.47
150	9872.52
200	15196.81

Species Tag: 64001	Page 1 of 1	Version: 1	Date: Oct. 1979
Species Name: Diatomic Sulfur		Author: H. M. Pickett	
$v = 0, {}^3\Sigma_g^-$ ground state		Min. Int. = $4.0 \times 10^{-9}$ cm <sup>2</sup> /MHz	
Q (Spin-Rot., T = 300K) = 965.37		J Max. = 35	Lines Listed = 34
Dipole Moments/Debye: $\mu_a =$ $\mu_b =$ magnetic $\mu_c =$			
Rot. Const./MHz: A = B = 8831.2 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  $S_2$ , the parameter  $\mu(1)$  is assumed to be zero. Only transitions between states with  $J = N$  and  $J = N - 1$  are listed because the energies of the  $J = N + 1$  states are uncertain by more than 1 GHz. All the neglected transitions from  $J = N + 1$  states lie above 450 GHz for  $J < 35$ .

The intensities of the magnetic dipole allowed transitions were calculated using the g values given in Pickett and Boyd. Hund's case (b) nomenclature is used even though the states are closer to Hund's case (a) for low J. The  $J = N + 1$  states correlate with  $\Sigma = 0$  and the  $J = N - 1$  and  $J = N$  states correlate with  $\Sigma = \pm 1$  states of  $p = \pm (-1)^J$  inversion parity, respectively.

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

Species Tag: 64002	Page 1 of 1	Version: 1	Date: Jan. 1980
Species Name: Sulfur Dioxide  SO <sub>2</sub>		Author: R. L. Poynter	
		Min. Int. = $5 \times 10^{-9}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 5898.91		J Max. = 40	Lines Listed = 1902
Dipole Moments/Debye: $\mu_a$ = 0. $\mu_b$ = 1.633 $\mu_c$ = 0.			
Rot. Const./MHz: A = 60778.558 B = 10317.913 C = 8799.652			

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:

F. J. Lovas, 1978, J. Phys. Chem. Ref. Data, 7, 1445. (A complete summary and references to all available data).

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

Species Tag: 75001	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Cyanodiacetylene  HC <sub>5</sub> N		Author: R. L. Poynter	
		Min. Int. = $2 \times 10^{-7}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 4695.48		J Max. = 99	Lines Listed = 99
Dipole Moments/Debye: $\mu_a$ = 4.330 $\mu_b$ = $\mu_c$ =			
Rot. Const./MHz: A =      B = 1331.33      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	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Cyanodiacetylene Carbon - 13 isotope on atom 1 HCCCC <sup>13</sup> CN		Author: R. L. Poynter	
		Min. Int. = $2 \times 10^{-7}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 4742.326		J Max. = 99	Lines Listed = 99
Dipole Moments/Debye: $\mu_a$ = 4.330 $\mu_b$ = $\mu_c$ =			
Rot. Const./MHz: A = B = 1318.18 C =			

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

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

Species Tag: 76002	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Cyanodiacetylene  Carbon - 13 isotope on atom 2 HCCC <sup>13</sup> CCN		Author: R. L. Poynter	
		Min. Int. = $2 \times 10^{-7}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 4699.78		J Max. = 99	Lines Listed = 99
Dipole Moments/ Debye: $\mu_a = 4.329$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A =      B = 1330.11      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	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Cyanodiacetylene  Carbon - 13 isotope on atom 3  HCC <sup>13</sup> CCCN	Author: R. L. Poynter		
	Min. Int. = 2 x 10 <sup>-7</sup> nm <sup>2</sup> MHz		
Q (Spin-Rot., T = 300K) = 4700.345	J Max. = 99	Lines Listed = 99	
Dipole Moments/Debye: $\mu_a$ = 4.329 $\mu_b$ = $\mu_c$ =			
Rot. Const./MHz: A = B = 1329.95 C =			

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

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



Species Tag: 76004	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Cyanodiacetylene Carbon - 13 isotope on atom 4 CH <sup>13</sup> CCCCN		Author: R. L. Poynter	
		Min. Int. = 2 x 10 <sup>-7</sup> nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 4744.09		J Max. = 99	Lines Listed = 99
Dipole Moments/Debye: $\mu_a$ = 4.329 $\mu_b$ = $\mu_c$ =			
Rot. Const./MHz: A = B = 1317.689 C =			

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

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

Species Tag: 76005	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Cyanodiacetylene Carbon - 13 isotope on atom 5 H <sup>13</sup> CCCCCN		Author: R. L. Poynter	
		Min. Int. = $2 \times 10^{-7}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 4820.96		J Max. = 99	Lines Listed = 99
Dipole Moments/Debye: $\mu_a$ 4.329 $\mu_b$ $\mu_c$			
Rot. Const./MHz: A = B = 1296.68 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	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Cyanodiacetylene Nitrogen - 15 isotope $\text{HC}_5^{15}\text{N}$		Author: R. L. Poynter	
		Min. Int. = $2 \times 10^{-7}$ cm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 4813.68		J Max. = 99	Lines Listed = 99
Dipole Moments/Debye: $\mu_a = 4.329$ $\mu_b$ $\mu_c =$			
Rot. Const./MHz: A =      B = 1298.639      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	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Cyanodiacetylene Deuterium isotope $\text{DC}_5\text{N}$		Author: R. L. Poynter	
		Min. Int. = $2 \times 10^{-7}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 4918.13		J Max. = 99	Lines Listed = 99
Dipole Moments/Debye: $\mu_a = 4.329$ $\mu_b =$ $\mu_c =$			
Rot. Const./MHz: A =      B = 1271.056      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: 80001	Page 1 of 1	Version: 1	Date: Feb. 1980
Species Name: Hydrogen Bromide Bromine - 79 isotope H <sup>79</sup> Br		Author: R. L. Poynter & H. M. Pickett	
		Min. Int. = $7 \times 10^{-3}$ cm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 101.214		J Max. =	Lines Listed = 19
Dipole Moments/Debye: $\mu_a$ = 0.828 $\mu_b$ = $\mu_c$ =			
Rot. Const./MHz: A =      B = 250357.6      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	Page 1 of 1	Version: 1	Date: Feb. 1980
Species Name: Hydrogen Bromide Bromine - 81 isotope $\text{H}^{81}\text{Br}$		Author: R. L. Poynter & H. M. Pickett	
		Min. Int. = $7 \times 10^{-3}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 101.257		J Max. =	Lines Listed = 19
Dipole Moments/Debye: $\mu_a$ = 0.828 $\mu_b$ = $\mu_c$ =			
Rot. Const./MHz: A =      B = 250250.2      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	Page 1 of 1	Version: 1	Date: Feb. 1980
Species Name: Bromine Monoxide Bromine - 79 isotope $2\Pi_{3/2}$ state 79 BrO		Author: H. M. Pickett	
		Min. Int. = $10^{-9}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 3897.60		J Max. = 49	Lines Listed = 850
Dipole Moments/Debye: $\mu_a$ = 1.765 $\mu_b$ = $\mu_c$ =			
Rot. Const./MHz: A = B = 12830.4 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	Page 1 of 1	Version: 1	Date: Feb. 1980
Species Name: Bromine Monoxide  Bromine - 81 isotope  $^2\Pi_{3/2}$ state 81 BrO		Author: H. M. Pickett	
		Min. Int. = $10^{-9}$ nm <sup>2</sup> MHz	
Q (Spin-Rot., T = 300K) = 3913.9		J Max. = 49	Lines Listed = 850
Dipole Moments/Debye: $\mu_a$ = 1.794 $\mu_b$ = $\mu_c$ =			
Rot. Const./MHz: A =      B = 12777.08      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.