JPL PUBLICATION 80-23, REVISION 1

(NASA-CR-164357) SUBMILLIMETER, MILLIMETER, AND MICROWAVE SPECTRAL LINE CATALOGUE (Jet Propulsion Lab.) 151 p HC A08/MF A01 CSCL 20N

N81-24323

Unclas
G3/32 42473

Submillimeter, Millimeter, and Microwave Spectral Line Catalogue

R. L. Poynter
H. M. Pickett

June 1, 1981

National Aeronautics and
Space Administration

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The research described in this publication was carried out by the Jet Propulsion Laboratory, California Institute of Technology, under NASA Contract No. NAS7-100.

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 μm) The catalogue can be used as a planning guide or as an aid in the identification and analysis of observed spectral lines. The information listed for each spectral line includes the frequency and its estimated error, the intensity, lower state energy, and quantum number assignment.

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

- NH2D
- H2O-V2
- H2O2
- CH3CHO-E
- O3-V2
- O3-V13
- HOCL
- HOCL-37
- HNO3

Revised Species (24)

- NH3
- N-15-H3
- H2O
- CH2NH
- CH2ND
- O2
- O2-V1
- O-18-O
- CH3OH
- H2S
- PH3
- NH2CHO
- CLO
- CL-37-O
- C2H5CN
- CH3CH2C-13-N
- CH3C-13-H2CN
- CH2DCH2CN-S
- CH2DCH2CN-A
- OCS
- OC-13-S
- OCS-34
- O-18-CS

CONTENTS

Tables

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 100μm). 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    , 12I2, 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 nm^2 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 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, nm^2 MHz, are based on the integral of the absorption cross section over the spectral lineshape. The value of the intensity is calculated for 300K and is directly comparable with the common infrared intensity unit of $cm^{-1}/(molecule/cm^2)$. The latter is obtainable by dividing the catalogue intensity by 2.9979 x 10^{+18}.

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

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

where ν_{ba} is the line frequency, ${}^{x}S_{ba}$ is the line strength, μ_x is the dipole moment along the molecular axis x, E" and E' are the lower and upper state energies respectively, and Q_{rs} is the rotation-spin partition function (using the same zero of energy as E' and E"). Care must be taken to assure that ${}^{x}S_{ba}$ and Q_{rs} are determined with same state degeneracies. Note that with this definition the intensities are defined with respect to the total concentration of the vibration electronic state of the species. No vibrational partition function or vibrational Boltzmann factor is included. For the catalogue, Eq. (1) is evaluated for T=300K.

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

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

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

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

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

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

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

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

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

in which p is the partial pressure of absorber in torr, and m is the mass of the absorber (in atomic mass units). In Eq. (4) - (6), ν_{ba} is the line frequency in MHz.

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

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

The inverse of σ_{ba} is the column density per unit optical depth in the same 1 km/s velocity interval.

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

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

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

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:

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

in which ϵ_n is the estimated error of frequency ν_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

$$\left(V^{-1}\right)_{k\ell} = \sum_m \frac{\partial \nu_m}{\partial p_k} \frac{\partial \nu_m}{\partial p_\ell} \epsilon_m^{-2} \qquad (8)$$

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

Experimental uncertainties in the literature vary from 1.6 σ estimates to 3 σ 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 ${}^{x}S_{ba}$ 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, I1 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)
Ω	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	QN	Remarks
A. Atoms		
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. Linear molecules and Diatomic molecules		
1XY	J', J'', x', x'', y', y''	$^1\Sigma$ state
2XY	$J' + \frac{1}{2}$, 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	$J' + \frac{1}{2}$, $\Omega' + \frac{1}{2}$, p', $J'' + \frac{1}{2}$, $\Omega'' + \frac{1}{2}$, p'', x', x'', y', y''	$^2\Pi$ state
6XY	J', Ω', p', J'', Ω'', p'', x', y'', y', y''	$^3\Pi$ state
7XY	J', Ω', p', J'', Ω'', p'', x', x'', y', y''	$^1\Delta$ state
C. Symmetric Rotors (3-fold symmetry or higher, S = 0)		
8XY	J', K', J'', K'', x', x'', y', y''	
D. Asymmetric Rotors		
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 must be zero)	$Y = 0$:	$y = 0$
$X = 1$:	$x = F+\frac{1}{2}$	(F half integer)	$Y = 1$:	$y = F_1 + \frac{1}{2}$ or $= F + \frac{1}{2}$ if $X = 4$
$X = 2$:	$x = F$	(F integer)		
$X = 4$:	$x = v$	vibrational state label (further specified in the species description)	$Y = 2$:	$y = F_1$ or $= F$ if $X = 4$

' signifies upper energy state, " signifies lower energy state

Table V-2: Special-Case Quantum Number Formats

QNFORM	QN	Remarks
1300	J,N	$^3\Sigma$ state "non-resonant" transition; frequency is $\lvert g\rvert J$ 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 magneticc 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
2001	D-Atom
3001	HD
12001	C-Atom
13001	C-13-Atom
14001	N-Atom
14002	N-Atom-D-State
16001	O-Atom
17001	HO
17002	NH3
17003	CH3D
18001	DO
18002	N-15-H3
18003	H2O
18004	NH2D
18005	H2O-ν2
19001	HO-18
19002	HDO
27001	HCN
27002	HNC
28001	CO
28002	HC-13-N
28003	HCN-15
28004	DCN
28005	HNC-13
28006	HN-15-C
28007	DNC
29001	C-13-O
29002	HCO+
29003	CH2NH
30001	CO-18
30002	HC-13-O+
30003	DCO+
30004	H2CO
30005	C-13-H2NH
30006	CH2N-15-H
30007	CH2ND
30008	NO
31001	HCO-18+
31002	H2C-13-O
32001	O2
32002	O2-v1
32003	CH3OH
32004	H2CO-18
34001	O-18-O
34002	H2S
34003	PH3
34004	H2O2
35001	HDS
36001	HCl
38001	HCl-37
40001	CH3CCH
41001	CH3CN
41002	CH3CC-13-H
41003	CH3C-13-CH
41004	C-13 H3CCH
41005	CH3CCD
41006	CH_2DCCH
42001	CH3CN-15
42002	CH2CO
43001	CHDCO
44001	CS
44002	SiO
44003	CH3CHO-A
44004	N2O
44005	CH_3CHO-E
45001	C-13-S
45002	Si-29-O
45003	NH2CHO
46001	CS-34
46002	Si-30-O
46003	H2CS
46004	C2H5OH
46005	HCOOH
47001	H2C-13-S
47002	HC-13-OOH
47003	DCOOH
47004	HCOOD
48001	SO
48002	SO-v1
48003	H2CS-34
48004	O3
48005	O3-ν2
48006	O3-ν1,3
50001	S-34-O
50002	SO-18
50003	O3-SYM-O-18
50004	O3-ASYM-O-18
51001	HCCCN
51002	ClO
52001	HCCC-13-N
52002	HCC-13-CN
52003	HC-13-CCN
52004	HCCCN-15
52005	DCCCN
52006	HOCl
53001	C2H3CN
53002	Cl-37-O
54001	CH2CHC-13-N
54002	CH2C-13-HCN
54003	C-13-H2CHCN
54004	CH2CDCN
54005	HOCl-37
55001	C2H5CN
56001	CH3CH2C-13-N
56002	CH3C-13-H2CN
56003	C-13-H3CH2CN
56004	C2H5CN-15
56005	CH2DCH2CN-S
56006	CH2DCH2CN-A
60001	OCS
60002	SiS
61001	OC-13-S
61002	O-18-CS
62001	Si-29-S
62002	O-18-CS
62003	Si-30-S
62004	SiS-34
63001	HNO3
64001	S2
64002	SO2
75001	HCCCCCN
76001	HCCCCC-13-N
76002	HCCCC-13-CN
76003	HCCC-13-CCN
76004	HCC-13-CCCN
76005	HC-13-CCCCN
76006	HCCCCCN-15
76007	DCCCCCN
80001	HBr-79
82001	HBr-81
95001	Br-79-O
97001	Br-81-O

Species Tag: 1001	Page 1 of 1	Version: 1	Date: Oct, 1979
Species Name: Atomic Hydrogen $^2S_{\frac{1}{2}}$ ground state		Author: H. M. Pickett Min. Int. = 8 X 10^{-10} nm^2MHz	
Q (Spin-Rot., T = 300K) = 4.0		J Max. = (½)	Lines Listed = 1
Dipole Moments/Debye: μ_a =		μ_b = magnetic	μ_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 X 10^{-15} sec $^{-1}$.

Species Tag: 2001	**Page** 1 **of** 1	**Version:** 1	**Date:** Oct. 1979
Species Name: Atomic Hydrogen Deuterium Isotope $^2S_{\frac{1}{2}}$ ground state		**Author:** H. M. Pickett **Min. Int.** = 5×10^{-11} nm^2MHz	
Q (Spin-Rot., T = 300K) = 6.0		**J Max.** = (½)	**Lines Listed** = 1
Dipole Moments/Debye: μ_a =		μ_b = magnetic	μ_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 4.695×10^{-17} sec $^{-1}$.

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} $\mathrm{nm}^2\mathrm{MHz}$	
Q (Spin-Rot., T = 300K) = 5.016		**J Max.** = (1)	**Lines Listed** = 1
Dipole Moments/Debye: μ_a = 5.85 X 10^{-4}	μ_b =	μ_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.

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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^2MHz	
Q (Spin-Rot., T - 300K) = 7.8330		**J Max.** = (2)	**Lines Listed** = 2
Dipole Moments/Debye: μ_a =		μ_b = magnetic	μ_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:

J	Energy	Degeneracy
0	0.0 cm^{-1}	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}C isotope		**Author:** H. M. Pickett **Min. Int. =** 10^{-16} nm^2MHz	
Q (Spin-Rot., T = 300K) = 15.666		J Max. = (2)	Lines Listed = 7
Dipole Moments/Debye: μ_a =		μ_b = magnetic	μ_c =
Rot. Const./MHz: A =		B =	C =

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

Species Tag: 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^2MHz	
Q (Spin-Rot., T = 300K) = 12.0		**J Max.** = (3/2)	**Lines Listed** = 2
Dipole Moments/Debye: μ_a =		μ_b = magnetic	μ_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 ^{2}D excited state		**Author:** H. M. Pickett **Min. Int.** = 10^{-8} nm^{2}MHz	
Q (Spin-Rot., T = 300K) = 29.510		J Max. = (5/2)	Lines Listed = 6
Dipole Moments/Debye: μ_a =		μ_b =	magnetic μ_c =
Rot. Const./MHz: A =		B =	C =

The $^2D_{5/2}$ state is 19223 cm^{-1} above the ground $^4S_{3/2}$ state. (C. E. Moore, 1949, Atomic Energy Levels I, 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 ± 600 MHz, but the hyperfine structure intervals are uncertain by less than 1 MHz. (H. E. Radford and K. M. Evenson, 1968, Phys. Rev. 168, 70). The average spontaneous emission rate from the ^2D states to the ^4S states is 1.06×10^{-6} sec^{-1}. In contrast, the spontaneous emission rate from $^2D_{3/2}$ F = 5/2 to $^2D_{5/2}$ F = 7/2 is 3.15×10^{-9} sec^{-1}.

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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^2MHz

Q (Spin-Rot., T = 300K) = 7.4943
J Max. = (2)
Lines Listed = 1

Dipole Moments/Debye: μ_a = μ_b = magnetic μ_c =

Rot. Const./MHz: A = B = C =

The 68 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:

J	Energy	Degeneracy
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. Pickett **Min Int.** = 10^{-13} nm^2MHz	
Q (Spin-Rot., T = 300K) = 83.328		**J Max.** = 19.5	**Lines Listed** = 125
Dipole Moments/Debye: μ_a = 1.667	μ_b =	μ_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_3, ground inversion states		**Author:** R.L. Poynter & H.M. Pickett **Min. Int.** = 10^{-17} nm^2MHz	
Q (Spin-Rot., T = 300K) = 578.984		**J Max.** = 20	**Lines Listed** = 235
Dipole Moments/Debye: μ_a =	μ_b =	μ_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:

T	Q
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_3D		**Author:** R. L. Poynter **Min. Int.** = 10^{-8} nm^2MHz	
Q (Spin-Rot., T - 300K) = 402.166		**J Max.** = 13	**Lines Listed** = 80
Dipole Moments/Debye: μ_a = 5.6 x 10^{-3}	μ_b =	μ_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. Muenter, 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} nm^2MHz	
Q (Spin-Rot., T = 300K) = 215.558		**J Max. =** 19.5	**Lines Listed =** 235
Dipole Moments/Debye: μ_a = 1.653	μ_b =	μ_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 $Q=6\ Q_{rot}\ [1 + \exp(-188.112/T)]$, in which Q_{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, $^{15}NH_3$ ground inversion states		**Author:** R. Poynter **Min. Int. =** 10^{-17} $nm^2 MHz$	
Q (Spin-Rot., T = 300K) = 575.808		**J Max. =** 20	**Lines Listed =** 235
Dipole Moments/Debye: μ_a =	μ_b =	μ_c = 1.476	
Rot. Const./MHz. A = B	**B =** 297390.8	**C =** 186711.	

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

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

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

T	Q
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_2O		Author: R.L. Poynter & H.M. Pickett	
		Min. Int. = 10^{-9} nm^2MHz	
Q (Spin-Rot., T - 300K) = 178.037		J Max. = 15	Lines Listed = 151
Dipole Moments/Debye: μ_a = 0		μ_b = 1.855	μ_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:

T	Q
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_2D, ground vibrational states		**Author:** H. M. Pickett **Min. Int. =** 10^{-10} nm^2MHz	
Q (Spin-Rot., T = 300K) = 1258.		**J Max. =** 14	**Lines Listed =** 5036
Dipole Moments/Debye: μ_a = -0.18	μ_b = 0.	μ_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 $P_aP_c + P_cP_a$ interaction term. The relative sign of the dipoles is determinable and is important for intensities because of mixing by the interaction term.

Species Tag: 18005	**Page** 1 **of** 1	**Version:** 1	**Date:** Jan. 1981
Species Name: Water excited bending state, ν_2 or (010) H_2O		**Author:** H. M. Pickett **Min. Int. =** 10^{-10} nm^2MHz	
Q (Spin-Rot., T - 300K) = 169.226		**J Max. =** 12	**Lines Listed =** 122
Dipole Moments/Debye: μ_a = 0		μ_b = 1.855	μ_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:

T	Q
10	1.325
30	5.983
60	15.964
100	33.350
150	60.446

The zero of energy is 1594.75 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}OH		**Author:** R. L. Poynter & H. M. Pickett **Min. Int.** = 10^{-13} nm^2MHz	
Q (Spin-Rot., T = 300K) = 83.882		**J Max.** = 20	**Lines Listed** = 113
Dipole Moments/Debye: μ_a = 1.667	μ_b =	μ_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}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^2MHz	
Q (Spin-Rot., T = 300K) = 146.05		J Max. = 13	Lines Listed = 221
Dipole Moments/Debye: μ_a = 0.657	μ_b = 1.732	μ_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^2MHz	
Q (Spin-Rot., T = 300K) = 424.154		J Max. = 34	Lines Listed = 45
Dipole Moments/Debye: μ_a = 2.984 μ_b = μ_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} $nm^2 MHz$	
Q (Spin-Rot., T = 300K) = 138.223		J Max. = (34)	Lines Listed = 34
Dipole Moments/Debye: μ_a = 2.699		μ_b =	μ_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^{-5} nm^2MHz	
Q (Spin-Rot., T = 300K) = 108.787		J Max. = (26)	Lines Listed = 26
Dipole Moments/Debye: μ_a = 0.1098		μ_b =	μ_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. Muenter, 1975, J. Mol. Spect. 55, 490.

Species Tag: 28002	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Hydrogen Cyanide		Author: R. L. Poynter	
Carbon - 13 isotope $H^{13}CN$		Min. Int. = 10^{-4} nm^2MHz	
Q (Spin-Rot., T = 300K) = 435.385		J Max. = 34	Lines Listed = 45
Dipole Moments/Debye: μ_a = 2.984	μ_b =	μ_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 $HC^{15}N$		Author: R. L. Poynter Min. Int. = 3×10^{-3} nm^2MHz	
Q (Spin-Rot., T = 300K) = 435.204		J Max. = 35	Lines Listed = 35
Dipole Moments/Debye: μ_a = 2.984	μ_b =	μ_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. = 7×10^{-5} nm^{2}MHz	
Q (Spin-Rot., T = 300K) = 518.916		J Max. = 41	Lines Listed = 54
Dipole Moments/Debye: μ_a = 2.984		μ_b =	μ_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 $HN^{13}C$		Author: R. L. Poynter	
		Min. Int. = 2×10^{-3} nm^2MHz	
Q (Spin-Rot., T = 300K) = 143.880		J Max. = (35)	Lines Listed = 35
Dipole Moments/Debye: μ_a = 2.699	μ_b =	μ_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 $H^{15}NC$		Author: R. L. Poynter Min. Int. = 2×10^{-3} $nm^2 MHz$	
Q (Spin-Rot., T = 300K) = 141.013		J Max. = (33)	Lines Listed = 33
Dipole Moments/Debye: μ_a = 2.699	μ_b =	μ_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^2MHz	
Q (Spin-Rot., T = 300K) = 164.169		J Max. = (39)	Lines Listed = 39
Dipole Moments/Debye: μ_a = 2.699	μ_b =	μ_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}CO		Author: R. L. Poynter Min. Int. = 8×10^{-6} nm^2MHz	
Q (Spin-Rot., T = 300K) = 113.776		J Max. = (27)	Lines Listed = 27
Dipole Moments/Debye: μ_a = 0.110 μ_b = μ_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^+		Author: R. L. Poynter Min. Int. = 10^{-3} nm^2MHz	
Q (Spin-Rot., T = 300K) = 140.504		J Max. = (33)	Lines Listed = 33
Dipole Moments/Debye: μ_a = 3.30	μ_b =	μ_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_2NH		**Author:** R. Poynter	
		Min. Int. = 10^{-8} below 120 GHz 10^{-5} above 120 GHz nm^2MHz	
Q (Spin-Rot., T = 300K) = 5892.86		**J Max.** = 33	**Lines Listed** = 2834
Dipole Moments/Debye: μ_a = 1.325	μ_b = 1.530	μ_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, <u>2</u>, 1.

Additional values of the partition function are:

T	Q
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. = 8×10^{-6} nm^2MHz	
Q (Spin-Rot., T = 300K) = 114.2096		J Max. = (27)	Lines Listed = 27
Dipole Moments/Debye: μ_a = 0.110	μ_b =	μ_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 $H^{13}CO^+$		Author: R. L. Poynter Min. Int. = 3×10^{-3} nm^2MHz	
Q (Spin-Rot., T = 300K) = 144.437		J Max. = (34)	Lines Listed = 34
Dipole Moments/Debye: μ_a = 3.30		μ_b =	μ_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		Author: R. L. Poynter	
Deuterium isotope DCO^+		Min. Int. = 2×10^{-3} nm^2MHz	
Q (Spin-Rot., T = 300K) = 173.872		J Max. = (42)	Lines Listed = 41
Dipole Moments/Debye: μ_a = 3.30	μ_b =	μ_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^2MHz	
Q (Spin-Rot., T = 300K) = 2876.7		J Max. = 40	Lines Listed = 611
Dipole Moments/Debye: μ_a = 2.331	μ_b = 0.	μ_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 $^{13}CH_2NH$		Author: R. L. Poynter Min. Int. = 10^{-8} nm^2MHz	
Q (Spin-Rot., T = 300K) = 2012.45		J Max. = 10	Lines Listed = 439
Dipole Moments/Debye: μ_a = 1.325	μ_b = 1.530	μ_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, CH_2NH. The data are from R. Pearson, Jr. and F. J. Lovas, 1977, J. Chem. Phys. 66, 4149. The dipole moment has been assumed the same as for the parent species.

Species Tag: 30006	**Page 1 of 1**	**Version:** 1	**Date:** Jan. 1980
Species Name: Methylenimine Nitrogen - 15 isotope $CH_2{}^{15}NH$		**Author:** R. L. Poynter	
		Min. Int. = 10^{-8} nm^2MHz	
Q (Spin-Rot., T = 300K) = 2015.792		**J Max.** = 10	**Lines Listed** = 440
Dipole Moments/Debye: μ_a = 1.325 μ_b = 1.530 μ_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, CH_2NH. The data are from R. Pearson, Jr. and F. J. Lovas, 1977, J. Chem. Phys. 66, 4149. The dipole moment has been assumed the same as for the parent species.

Species Tag: 30007 | **Page** 1 **of** 1 | **Version:** 2 | **Date:** Feb 1981

Species Name: Methylenimine
Deuterium on nitrogen atom
CH_2ND

Author: R. L. Poynter

Min. Int. = 10^{-8} below 120 GHz, 10^{-5} above 120 GHz nm^2MHz

Q (Spin-Rot., T = 300K) = 2393.69

J Max. = 14

Lines Listed = 1834

Dipole Moments/Debye: μ_a = 1.325 μ_b = 1.530 μ_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, CH_2NH. The data are from R. Pearson, Jr. and F. J. Lovas, 1977, J. Chem. Phys. 66, 4149.

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

Additional values of the partition function are:

T	Q
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^2MHz	
Q (Spin-Rot., T = 300K) = 1159.464		J Max. = 35.5	Lines Listed = 1909
Dipole Moments/Debye: μ_a = 0.15872		μ_b = 0.	μ_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:

T	Q
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 $HC\,^{18}O^+$		Author: R. L. Poynter Min. Int. = 3×10^{-3} nm^2MHz	
Q (Spin-Rot., T = 300K) = 145.427		J Max. = (34)	Lines Listed = 34
Dipole Moments/Debye: μ_a =		μ_b = 3.30	μ_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. = 5×10^{-10} nm^2MHz	
Q (Spin-Rot., T = 300K) = 2949.7		J Max. = 40	Lines Listed = 601
Dipole Moments/Debye: μ_a = 2.331	μ_b = 0.	μ_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 $^{16}O_2$ v = 0 state of ground $^3\Sigma_g^-$ electronic state		**Author:** H. M. Pickett **Min. Int.** = 10^{-32} nm^2MHz	
Q (Spin-Rot., T - 300K) = 218.529		J Max. = 60	Lines Listed = 174
Dipole Moments/Debye: μ_a =		μ_b = magnetic	μ_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 O_2 (M. Loete and H. Berger, 1977, J. Mol. Spectroscopy 68, 317) were used with the millimeter wavelength measurements and the submillimeter-line of W. Steinbach and W. Gordy (1973, Phys. Rev A 8, 1953) in a combined fit of the v = 0 and v = 1 transitions. The intensities of the magnetic dipole transitions have been calculated using the g values obtained from magnetic resonance by K. D. Bowers, R. A. Kamper and C. D. Lustig, 1959, Proc. Roy. Soc. (Lond.) A251, 565. The zero-frequency absorption is included but the frequency is set to a synthetic frequency of |g|J for the given level.

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

T	Q
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 $^{16}O_2$ v = 1 state of the ground $^{3}\Sigma_g^-$ state		**Author:** H. M. Pickett **Min. Int.** = 10^{-10} nm^{2}MHz	
Q (Spin-Rot., T = 300K) = 220.918		**J Max.** = (40)	**Lines Listed** = 63
Dipole Moments/Debye: μ_a =	μ_b = magnetic	μ_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 ± 0.01 cm^{-1} above the ground state (M. Loete and H. Berger, 1977, J. Molec. Specty. 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:

T	Q
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) CH_3OH lowest A, E_1, and E_2 vibrational states		**Author:** H. M. Pickett **Min. Int.** = 10^{-10} nm^2MHz	
Q (Spin-Rot., T - 300K) = 6414.2516		**J Max.** = 12	**Lines Listed** = 709
Dipole Moments/Debye: μ_a = 0.885		μ_b = 1.440	μ_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 v quantum numbers in the catalogue are:

v	species	asymmetric rotor correspondence
1	A+	upper K state for K even, lower for K odd
2	A-	upper K state for K odd, lower for K even
3	E_1	no direct correspondence
4	E_2	no direct correspondence

Species Tag: 32004	**Page** 1 **of** 1	**Version:** 1	**Date:** Feb. 1980
Species Name: Formaldehyde Oxygen - 18 isotope $H_2C^{18}O$		**Author:** R. L. Poynter **Min. Int.** = 10^{-9} nm^2MHz	
Q (Spin-Rot., T = 300K) = 3017.226		**J Max.** = 20	**Lines Listed** = 449
Dipole Moments/Debye: μ_a = 2.331	μ_b = 0.	μ_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: $^{18}O\ ^{16}O$ Molecular Oxygen - O^{18} species ground state		**Author:** H. M. Pickett **Min. Int.** = 2.5×10^{-11} nm^2MHz	
Q (Spin-Rot., T = 300K) = 462.32		**J Max.** = (42)	**Lines Listed** = 132
Dipole Moments/Debye: μ_a =		μ_b = magnetic	μ_c =
Rot. Const./MHz: A =		B = 40708.	C =

The measurements and calculational method are from T. Amano and E. Hirota, 1974, J. Mol. Spectroscopy <u>53</u>, 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.) <u>A251</u>, 565. The zero-frequency absorption is included but the frequency is set to a synthetic frequency of $|g|J$ for the given level.

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

T	Q
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^2MHz	
Q (Spin-Rot., T - 300K) = 514.197		J Max. = 15	Lines Listed = 311
Dipole Moments/Debye: μ_a = 0.		μ_b = 0.974	μ_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:

T	Q
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 PH_3		**Author:** R. L. Poynter **Min. Int.** = 10^{-17} nm^2MHz	
Q (Spin-Rot., T = 300K) = 608.55		**J Max.** = (19)	**Lines Listed** = 142
Dipole Moments/Debye: μ_a = $^*7.2 \times 10^{-5}$	μ_b =	μ_c = 0.574	
Rot. Const./MHz: A =	*centrifugally induced 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 ± 0.0003D.

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

Other values of the partition function are:

T	Q
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_2O_2		**Author:** H. M. Pickett **Min. Int. =** 10^{-8} nm^2MHz	
Q (Spin-Rot., T = 300K) = 7651.8		**J Max. =** 24	**Lines Listed =** 883
Dipole Moments/Debye: μ_a =	μ_b =	μ_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 τ = 1, 2 and v = 1 for τ = 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. = 4×10^{-12} nm^2MHz	
Q (Spin-Rot., T - 300K) = 430.900		J Max. = 20	Lines Listed = 1138
Dipole Moments/Debye: μ_a = 0.470	μ_b = 0.974	μ_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. Steenbeckliers, 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 $H\ ^{35}Cl$		Author: R. L. Poynter & H. M. Pickett Min. Int. = 5×10^{-2} nm^2MHz	
Q (Spin-Rot., T = 300K) = 81.232		J Max. = 4	Lines Listed = 17
Dipole Moments/Debye: μ_a = 1.109	μ_b = 0	μ_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 $H^{37}Cl$		Author: R. L. Poynter & H. L. Pickett Min. Int. = 5×10^{-2} nm^2MHz	
Q (Spin-Rot., T = 300K) = 81.352		J Max. = 4	Lines Listed = 17
Dipole Moments/Debye: μ_a = 1.109	μ_b =	μ_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_3 CCH		Author: R. L. Poynter Min. Int. = 3×10^{-5} nm^2MHz for J > 14	
Q (Spin-Rot., T = 300K) = 5428.80		J Max. = 80	Lines Listed = 813
Dipole Moments/Debye: μ_a = 0.750	μ_b =	μ_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. Muenter 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_3 CN ground state		**Author:** R. L. Poynter **Min. Int. =** 3×10^{-5} nm^2MHz for J > 14	
Q (Spin-Rot., T = 300K) = 15145.		**J Max. =** 82	**Lines Listed =** 1441
Dipole Moments/Debye: μ_a = 3.919	μ_b =	μ_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. Kukolich, D. J. Ruben, J. H. S. Wang, and J. R. Williams, 1973, J. Chem. Phys. 58, 3155.

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

Species Tag: 41002	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Propyne, Carbon - 13 isotope on atom 1 $CH_3 C\ {}^{13}CH$		Author: R. L. Poynter Min. Int. = 3×10^{-5} nm^2MHz for J > 14	
Q (Spin-Rot., T = 300K) = 5596.11		J Max. = 80	Lines Listed = 822
Dipole Moments/Debye: μ_a = 0.750	μ_b =	μ_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 $CH_3\,^{13}CCH$		Author: R. L. Poynter	
		Min. Int. = 3×10^{-5} nm^2MHz for J > 14	
Q (Spin-Rot., T = 300K) = 5431.06		J Max. = 79	Lines Listed = 813
Dipole Moments/Debye: μ_a = 0.750	μ_b =	μ_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: ec. 1979
Species Name: Propyne, carbon - 13 isotope on atom 3 $H_3{}^{13}CCCH$		Author: R. L. Poynter Min. Int. = 3×10^{-5} nm^{2}MHz for J > 14	
Q (Spin-Rot., T = 300K) = 5580.65		J Max. = 80	Lines Listed = 821
Dipole Moments/Debye: μ_a = 0.750	μ_b =	μ_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_3 CCD		Author: R. L. Poynter Min. Int. = 3 x 10^{-5} nm^2MHz for J > 14	
Q (Spin-Rot., T = 300K) = 5956.732		J Max. = 82	Lines Listed = 800
Dipole Moments/Debye: μ_a = 0.750	μ_b =	μ_c =	
Rot. Const./MHz: A = 158590.0	B = 7788.158	C = B	

The experimental measurements are from J. S. Muenter and V. W. Laurie, 1966, J. Chem. Phys. 45, 855; L. F. Thomas, E. I. Sherrard, and J. Sheridan, 1955, Trans. Far. Soc. 51, 619.

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 Muenter 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 $CH_2D\ CCH$		Author: R. L. Poynter Min. Int. = 2×10^{-10} nm^2MHz	
Q (Spin-Rot., T = 300K) = 9982.44		J Max. = 15	Lines Listed = 223
Dipole Moments/Debye: μ_a = 0.750	μ_b = 0.	μ_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 $CH_3\ C\ ^{15}N$		Author: R. L. Poynter Min. Int. = 2×10^{-5} $nm^2 MHz$ for $J > 14$	
Q (Spin-Rot., T = 300K) = 15145		J Max. = 90	Lines Listed = 2755
Dipole Moments/Debye: μ_a = 3.919	μ_b =	μ_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. = 3×10^{-15} nm^2MHz	
Q (Spin-Rot., T = 300K) = 10322.9		J Max. = 29	Lines Listed = 835
Dipole Moments/Debye:	μ_a = 1.422	μ_b = 0	μ_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. Muenter, 1977, J. Chem. Phys. 67, 1576.
J. W. C. Johns, J. M. R. Stone, and G. Winnewisser, 1972, J. Mol. Spect. 42, 523.
H. R. Johnson and M. W. P. Strandberg, 1952, J. Chem. Phys. 20, 687.

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

Species Tag: 43001	Page 1 of 1	Version: 1	Date: Jan. 1980
Species Name: Ketene Deuterium isotope HDCCO		Author: R. L. Poynter	
		Min. Int. = 10^{-23} nm^2MHz	
Q (Spin-Rot., T = 300K) = 6682.68		J Max. = 29	Lines Listed = 886
Dipole Moments/Debye: μ_a = 1.422		μ_b = 0.	μ_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. = 4×10^{-5} nm^2MHz	
Q (Spin-Rot., T = 300K) = 255.515		J Max. = (60)	Lines Listed = 60
Dipole Moments/Debye: μ_a = 1.957	μ_b =	μ_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, 1963, 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}Si O		Author: R. L. Poynter	
		Min. Int. = 3×10^{-5} nm^2MHz	
Q (Spin-Rot., T = 300K) = 287.232		J Max. = 66	Lines Listed = 66
Dipole Moments/Debye: μ_a = 3.098	μ_b =	μ_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. Muenter, 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_3CHO		Author: R. L. Poynter Min. Int. = 6×10^{-9} nm^2MHz	
Q (Spin-Rot., T = 300K) = 12112.28		J Max. = 20	Lines Listed = 1347
Dipole Moments/Debye: μ_a = 2.550	μ_b = 0.870	μ_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. = 2×10^{-7} nm^2MHz	
Q (Spin-Rot., T = 300K) =		J Max. = 61	Lines Listed = 61
Dipole Moments/Debye: μ_a = .1608 μ_b = μ_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_3CHO		**Author:** H. M. Pickett **Min. Int. =** 10^{-10} nm^2MHz	
Q (Spin-Rot., T - 300K) = 12112.3		**J Max. =** 15	**Lines Listed =** 691
Dipole Moments/Debye: $\mu_a = 2.55$	$\mu_b = 0.870$	$\mu_c = 0$	
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_aP^2, P_aP^4, P_a^3, $P_a^3P^2$, and P_a^5 terms. The fit produced observed - calculated frequencies which were 3.5 times the experimental uncertainties in an rms sense. Calculated values of μ^2 S agree with those of Bauder et al. The reference energy is located at the J=0 level of the A state, but intensities are based on E state concentrations.

Species Tag: 45001	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Carbon Monosulfide Carbon - 13 isotope ^{13}CS		Author: R. L. Poynter Min. Int. = 3×10^{-5} nm^2MHz	
Q (Spin-Rot., T = 300K) = 270.652		J Max. = (62)	Lines Listed = 62
Dipole Moments/Debye: μ_a = 1.957	μ_b =		μ_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}Si O		Author: R. L. Poynter Min. Int. = 4×10^{-5} nm^2MHz	
Q (Spin-Rot., T = 300K) = 290.878		J Max. = 66	Lines Listed = 66
Dipole Moment/Debye: μ_a = 3.098	μ_b =	μ_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. Muenter, 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

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Version: 2

Date: Jan. 1981

Species Name: Formamide, NH_2CHO

Author: R. Poynter

Min. Int. = 10^{-8} below 120 GHz, 10^{-5} above 120 GHz nm^2MHz

Q (Spin-Rot., T = 300K) = 29155.55

J Max. = 30

Lines Listed = 3476

Dipole Moments/Debye: μ_a = 316.6 μ_b = 0.852 μ_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. Costain and J. M. Dowling, 1960, J. Chem. Phys. 32, 290.

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

W. H. Kirchhoff and D. R. Johnson, 1973, J. Mol. Spect. 45, 159.

S G. Kukolich and A. C. Nelson, 1971, Chem. Phys. Lett. 11, 383.

R. J. Kurland and E. B. Wilson, Jr., 1957, J. Chem. Phys. 27, 585.

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

Additional values of the partition function are:

T	Q
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 $C\ ^{34}S$		Author: R. L. Poynter Min. Int. = 3×10^{-5} nm^2MHz	
Q (Spin-Rot., T = 300K) = 259.665		J Max. = (61)	Lines Listed = 61
Dipole Moments/Debye: μ_a = 1.957		μ_b =	μ_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}Si O		Author: R. L. Poynter Min. Int. = 3 x 10^{-5} nm^2MHz	
Q (Spin-Rot., T = 300K) = 294.358		J Max. = 67	Lines Listed = 67
Dipole Moments/Debye: μ_a = 3.098	μ_b =	μ_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. Muenter, 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. = 8×10^{-10} nm^2MHz	
Q (Spin-Rot., T = 300K) = 5984.646		J Max. = 27	Lines Listed = 517
Dipole Moments/Debye: μ_a = 1.649	μ_b = 0.	μ_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. Muenter, 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. = 3×10^{-10} nm^2MHz	
Q (Spin-Rot., T = 300K) = 17010.5		J Max. = 20	Lines Listed = 1236
Dipole Moments/Debye: μ_a = 0.046	μ_b = 1.438	μ_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 x 10^{-10} nm^2MHz	
Q (Spin-Rot., T = 300K) = 8884.2		J Max. = 20	Lines Listed = 1888
Dipole Moments/Debye: μ_a = 1.396	μ_b = 0.260	μ_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. Hearns, 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. Muenter, 1968, J. Chem. Phys. 48, 4544).

Species Tag: 47001	Page 1 of 1	Version: 1	Date: Jan. 1980
Species Name: Thioformaldehyde Carbon - 13 isotope $H_2{}^{13}CS$		Author: R. L. Poynter Min. Int. = 2×10^{-9} nm^2MHz	
Q (Spin-Rot., T = 300K) = 6219.87		J Max. = 10	Lines Listed = 110
Dipole Moments/Debye:	μ_a = 1.649	μ_b = 0.	μ_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 $H\,^{13}COOH$		Author: R. L. Poynter Min. Int. = 10^{-10} nm^2MHz	
Q (Spin-Rot., T = 300K) = 8896.76		J Max. = 20	Lines Listed = 1194
Dipole Moments/Debye: μ_a = 1.396	μ_b = 0.260	μ_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. = 2×10^{-9} nm^{2}MHz	
Q (Spin-Rot., T = 300K) = 10531.19		J Max. = 20	Lines Listed = 628
Dipole Moments/Debye: μ_a = 1.396	μ_b = 0.260	μ_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. Deldalle, C. Samson, G. Steenbeckeliers, and R. Wertheimer, 1971, J. Mol. Structure, 9, 65.

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

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

Species Tag: 47004	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^2MHz	
Q (Spin-Rot., T = 300K) = 9954.87		J Max. = 20	Lines Listed = 612
Dipole Moments/Debye: μ_a = 1.396	μ_b = 0.260	μ_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 $^3\Sigma$ ground state		**Author:** H. M. Pickett **Min. Int.** = 10^{-6} nm^2MHz	
Q (Spin-Rot., T = 300K) = 850.099		**J Max.** = 50	**Lines Listed** = 330
Dipole Moments/Debye: μ_a = 1.55	μ_b =	μ_c =	
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

T	Q
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. = 4×10^{-6} nm^2MHz

Q (Spin-Rot., T = 300K) = 856.726

J Max. = 50

Lines Listed = 261

Dipole Moments/Debye: μ_a = 1.55 μ_b = μ_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 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:

T	Q
10K	17.341
30	69.781
60	155.452
100	271.644
150	417.628

Species Tag: 48003	Page 1 of 1	Version: 1	Date: Jan. 1980
Species Name: Thioformaldehyde Sulfur - 34 isotope $H_2C\ ^{34}S$		Author: R. L. Poynter Min. Int. = 3×10^{-9} nm^2MHz	
Q (Spin-Rot., T = 300K) = 6084.57		J Max. = 10	Lines Listed = 111
Dipole Moments/Debye: μ_a = 1.647	μ_b = 0.	μ_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 $^{16}O_3$		Author: R. L. Poynter and H. M. Pickett Min. Int. = 3×10^{-10} nm^2MHz	
Q (Spin-Rot., T = 300K) = 3378.28		J Max. = 40	Lines Listed = 1465
Dipole Moments/Debye: μ_a = 0.	μ_b = 0.5324	μ_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. Duterage, and M. J. Bellet, 1977, J. Quant. Spect. Radiat. Transfer 17, 519. Additional lines are cited in F. J. Lovas, 1978, J. Phys. Chem. Ref. Data 7, 1445.

Species Tag: 48005	**Page** 1 **of** 1	**Version:** 1	**Date:** Jan. 1981
Species Name: Ozone, ν_2 vib. state $^{16}O_3$, (010) state		**Author:** R. Poynter	
		Min. Int. = 10^{-8} below 120 GHz 10^{-5} above 120 GHz nm^2MHz	
Q (Spin-Rot., T = 300K) = 3367.8162		**J Max.** = 30	**Lines Listed** = 734
Dipole Moments/Debye: μ_a =		μ_b = 0.5324	μ_c =
Rot. Const./MHz: A = 108137.979		B = 13311.143	C = 11765.222

The ν_2 ozone lines were derived from a fit of the data given by M. J. C. Depannemaecker, B. Duterage, and M. J. Bellet, 1977, J. Quant. Spect. and Radiat. Transfer 17, 519. Additional lines are listed in F. J. Lovas, 1978, J. Phys. Chem. Ref. Data., 7, 1445.

Additional values of the partition function are:

T	Q
10	20.88
30	107.12
60	302.01
150	1191.47
200	1833.80

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

Species Tag: 48006	**Page** 1 **of** 1	**Version:** 1	**Date:** Dec. 1980
Species Name: Ozone, O_3 excited stretching states ν_1, ν_3 or (100) and (001)		**Author:** H. M. Pickett	
		Min. Int. = 10^{-8} nm^2MHz	
Q (Spin-Rot., T - 300K) = 6828.0		**J Max.** = 31	**Lines Listed** = 3686
Dipole Moments/Debye: μ_a = 0		μ_b = 0.5324	μ_c = 0
Rot. Const./MHz: A = 106626.6 104943.4		**B** = 13272.8 13229.8	**C** = 11763.1 11727.5

The rotational lines were determined by T. Tanaka and Y. Morino, 1970, J. Mol. Spec. 33, 538 and A. Barbe, et al., 1977, J. Mol. Spec. 64, 343. The rotational lines were fit with the Hamiltonian of Barbe, et al., in which the interaction terms were fixed to the values of Barbe, et al., but all centrifugal terms (up to sixth power in angular momentum) were fit. The zero of energy is 1042.08 cm^{-1} above the zero of energy for the ground state species. The ν states (100) have v = 1 and the ν_3 state (001) have v = 3 in the 940 quantum number format in the catalogue.

Species Tag: 50001	**Page** 1 of 1	**Version:** 1	**Date:** Dec. 1979
Species Name: Sulfur Monoxide Sulfur 34 isotope $^3\Sigma$ ground state ^{34}SO		**Author:** H. M. Pickett **Min. Int.** = 10^{-6} nm^2MHz	
Q (Spin-Rot., T = 300K) = 866.870		**J Max.** = 50	**Lines Listed** = 280
Dipole Moments/Debye: μ_a = 1.55		μ_b =	μ_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:

T	Q
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^{2}MHz	
Q (Spin-Rot., T = 300K) = 917.393		J Max. = 50	Lines Listed = 179
Dipole Moments/Debye: μ_a = 1.55	μ_b =	μ_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 μ was fixed at -156.51 MHz and $\mu(1)$ was set to zero. Both electric dipole and magnetic dipole transitions are listed in the catalogue. The data used is listed in E. Tiemann, 1974, J. Phys. Chem. Ref. Data. 3, 259.

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

T	Q
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}O Ozone ground state $^{16}O-^{18}O-^{16}O$		Author: H. M. Pickett & R. L. Poynter Min. Int. = 10^{-9} nm^{2}MHz	
Q (Spin-Rot., T = 300K) = 3525.63		J Max. = 40	Lines Listed = 1568
Dipole Moments/Debye: μ_a = 0.		μ_b = 0.5324	μ_c = 0.
Rot. Const./MHz: A = 98646.687		B = 13352.732	C = 11731.767

The catalog of symmetric ^{18}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 $^{16}O_3$ value.

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

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

Species Tag: 51001	Page 1 of 1	Version: 1	Date: Dec. 1979
Species Name: Cyanoacetylene HCCCN		Author: R. L. Poynter Min. Int. = 2×10^{-7} nm^2MHz	
Q (Spin-Rot., T = 300K) = 4123.26		J Max. = 99	Lines Listed = 154
Dipole Moments/Debye: μ_a = 3.599		μ_b =	μ_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 3.724D. 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: 51002	**Page** 1 **of** 1	**Version:** 2	**Date:** Oct. 1980
Species Name: Chlorine Monoxide $^2\Pi$ states ^{35}ClO $v = o$		**Author:** H. M. Pickett **Min. Int.** = 10^{-10} nm^2MHz	
Q (Spin-Rot., T - 300K) = 3291.80		J Max. = 87.5	Lines Listed = 2610
Dipole Moments/Debye: μ_a = 1.239 μ_b = μ_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, η_1, η_2, and η_3. The partition function was determined by a sum over states to F = 86 for both the Ω = 1/2 and Ω = 3/2 states. Other values are:

T	Q
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 $H^{13}CCN$		Author: R. L. Poynter Min. Int. = 2×10^{-7} nm^2MHz	
Q (Spin-Rot., T = 300K) = 4140.42		J Max. = 99	Lines Listed = 152
Dipole Moments/Debye: μ_a = 3.599		μ_b =	μ_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 $HC^{13}CCN$		Author: R. L. Poynter Min. Int. ~ 2×10^{-7} nm^2MHz	
Q (Spin-Rot., T = 300K) = 4140.82		J Max. = 99	Lines Listed = 146
Dipole Moments/Debye: μ_a = 3.599		μ_b =	μ_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 $H^{13}CCCN$		Author: R. L. Poynter Min. Int. = 2×10^{-7} nm^2MHz	
Q (Spin-Rot., T = 300K) = 4254.,5		J Max. = 99	Lines Listed = 144
Dipole Moments/Debye: μ_a = 3.599	μ_b =	μ_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, $HCCC^{15}N$		Author: R. L. Poynter Min. Int. = 4×10^{-6} $nm^2 MHz$	
Q (Spin-Rot., T = 300K) = 1415.581		J Max. = 99	Lines Listed = 99
Dipole Moments/Debye: μ_a = 3.599		μ_b =	μ_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} nm^2MHz	
Q (Spin-Rot., T = 300K) = 4443.03		J Max. = 99	Lines Listed = 156
Dipole Moments/Debye: μ_a = 3.724	μ_b =	μ_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, $HO^{35}Cl$

Author: R. Poynter

Min. Int. = $1.0x10^{-8}$ below 120 GHz, nm^2MHz
$10^{-5}mm^2$ MHz above this frequency

Q (Spin-Rot., T = 300K) = 9481.708
J Max. = 20
Lines Listed = 671

Dipole Moments/Debye: μ_a = 1.3 μ_b = 0.367 μ_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:

T	Q
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_2H_3CN		Author: R. L. Poynter Min. Int. = 10^{-9} nm^2MHz	
Q (Spin-Rot., T = 300K) = 26198.1		J Max. = 40	Lines Listed = 3697
Dipole Moments/Debye: μ_a = 3.68	μ_b = 1.25	μ_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 $^2\Pi$ states Chlorine - 37 isotope ^{37}ClO $\nu = o$		**Author:** H. M. Pickett **Min. Int. =** 10^{-10} nm^2MHz	
Q (Spin-Rot., T - 300K) = 3348.0		**J Max. =** 83	**Lines Listed =** 2645
Dipole Moments/Debye: μ_a = 1.239	μ_b =	μ_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, η_1, η_2, and η_3. The partition function was determined by a sum over states to F = 86 for both the Ω = 1/2 and Ω = 3/2 states. Other values are:

T	Q
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 $CH_2\ CH^{13}CN$		Author: R. L. Poynter Min. Int. = 4×10^{-9} nm^2MHz	
Q (Spin-Rot., T = 300K) = 26333.		J Max. = 10	Lines Listed = 118
Dipole Moments/Debye: μ_a = 3.68		μ_b = 1.25	μ_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

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Version: 1

Date: Jan. 1980

Species Name: Acrylonitrile

carbon - 13 isotope on atom 2

$CH_2\,^{13}CHCN$

Author: R. L. Poynter

Min. Int. = 3×10^{-9} nm^2MHz

Q (Spin-Rot., T = 300K) = 26665.

J Max. = 10

Lines Listed = 117

Dipole Moments/Debye: μ_a = 3.68 μ_b = 1.25 μ_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 $^{13}CH_2CHCN$		Author: R. L. Poynter Min. Int. = 3×10^{-9} nm^2MHz	
Q (Spin-Rot., T = 300K) = 27087.5		J Max. = 10	Lines Listed =
Dipole Moments/Debye: μ_a = 3.68		μ_b = 1.25	μ_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_2CDCN		Author: R. L. Poynter Min. Int. = 9×10^{-10} nm^2MHz	
Q (Spin-Rot., T = 300K) = 29697.8		J Max. = 10	Lines Listed = 322
Dipole Moments/Debye: μ_a = 3.68	μ_b = 1.25	μ_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, $HO^{37}Cl$

Author: R. Poynter

Min. Int. = 10^{-8} below 120 GHz; nm^{2}MHz
10^{-5}mm^{2}MHz above this frequency

Q (Spin-Rot., T = 300K) = 9657.239

J Max. = 20

Lines Listed = 673

Dipole Moments/Debye: μ_a = 1.3 μ_b = .367 μ_c =

Rot. Const./MHz: A = 613455.020 B = 14851.929 C = 14471.418

The comments made for $HO^{35}Cl$ (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 $HO^{35}Cl$. Quadrupole splittings were only computed up through J = 5, as for $HO^{35}Cl$.

Other values of the partition function are:

T	Q
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^{2}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: μ_a = 3.850	μ_b = 1.23	μ_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:

T	Q
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 $CH_3CH_2{}^{13}CN$		**Author:** R. L. Poynter **Min. Int.** = 10^{-9} below 160 GHz, 10^{-5} above 160 GHz $nm^2 MHz$	
Q (Spin-Rot., T = 300K) = 112465.7		J Max. = 10	Lines Listed = 1183
Dipole Moments/Debye: μ_a = 3.840	μ_b = 1.370	μ_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:

T	Q
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 $CH_3{}^{13}CH_2CN$		Author: R. L. Poynter Min. Int. = 10^{-9} below 160 GHz, 10^{-5} above 160 GHz nm^2MHz	
Q (Spin-Rot., T = 300K) = 113691.5		J Max. = 10	Lines Listed = 1252
Dipole Moments/Debye: μ_a = 3.840	μ_b = 1.370	μ_c = 0.	
Rot. Const./MHz: A = 27045.40	B = 4697.868	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:

T	Q
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 $^{13}CH_3CH_2CN$		**Author:** R. L. Poynter **Min. Int.** = 10^{-9} below 160 GHz 10^{-5} above 160 GHz nm^2MHz	
Q (Spin-Rot., T = 300K) = 115303.9		**J Max.** = 10	**Lines Listed** = 1183
Dipole Moments/Debye: μ_a = 3.840	μ_b = 1.370	μ_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:

T	Q
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** $CH_3CH_2C^{15}N$		Author: R. L. Poynter Min. Int. = 2×10^{-9} nm^2MHz	
Q (Spin-Rot., T = 300K) = 38458.		J Max. = 20	Lines Listed = 1621
Dipole Moments/Debye: μ_a = 3.840	μ_b = 1.370	μ_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.

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
$CH_2D\ CH_2CN$ - S

Author: R. L. Poynter

Min. Int. = 10^{-9} below 160 GHz
10^{-5} above 160 Ghz nm^2MHz

Q (Spin-Rot., T = 300K) = 118802.0
J Max. = 10
Lines Listed = 1166

Dipole Moments/Debye: μ_a = 3.840 μ_b = 1.370 μ_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. <u>41</u>, 333 and W. H. Kirchhoff and D. R. Johnson, 1973, J. Mol. Spect. <u>45</u>, 159. The measurements were taken from the following papers:

H. Mader, H. M. Heise, and H. Dreizler, 1973, Z. Naturforsch. <u>29a</u>, 164.

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

Additional values of the partition function are:

T	Q
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
CH_2DCH_2CN-a

Author: R. L. Poynter

Min. Int. 10^{-9} below 160 GHz, 10^{-5} above 160 GHz nm^2MHz

Q (Spin-Rot., T = 300K) = 121064.4 | **J Max.** = 10 | **Lines Listed** = 1286

Dipole Moments/Debye: μ_a = 3.840 μ_b = 1.370 μ_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:

T	Q
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. =** 4×10^{-7} nm^2MHz	
Q (Spin-Rot., T = 300K) = 1028.17		**J Max. =** 99	**Lines Listed =** 99
Dipole Moments/Debye: μ_a =	μ_b = .715	μ_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:

T	Q
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 $^{28}Si\ ^{32}S$		Author: R. L. Poynter Min. Int. = 9×10^{-6} nm^2MHz	
Q (Spin-Rot., T = 300K) = 688.940		J Max. = 97	Lines Listed = 97
Dipole Moments/Debye: μ_a = 1.730	μ_b =	μ_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.** = 4×10^{-7} nm^2MHz	
Q (Spin-Rot., T = 300K) = 1031.491		J Max. = 99	Lines Listed = 99
Dipole Moments/Debye: μ_a =		μ_b = 0.715	μ_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:

T	Q
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 $^{29}Si\ ^{32}S$		Author: R. L. Poynter Min. Int. = 9×10^{-6} nm^2MHz	
Q (Spin-Rot., T = 300K) = 701.830		J Max. = 98	Lines Listed = 98
Dipole Moments/Debye: μ_a = 1.730		μ_b =	μ_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: $OC^{34}S$, Carbonyl Sulfide ^{34}S isotope species		**Author:** R. L. Poynter **Min. Int.** = 4×10^{-7} nm^2MHz	
Q (Spin-Rot., T = 300K) = 1053.928		**J Max.** = 99	**Lines Listed** = 99
Dipole Moments/Debye: μ_a =	μ_b = .715	μ_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:

T	Q
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: ^{18}OCS, Carbonyl Sulfide ^{18}O isotopic modification		**Author:** R. L. Poynter	
		Min. Int. = 4 x 10^{-7} nm^{2}MHz	
Q (Spin-Rot., T = 300K) = 1096.031		**J Max. =** 99	**Lines Listed =** 99
Dipole Moments/Debye: μ_a =		μ_b = .715	μ_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:

T	Q
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 Silicon - 30 isotope ^{30}Si ^{32}S		Author: R. L. Poynter	
		Min. Int. = 8×10^{-6} nm^2MHz	
Q (Spin-Rot., T = 300K) = 714.275		J Max. = 99	Lines Listed = 99
Dipole Moments/Debye: μ_a = 1.730	μ_b =	μ_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 $^{28}Si\ ^{34}S$		Author: R. L. Poynter Min. Int. = 9×10^{-6} nm^{2}MHz	
Q (Spin-Rot., T = 300K) = 708.329		J Max. = 99	Lines Listed = 99
Dipole Moments/Debye: μ_a = 1.730		μ_b =	μ_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 HNO_3		Author: R. Poynter Min. Int. = 10^{-8} nm^2MHz	
Q (Spin-Rot., T - 300K) = 27912.921		J Max. = 40	Lines Listed = 7259
Dipole Moments/Debye: μ_a = 1.986		μ_b = .882	μ_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 v = 0, $^3\Sigma_g^-$ ground state		Author: H. M. Pickett Min. Int. = 4.0×10^{-9} nm^{2}MHz	
Q (Spin-Rot., T = 300K) = 965.37		J Max. = 35	Lines Listed = 34
Dipole Moments/Debye: μ_a =	μ_b = magnetic	μ_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. Specty. 75, 53. The calculational method used is from T. Amano and E. Hirota, 1974, J. Mol. Specty. 53, 346. For S_2, the parameter $\mu(1)$ 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_2		Author: R. L. Poynter Min. Int. = 5×10^{-9} nm^2MHz	
Q (Spin-Rot., T = 300K) = 5898.91		J Max. = 40	Lines Listed = 1902
Dipole Moments/Debye: μ_a = 0.	μ_b = 1.633	μ_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_5N		Author: R. L. Poynter Min. Int. = 2×10^{-7} nm^2MHz	
Q (Spin-Rot., T = 300K) = 4695.48		J Max. = 99	Lines Listed = 99
Dipole Moments/Debye: μ_a = 4.330		μ_b =	μ_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 $HCCCC\,^{13}CN$		Author: R. L. Poynter Min. Int. = 2×10^{-7} nm^2MHz	
Q (Spin-Rot., T = 300K) = 4742.326		J Max. = 99	Lines Listed = 99
Dipole Moments/Debye: μ_a = 4.330	μ_b =	μ_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 ^{13}CCN		Author: R. L. Poynter Min. Int. = 2×10^{-7} nm^2MHz	
Q (Spin-Rot., T = 300K) = 4699.78		J Max. = 99	Lines Listed = 99
Dipole Moments/ Debye: μ_a = 4.329		μ_b =	μ_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 $HCC^{13}CCCN$		Author: R. L. Poynter Min. Int. = 2×10^{-7} nm^2MHz	
Q (Spin-Rot., T = 300K) = 4700.345		J Max. = 99	Lines Listed = 99
Dipole Moments/Debye: μ_a = 4.329		μ_b =	μ_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 $CH^{13}CCCCN$		Author: R. L. Poynter Min. Int. = 2×10^{-7} nm^2MHz	
Q (Spin-Rot., T = 300K) = 4744.09		J Max. = 99	Lines Listed = 99
Dipole Moments/Debye: μ_a = 4.329		μ_b =	μ_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 ^{13}CCCCCN		Author: R. L. Poynter Min. Int. = 2×10^{-7} nm^{2}MHz	
Q (Spin-Rot., T = 300K) = 4820.96		J Max. = 99	Lines Listed = 99
Dipole Moments/Debye: μ_a 4.329		μ_b	μ_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 $HC_5{}^{15}N$		Author: R. L. Poynter Min. Int. = 2×10^{-7} nm^2MHz	
Q (Spin-Rot., T = 300K) = 4813.68		J Max. = 99	Lines Listed = 99
Dipole Moments/Debye: μ_a = 4.329		μ_b	μ_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 DC_5N		Author: R. L. Poynter Min. Int. = 2×10^{-7} nm^2MHz	
Q (Spin-Rot., T = 300K) = 4918.13		J Max. = 99	Lines Listed = 99
Dipole Moments/Debye: μ_a = 4.329		μ_b =	μ_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. <u>62</u>, 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 $H^{79}Br$		Author: R. L. Poynter & H. M. Pickett Min. Int. = 7×10^{-3} nm^2MHz	
Q (Spin-Rot., T = 300K) = 101.214		J Max. =	Lines Listed = 19
Dipole Moments/Debye: μ_a = 0.828	μ_b =	μ_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 $H^{81}Br$		Author: R. L. Poynter & H. M. Pickett Min. Int. = 7×10^{-3} nm^2MHz	
Q (Spin-Rot., T = 300K) = 101.257		J Max. =	Lines Listed = 19
Dipole Moments/Debye: μ_a = 0.828	μ_b =	μ_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^2MHz	
Q (Spin-Rot., T = 300K) = 3897.60		J Max. = 49	Lines Listed = 850
Dipole Moments/Debye: μ_a = 1.765	μ_b =	μ_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

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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^2MHz

Q (Spin-Rot., T = 300K) = 3913.9

J Max. = 49

Lines Listed = 850

Dipole Moments/Debye: μ_a = 1.794 μ_b = μ_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.