Submillimeter, Millimeter, and Microwave Spectral Line Catalogue

R.L. Poynter
H.M. Pickett

June 1, 1984

NASA
National Aeronautics and Space Administration
Jet Propulsion Laboratory
California Institute of Technology
Pasadena, California
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ABSTRACT

This report describes a computer accessible catalogue of submillimeter, millimeter, and microwave spectral lines in the frequency range between 0 and 10000 GHz (i.e., wavelengths longer than 30 μm). The catalogue can be used as a planning guide or as an aid in the identification and analysis of observed spectral lines. The information listed for each spectral line includes the frequency and its estimated error, the intensity, lower state energy, and quantum number assignment.

The catalogue has been constructed by using theoretical least squares fits of published spectral lines to accepted molecular models. The associated predictions and their estimated errors are based upon the resultant fitted parameters and their covariances. Future versions of this catalogue will add more atoms and molecules and update the present listings (151 species) as new data appear.

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

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

New Species, Rev. 2 (18)

<table>
<thead>
<tr>
<th>TAG NAME</th>
<th>TAG NAME</th>
</tr>
</thead>
<tbody>
<tr>
<td>13002 CH</td>
<td>29004 HC0</td>
</tr>
<tr>
<td>17004 NH3-V2</td>
<td>29005 NNH+</td>
</tr>
<tr>
<td>20001 D20</td>
<td>30009 NND+</td>
</tr>
<tr>
<td>25001 CCH</td>
<td>33001 HO2</td>
</tr>
<tr>
<td>26001 CN</td>
<td>46006 NO2</td>
</tr>
<tr>
<td>26002 CN-V1</td>
<td>48007 03-2V2</td>
</tr>
</tbody>
</table>

Revised Species, Rev. 2 (30)

<table>
<thead>
<tr>
<th>TAG NAME</th>
<th>TAG NAME</th>
</tr>
</thead>
<tbody>
<tr>
<td>16001 O-ATOM</td>
<td>30002 HC-13-0+</td>
</tr>
<tr>
<td>17001 OH</td>
<td>30003 DCO+</td>
</tr>
<tr>
<td>17002 NH3</td>
<td>31001 HCO-18+</td>
</tr>
<tr>
<td>18001 OD</td>
<td>32001 02</td>
</tr>
<tr>
<td>18003 H2O</td>
<td>32002 02-V1</td>
</tr>
<tr>
<td>18005 H2O-V2</td>
<td>34001 0-18-0</td>
</tr>
<tr>
<td>19001 HO-18</td>
<td>41005 CH3CCU</td>
</tr>
<tr>
<td>19002 HD0</td>
<td>44001 CS</td>
</tr>
<tr>
<td>27001 HCN</td>
<td>44002 S10</td>
</tr>
<tr>
<td>29002 HCO+</td>
<td>45001 C-13-S</td>
</tr>
</tbody>
</table>

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

New Species, Rev. 1 (9)

<table>
<thead>
<tr>
<th>TAG NAME</th>
<th>TAG NAME</th>
</tr>
</thead>
<tbody>
<tr>
<td>18004 NH2D</td>
<td>44005 CH3CHO-E</td>
</tr>
<tr>
<td>18005 H2O-V2</td>
<td>48005 03-V2</td>
</tr>
<tr>
<td>34004 H2O2</td>
<td>48006 03-V1,3</td>
</tr>
</tbody>
</table>

Revised Species, Rev. 1 (24)

<table>
<thead>
<tr>
<th>TAG NAME</th>
<th>TAG NAME</th>
</tr>
</thead>
<tbody>
<tr>
<td>17002 NH3</td>
<td>34001 0-18-0</td>
</tr>
<tr>
<td>18002 N-15-H3</td>
<td>34002 H2S</td>
</tr>
<tr>
<td>18003 H2O</td>
<td>34003 PH3</td>
</tr>
<tr>
<td>29003 CH2NH</td>
<td>45003 NH2CHO</td>
</tr>
<tr>
<td>30007 CH2ND</td>
<td>51002 CL0</td>
</tr>
<tr>
<td>32001 02</td>
<td>53002 CL-37-0</td>
</tr>
<tr>
<td>32002 02-V1</td>
<td>55001 C2H5CN</td>
</tr>
<tr>
<td>32003 CH3OH</td>
<td>56001 CH3CH2C-13-N</td>
</tr>
</tbody>
</table>

iv
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    (listed in order of species tag)
I. Introduction

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

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

The catalogue is available as a magnetic data tape recorded in card images, with one card image per spectral line. The authors will reproduce the catalogue onto a tape furnished by the user without charge on a limited basis. The format of the data is given in Section II. Section III gives conversions between different measures of spectral line intensity. General comments on the precision of the spectral line positions and intensities are given in Section IV, while species specific comments are reserved for Section VI. Section V gives the format of quantum numbers as they appear in the catalogue. Documentation for each molecular or atomic species is listed in Section VI in order of the "species tag". This tag is a six digit number in which the three most significant digits represent the mass number of the molecule or atom and the last three digits are an accession number for the given mass. Usually there is a separate tag for each vibration-electronic state of a particular molecule.

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

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

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

(F13.4, F8.4, F8.4, I2, F10.4, I3, I7, I4, 612, 612, X)

FREQ: Frequency of the line in MHz.
ERR: Estimated or experimental error of FREQ in MHz.
LGINT: Base 10 logarithm of the integrated intensity in units of \( \text{nm}^2 \text{ MHz at 300 K} \). (See Section III for conversions to other units.)
DR: Degrees of freedom in the rotational partition function (0 for atoms, 2 for linear molecules, 3 for non-linear molecules).
ELOW: Lower state energy in cm\(^{-1}\) relative to the ground state.
GUP: Upper state degeneracy.
TAG: Species tag or molecular identifier. A negative value flags that the line frequency has been measured in the laboratory. The absolute value of TAG is then the species tag and ERR is the reported experimental error. The three most significant digits of the species tag are coded as the mass number of the species as explained above.
QNFORM: Identifies the format of the quantum numbers given in the field QN. These quantum number formats are given in Section V. (They are different from previous editions.)
QN': Quantum numbers for the upper state coded according to QNFORM.
QN'': Quantum numbers for the lower state.
The catalogue data tape also contains a second file with a species directory. Each element of this directory is an 80 character record with the following format:

```
TAG, NAME, NLINE, QLOG, VERSION
(I6, X, A14, I5, 7F7.4, I2)
```

**NAME:** an ASCII name for the species

**NLINE:** number of lines in catalogue

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

**VERSION:** version of the calculation for this species in the catalogue.
Physical Format of Tape

Density: 800 or 1600 bytes/inch on 9 tracks

Encoding: ASCII

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

First file (catalogue):

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

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

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

Second file (directory):

Blocking: 80 characters per block

Length: 151 blocks followed by end of file mark

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

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

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

\[
I_{ba}(T) = \left( \frac{8s^3}{3hc} \right) v_{ba} \times S_{ba} \mu_x^2 \left[ \exp \left( \frac{-E''}{kT} \right) - \exp \left( \frac{-E'}{kT} \right) \right] / Q_{rs} \tag{1}
\]

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

\[
I_{ba}(T) = I_{ba}(300K) \left[ Q_{rs}(300)/Q_{rs}(T) \right] \left[ \exp( -E''/kT ) - \exp( -E'/kT ) \right] / \left[ \exp( -E''/k*300K ) - \exp( -E'/k*300K ) \right] \tag{2}
\]

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

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

(3)

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

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

(4)

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

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

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

(5)

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

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

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

(6)

\[
\equiv I_{ba}(300K) \nu_{ba} [Q_{RS}(300K)/g'] \exp[E'/k*300K] \times 1.748 \times 10^{-9} \text{ sec}^{-1}
\]  

(6a)

in which \( g' \) is the degeneracy of the upper state. The value of \( g' \) is listed as part of the spectral line information in the catalogue. Values of \( Q_{RS} \) are listed in Section VI.
IV. General Comments on Precision

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

\[ \varepsilon_n^2 = \sum_{kj} \frac{3\nu_n}{\partial p_k} \frac{3\nu_n}{\partial p_j} V_{kj} \]  

(7)

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

\[ (V^{-1})_{kj} = \sum_m \frac{3\nu_m}{\partial p_k} \frac{3\nu_m}{\partial p_j} \varepsilon_m^{-2} \]  

(8)

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

The experimental uncertainties generally given in the literature vary from 1.6 \( \sigma \) estimates to 3 \( \sigma \) estimates and are more usually "guesstimates". Unfortunately, many authors do not even report their experimental uncertainties. Therefore, the expected errors in predicted lines obtained from fits based on such data will usually reflect this ambiguity in laboratory uncertainties through Eq. (7) and (8). In some cases, the quality of the least squares fit of the parameters to the experimental lines can be a guide to the statistical nature of the experimental uncertainties. Whenever possible, the expected errors in this catalog will reflect an expected 95% confidence interval based on the model used to fit the data. However, the errors can be different from this design goal by factors of three just due to the quality of input error estimates. Lines with an expected error greater than 1 GHz have been dropped from the catalogue.
The expected errors can only be computed relative to the model used. There are at least two ways the model can be "wrong" for the predicted frequencies. First, higher-order centrifugal distortion terms may no longer be negligible for the predicted frequencies. This effect will generally be important for lines of higher J or K than the laboratory-determined data set. In a sense, the predictions are then a form of extrapolation rather than interpolation and are therefore more suspect. A second factor leading to discrepancies in the predicted frequencies comes from "resonances". These resonances come from a near overlap of energy states that are coupled by elements of the Hamiltonian matrix. Poor predictability comes when these elements are neglected in the model or are treated inadequately by some form of perturbation theory. Such a neglect of coupling elements is always necessary at some level in any practical calculation. A major contributing problem is that often the existing data set is not sensitive to the parameters which are needed to characterize the resonances.

Precision in the intensity estimates is generally less critical than precision in the frequency. Contributing to intensity uncertainty are errors in the dipole moment, errors in the line strength, errors in the rotation-spin partition function. (The vibration-electronic partition function does not enter directly because the catalogue intensities are defined on the basis of concentrations of the given vibration-electronic state.) Dipole moment errors come directly from the experimental determination and indirectly from the J dependence of the dipole moment due to centrifugal mixing of vibrational states. Line strength errors can come from deficiencies in the model Hamiltonian and are particularly severe when resonances have been inadequately accounted for. Partition function errors are relatively benign but can become significant if the classical formulae are used at low temperatures for small molecules. With the exception of unanticipated resonances and poorly determined dipole moments, worst case errors in the intensity will generally be at the 1% level or lower.
There are many molecular models that are found in the literature. In principle, a very general model should be able to treat every possible case. In practice this is hardly ever done. A specific model is most frequently used for every case, mainly because every author starts with a different viewpoint of the problem. In our case, we have tried to develop a program that will treat a wide variety of problems with a minimum of adaptation. This saves a great deal of time in the initial set up, and provides a uniform output format for the final results. Most important, the basic treatment is the same for every molecule, regardless of the model used, so that a high degree of consistency can be maintained, facilitating comparisons between different molecules. The particular model needed to analyze a specific problem is treated as a subroutine. For certain problems, this subroutine can be quite simple, which for others it is more complex.

Simple singlet sigma diatomic, linear and symmetric rotor molecules are treated together. Asymmetric rotors with and without various complicating interactions are treated exactly, without any perturbation expansions. This is done by employing the Hamiltonian operators to generate the matrix elements. All possible operators can be used, so any conceivable interaction can be included initially.

Comments on specific models are given for the individual species.
V. Format of Quantum Numbers

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

\[ QNFORM = Q \times 100 + H \times 10 + NQN \]

in which Q determines the type of molecule (see table below), H determines the coding of half integer quantum numbers, and NQN is the number of quantum numbers for each state. Q is defined so that MOD(Q, 5) is the number of primary quantum numbers. If NQN is greater than the number of primary quantum numbers, the degeneracy is derived from the last quantum number. Otherwise the degeneracy is derived from the first quantum number. H is a 3 bit binary code for the existence of half integer quantum numbers for the last three quantum numbers. The least significant bit refers to quantum number NQN and is 1 if the last quantum number is half integer. In the catalogue all half integer quantum numbers are rounded up to the next integer.
<table>
<thead>
<tr>
<th>type</th>
<th>Q</th>
<th>ITD</th>
<th>quantum order</th>
</tr>
</thead>
<tbody>
<tr>
<td>atom</td>
<td>0</td>
<td>0</td>
<td>(J),(F),.....</td>
</tr>
<tr>
<td>linear - Σ</td>
<td>1</td>
<td>2</td>
<td>N,(J),(F1),(F2),(F)</td>
</tr>
<tr>
<td>linear - case b</td>
<td>2</td>
<td>2</td>
<td>N,A,(F1),(F2),(F)</td>
</tr>
<tr>
<td>linear - case a-2S+1 odd</td>
<td>3</td>
<td>2</td>
<td>J,Ω,A,(F1),(F2),(F)</td>
</tr>
<tr>
<td>linear - case a-2S+1 even</td>
<td>3</td>
<td>2</td>
<td>J+1/2,Ω+1/2,A,(F1),(F2),(F)</td>
</tr>
<tr>
<td>symmetric rotor</td>
<td>2</td>
<td>3</td>
<td>N,K,(J),(F1),(F2),(F)</td>
</tr>
<tr>
<td>symmetric rotor with vibration</td>
<td>13</td>
<td>3</td>
<td>N,K,v,(J),(F1),(F)</td>
</tr>
<tr>
<td>asymmetric rotor</td>
<td>3</td>
<td>3</td>
<td>N,K-1,K+1,(J),(F1),(F)</td>
</tr>
<tr>
<td>asymmetric rotor with vibration</td>
<td>14</td>
<td>3</td>
<td>N,K-1,K+1,v,(J),(F)</td>
</tr>
</tbody>
</table>

conventions:
1. Half integer quantum numbers rounded up
2. The sign of Λ and K refers to parity under inversion not sign of operator. NOTE: Wang symmetry is related to parity by (-1)^J+S+e or (-1)^N+e where e=0 for all states except Σ^- states
3. Quantum numbers in parentheses optional
VI. Documentation by Species

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

\[ 10^{\text{LGINT}} > 10^{\text{LOGSTRO}} + (\nu/300 \text{ GHz})^2 \times 10^{\text{LOGST1}} \]

A blank entry for LOGSTRI means that the second term was not included. The partition functions listed (Q) include rotation and spin statistics but usually do not include vibrational corrections. (Exceptions are H2O and O3.) Calculation of Q is based on a sum over states. At higher temperatures, the sum-over-states calculation is replaced by a classical calculation when the latter is larger due to a limited number of states in the catalogue. The spin statistics included are only a partial set but are consistent with the intensities in the catalogue.

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

<table>
<thead>
<tr>
<th>Element</th>
<th>log (rel. abundance)</th>
<th>log (rel. abundance)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^1\text{H}$</td>
<td>0.</td>
<td>$^{29}\text{Si}$</td>
</tr>
<tr>
<td>$^2\text{H}$</td>
<td>-3.824</td>
<td>$^{30}\text{Si}$</td>
</tr>
<tr>
<td>$^{12}\text{C}$</td>
<td>0.</td>
<td>$^{32}\text{S}$</td>
</tr>
<tr>
<td>$^{13}\text{C}$</td>
<td>-1.955</td>
<td>$^{33}\text{S}$</td>
</tr>
<tr>
<td>$^{14}\text{N}$</td>
<td>0.</td>
<td>$^{34}\text{S}$</td>
</tr>
<tr>
<td>$^{15}\text{N}$</td>
<td>-2.432</td>
<td>$^{35}\text{Cl}$</td>
</tr>
<tr>
<td>$^{16}\text{O}$</td>
<td>0.</td>
<td>$^{37}\text{Cl}$</td>
</tr>
<tr>
<td>$^{17}\text{O}$</td>
<td>-3.432</td>
<td>$^{79}\text{Br}$</td>
</tr>
<tr>
<td>$^{18}\text{O}$</td>
<td>-2.690</td>
<td>$^{81}\text{Br}$</td>
</tr>
<tr>
<td>$^{28}\text{Si}$</td>
<td>-0.035</td>
<td></td>
</tr>
</tbody>
</table>
Species List

001 H-ATOM 32002 02-V1
2001 D-ATOM 32003 CH3OH
3001 HD 32004 H2O
12001 C-ATOM 33001 H2
13001 C-13-ATOM 34001 O-18-O
13002 CH 34002 H2S
14001 N-ATOM 34003 PH3
14002 N-ATOM-D-STATE 34004 H2J2
16001 O-ATOM 35001 HDS
17001 OH 36001 HCl
17002 NH3 38001 HCl-37
17003 CH3 40001 CH3CH
17004 NH3-V2 41001 CH3CN
18001 N-15-H3 42001 CH3CN-15
18002 H2O 43001 CH2CO
18003 H2O-V2 44001 CH3CHO
19001 HO-18 45001 C-13-S
20001 HDO 46001 CH3CHO
25001 CH4 47001 HC1-13-S
26001 CN-V1 48001 H2S
27001 HCN 49001 HCN
27002 HNC 50001 H2CO
28001 CO 50002 H2CO
28002 HC-13-N 51001 HNCN
28003 HCN-15 52001 HCCCN
28004 DCN 53001 HCCCN
28005 HNC-13 54001 HCCCN
28006 HN-15-C 55001 HCCCN
28007 DNC 56001 HCCCN
29001 C-13-O 57001 HCCCN
29002 HCO+ 58001 HCCCN
29003 CH2NH 59001 HCCCN
29004 HCO 60001 HCCCN
29005 NH+ 61001 HCCCN
30001 CO-18 62001 HCCCN
30002 HC-13-O+ 63001 HCCCN
30003 DC0+ 64001 HCCCN
30004 H2CO 65001 HCCCN
30005 C-13-H2NH 66001 HCCCN
30006 CH2N-15-H 67001 HCCCN
30007 CH2ND 68001 HCCCN
30008 NO 69001 HCCCN
30009 ND+ 70001 HCCCN
31001 HCO-18+ 71001 HCCCN
31002 H2C-13-O 72001 HCCCN
32001 O2 73001 HCCCN

-14-
The atomic hydrogen line at 21 cm has been measured to a precision of 0.001 Hz (L. Essen, R. W. Donaldson, M. J. Bangham, and E. G. Hope, 1971, Nature 229, 110). The average spontaneous emission lifetime of the three $F = 1$ states is $2.876 \times 10^{-15}$ sec$^{-1}$.
Species Tag: 2001  
Version: 1  
Date: Oct 1979  
Contributor: H. M. Pickett

| Lines Listed | Q(300.) | 6. |
| Max. Frequency | 0.3 GHz | Q(225.) | 6. |
| LOGSTR | -10.3 | Q(75.) | 6. |
| LOGSTR1 | | Q(37.5) | 6. |
| Isotope Correction | -3.824 | Q(18.25) | 6. |
| Minimum Energy | 0 cm\(^{-1}\) | Q(9.375) | 6. |

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

The atomic deuterium line at 327 MHz has been measured to an accuracy of 0.002 Hz (D. J. Wineland and N. F. Ramsey, 1972, Phys. Rev. A 5, 821). The average spontaneous emission lifetime for the four \(F = 3/2\) states is \(4.695 \times 10^{-17}\) sec\(^{-1}\).
Species Tag: 3001
Species Name: HD

Version: 1
Date: Oct. 1979
Contributor: H. M. Pickett

Lines Listed = 1
Max. Frequency = 2676. GHz
Max. J = 1
LOGSTR = -5.6
LOGSTRH = 0.
Isotope Correction = -3.523
Minimum Energy = 0. cm⁻¹

Dipoles:
μ(a) = A
μ(b) = 0.000585
μ(c) = C

The dipole moment is from M. Trefler and H. P. Gush, 1968, Phys. Rev. Letters, 20, 703. The rotational constant is from R. A. Durie and G. Herzberg, 1960, Can. J. Phys. 38, 806. The frequency and its error limits were obtained from the difference of the S₁ (0) and R₁ (1) transitions listed by A. McKellar, 1974, Can. J. Phys. 52, 1144.
The lines of atomic carbon have been measured by Laser Magnetic Resonance (R. J. Saykally and K. M. Evenson, 1980, Ap. J. 238, L107.) Intensities were calculated using the free electron g factor.
Species Tag: 13001  
Species Name: Carbon atom  
Version: 1  
Date: Oct 1979  
Contributor: H. M. Pickett

Lines Listed = 7  
Max. Frequency = 810. GHz  
Max. J = 7  
LOGSTR = -16.  
LOGSTR1 =  
Isotope Correction = -1.955  
Minimum Energy = 0. cm⁻¹  
Dipoles:  
\( \mu(a) = \) A  
\( \mu(b) = \) B  
\( \mu(c) = \) C

The fine structure intervals of \( ^{12}\text{C} \) were multiplied by 0.999992967 to account for the isotope effect on the Rydberg constant. The hyperfine intervals of G. Wolber, H. Figger, R. A. Haberstroh and S. Penselin, 1969, Physics Letters A29, 461, were then used to compute the line frequencies. Intensities were calculated using the free electron g value.
<table>
<thead>
<tr>
<th>Species Tag:</th>
<th>13002</th>
<th>Species Name: CH radical ( \Sigma_{\Pi} ) states</th>
</tr>
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<tbody>
<tr>
<td>Version:</td>
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<tr>
<td>Date:</td>
<td>Feb 1984</td>
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<td>Contributor:</td>
<td>H. M. Pickett</td>
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<td>Lines Listed</td>
<td>= 324</td>
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<tr>
<td>Dipoles:</td>
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</tr>
<tr>
<td></td>
<td>( \mu(b) = )</td>
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</tr>
<tr>
<td></td>
<td>( \mu(c) = )</td>
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</table>


The hyperfine transitions of atomic nitrogen at 14.6 and 26.1 MHz were obtained from J. M. Hirsch, G. H. Zimmerman, III, D. J. Larson, and N. F. Ramsey, 1977, Phys. Rev. A 16, 484. Intensities were calculated using the experimental $g_J$ value.
Species Tag: 14002  Species Name: N-atom $^2$D state
Version: 2
Date: Aug 1963
Contributor: H. M. Pickett

Lines Listed = 6  Q(300.) = 29.51
Max. Frequency = 261. GHz  Q(225.) = 29.35
Max. J = 2.5  Q(150.) = 29.03
LOGSTR = -49.  Q(75.) = 28.15
LOGSTR1 = 26.58
Isotope Correction = 0.  Q(18.25) = 24.13
Minimum Energy = 19223. cm$^{-1}$  Q(9.375) = 21.12

The $^2$D$_{5/2}$ state is 19223 cm$^{-1}$ above the ground $^4$S$_{3/2}$ state (C. E. Moore, 1949, Atomic Energy Levels I, Nat. Bureau of Stds.). The $^2$D$_{3/2}$ - $^2$D$_{5/2}$ 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 $^2$D states to the $^4$S states is $1.06 \times 10^{-6}$ sec$^{-1}$. In contrast, the spontaneous emission rate from $^2$D$_{3/2}$ $F = 5/2$ to $^2$D$_{5/2}$ $F = 7/2$ is $3.15 \times 10^{-9}$ sec$^{-1}$. 

-22-
The 68 cm\(^{-1}\) J = 1-2 and the 158.3 cm\(^{-1}\) J=0-1 lines of oxygen have been measured by laser Magnetic Resonance (R. J. Saykally and K. M. Evenson, 1979, J. Chem Phys. 71, 1564). Intensities were calculated using the free electron g factor.

---

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

<table>
<thead>
<tr>
<th>Lines Listed</th>
<th>Max. Frequency</th>
<th>Max. J</th>
<th>LOGSTR</th>
<th>LOGSTR1</th>
<th>Isotope Correction</th>
<th>Minimum Energy</th>
<th>Dipoles: (\mu(a))</th>
<th>Dipoles: (\mu(b))</th>
<th>Dipoles: (\mu(c))</th>
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<tr>
<td>2</td>
<td>3000 GHz</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>A</td>
<td>B</td>
<td>C</td>
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Q(300.) = 6.7407  
Q(225.) = 6.3243  
Q(150.) = 5.7705  
Q(75.) = 5.1568  
Q(37.5) = 5.0  
Q(18.25) = 5.015  
Q(9.375) = 5.000
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<tr>
<td>Date:</td>
<td>May 1983</td>
<td></td>
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<tr>
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<tr>
<td>LOGSTR1</td>
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<tr>
<td>Minimum Energy</td>
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<tr>
<td>Dipoles:</td>
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<tr>
<td>(\mu(a))</td>
<td>1.667</td>
<td>(A)</td>
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<td>(\mu(b))</td>
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<td>(B) = 556141.</td>
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<tr>
<td>(\mu(c))</td>
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<td>(C)</td>
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</table>

The microwave data are reported in R. A. Beaudet and R. L. Poynter, 1978, J. Phys. Chem. Ref. Data 7, 311. The predictions of the rotational lines of J. M. Brown et al, Astrophysical J. 258, 899 were included in the fit. The calculation involved fitting the spectra to effective parameters for the two \(\Pi\) states.
The computational method and most of the microwave data are given in R. L. Poynter and R. K. Kakar, 1975, Ap. J. Suppl. 29, 87. Additional microwave transitions have been reported by B. V. Shinha and P. D. P. Smith, 1980, J. Mol. Spectrosc. 80, 231.

The rotational transitions and energy levels were taken from R. Poynter and J. S. Margolis, 1983, Mol. Phys. 48, 401. This analysis was based on a very extensive set of accurate v2 measurements reported by R. Poynter and J. S. Margolis, 1984, Mol. Phys. 51, 393, and upon a series of "forbidden" transitions in the v4 band, reported by E. A. Cohen, W. H. Weber, R. L. Poynter, and J. S. Margolis, 1983, Mol. Phys. 50, 727. The work of Cohen, et al. allowed the C, Dk, Hk, and Lk constants to be determined, thus fixing the energy level scale. The J = 1 + 0, k = 0 rotational transition was taken from P. Helminger, F. C. DeLucia, and W. Gordy, 1971, J. Mol. Spectr. 39, 94. Because of the important applications of these rotational lines, the upper frequency limit has been extended to 335 cm⁻¹ (9.5 THz). Hyperfine splittings have not been included.
Species Tag: 17003
Species Name: CH₃D
Version: 1
Date: Feb 1980
Contributor: R. L. Poynter

Lines Listed = 80
Max. Frequency = 3000. GHz
Max. J = 13
LOGSTR = -8
LOGSTRI = 0
Isotope Correction = -3.222
Minimum Energy = 0. cm⁻¹
Dipoles: \( \mu(a) = 0.0056 \)
\( \mu(b) = 0 \)
\( \mu(c) = 0 \)

Q(300.) = 402.17
Q(225.) = 315.14
Q(150.) = 142.69
Q(75.) = 51.09
Q(37.5) = 18.47
Q(18.25) = 7.03
Q(9.375) = 2.98

Species Tag: 17004
Species Name: NH₃, v₂ - 010 state
Version: 1
Date: Mar 1984
Contributor: R. L. Poynter

Lines Listed = 442
Max. Frequency = 11600 GHz
Max. J = 17
LOGSTR = -12
LOGSTRI =
Isotope Correction =
Minimum Energy = 0. cm⁻¹
Dipoles: 


The transition dipole moment was reported by B. J. Orr and T. Oka, 1977, J. Mol. Spect. 66, 302.
Species Tag: 18001  
Species Name: OD

Version: 1
Date: May 1983
Contributor: H. M. Pickett

Hydroxyl radical, deuterium isotope

Lines Listed = 912
Max. Frequency = 100000. GHz
Max. J = 15.5
LOGSTR = -10.
LOGSTR1 = -10
Isotope Correction = -3.824
Minimum Energy = 0. cm⁻¹
Dipoles:
  μ(a) = 1.653
  μ(b) = 0.
  μ(c) = 0.

Q(303.) = 212.42
Q(225.) = 153.388
Q(150.) = 97.477
Q(75.) = 48.966
Q(37.5) = 30.896
Q(18.25) = 25.020
Q(9.375) = 24.010

The microwave data are reported in R. A. Beaudet and R. L. Poynter, 1978, J. Phys. Chem. Ref. Data 7, 311. Additional data are reported in J. M. Brown and J. E. Schubert, 1982, J. Mol. Spec. 95, 194. Predictions of the rotational lines were included in the fit. The calculation involved fitting the spectra to effective parameters for the two Π states.
Species Tag: 18002
Version: 2
Date: Jan 1981
Contributor: R. L. Poynter

Species Name: Ammonia, $^{15}\text{NH}_3$

15 nitrogen isotope

Lines Listed = 235
Max. Frequency = 3000. GHz
Max. $J$ = 20
LOGSTR = -17
LOGSTR1 = 0.
Isotope Correction = -2.432
Minimum Energy = 0. cm$^{-1}$

Quanta:
$Q(300.) = 575.84$
$Q(225.) = 451.23$
$Q(150.) = 206.21$
$Q(75.) = 74.71$
$Q(37.5) = 27.669$
$Q(18.25) = 11.277$
$Q(9.375) = 5.415$

Dipoles:
$\mu(a) = 0$
$\mu(b) = 0.
\mu(c) = 1.476$

The same computational method was used here as for $^{14}\text{NH}_3$. These lines are based upon the precision molecular beam measurements by S. G. Kukolich, 1967, Phys. Rev. 156, 83 and 1968, Phys. Rev. 172, 59, and upon the most recent microwave measurements of H. Sasada, 1980, J. Mol. Spect. 83, 15. The energy levels were computed from the recent far IR measurements of M. Carlotti, A. Trombetti, B. Velino, and J. Vrbancich, 1980, J. Mol. Spect. 83, 401. The C rotational constant was assumed to be the same as in $^{14}\text{NH}_3$.

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

-29-
Species Tag: 18003  
Species Name: H₂O  
Version: 3  
Date: Dec 1983  
Contributor: R. L. Poynter and H. M. Pickett

<table>
<thead>
<tr>
<th>Lines Listed</th>
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<th>Max. J</th>
<th>LOGSTR</th>
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<th>Isotope Correction</th>
<th>Minimum Energy</th>
<th>Dipole:</th>
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<td>0.</td>
<td>0. cm⁻¹</td>
<td>0</td>
<td>3, 211</td>
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The data set used in this new fit is based upon both the microwave and submillimeter lines reported by J. K. Messer, F. C. DeLucia and P. Helming (1984), J. Mol. Spect. (in press), and on 720 ground state combination differences derived from the v2 data of G. Guelachvilli (1983), J. Opt. Soc. Am. 73, 137. All of the submillimeter/microwave lines fit to within an 0.05 MHz RMS deviation, while the combination differences fit to within an RMS deviation of 0.00015 cm⁻¹ (4 MHz). Because of the importance of this molecule in many applications, the upper frequency limit of the predicted lines has been extended to 10. THz (300 cm⁻¹). The details of the analysis will be reported shortly. The dipole moment is from T. R. Dyke and J. S. Muentor, (1973), J. Chem. Phys. 59, 3125. Other references are given in F. C. DeLucia, P. Helming and W. H. Kirchhoff, (1974), J. Phys. Chem. Ref. Data, 3, 211.

The partition function includes contributions from the v2 state.
<table>
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<th>Species Tag:</th>
<th>18004</th>
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<td>Date:</td>
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<table>
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<td>Minimum Energy</td>
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<td>Q(9.375)</td>
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<td>μ(a)</td>
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<td>110797</td>
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</table>

The experimental lines were measured by F. C. DeLucia and P. Helminger, 1975, J. Mol. Spec. 54, 200 and by E. A. Cohen and H. M. Pickett, 1982, J. Mol. Spect. 93, 83. The dipole moments and quadrupole splitting were also determined by Cohen and Pickett. The Hamiltonian included terms up to 8-th power in angular momentum as well as a PₐPₜₐ+PₜₐPₐ interaction term. The relative sign of the dipoles is determinable and is important for intensities because of mixing by the interaction term.

The partition function is the same as that used for the ground state.
Species Tag: 19001
Species Name: HO-18 Hydroxyl radical

Version: 2
Date: May 1983
Contributor: H. M. Pickett

Lines Listed = 295
Max. Frequency = 10000. GHz
Max. J = 13.5
LOGSTR = -10.
LOGSTR1 = -10.
Isotope Correction = -2.690
Minimum Energy = 0. cm⁻¹
Dipoles: μ(a) = 1.667
μ(b) =
μ(c) =
Q(300.) = 81.945
Q(225.) = 60.611
Q(150.) = 40.329
Q(75.) = 22.824
Q(37.5) = 17.054
Q(18.25) = 16.006
Q(9.375) = 15.930

The microwave data are reported in R. A. Beaudet and R. L. Poynter, 1978, J. Phys. Chem. Ref. Data 7, 311. The fit involved constraining the constants by isotope relations to the mean of those for OH and OD, since only λ doubling data is available.
The lines reported here were derived from a fit which included the microwave and submillimeter lines reported by J. K. Messer, F. C. DeLucia and P. Helminger (1984), J. Mol. Spect. (in press), and an extensive set of ground state energy levels obtained from new high resolution FTS measurements of the v2 band reported by R. A. Toch, 1984 (private communication). The RMS deviations of the submillimeter lines is almost the same as that reported above by Messer, et al., while the RMS deviations for the fit of the ground state energy levels is 0.00015 cm\(^{-1}\) (4 MHz).


Species Tag: 20001  
Version: 1  
Date: Feb 1984  
Contributor: R. L. Poynter  

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

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


and on the infrared \(v_2\) data of R. A. Toth, 1984, private communication.

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<td>H. M. Pickett</td>
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- **Lines Listed**: 114
- **Max. Frequency**: 3000 GHz
- **Max. \(F\)**: 28
- **LOGSTR**: -10
- **LOGSTR1**: -4
- **Isotope Correction**: 0
- **Minimum Energy**: 0 cm\(^{-1}\)
- **Dipoles**:
  - \(u(a)\) = 0.8 cm\(^{-1}\)
  - \(u(b)\) = 0
  - \(u(c)\) = 0

The spectral data and Hamiltonian are from C. A. Gottlieb, E. W. Gottlieb, and P. Thaddeus, Astrophys. J. 264, 740-745. The dipole moment is an assumed value.
<table>
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<th>Species Name:</th>
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<td>Date:</td>
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<tr>
<td>Contributor:</td>
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| Lines Listed    | 385         | Q(300.)        | 663.88     |
| Max. Frequency  | 3493. GHz   | Q(225.)        | 498.44     |
| Max. J          | 29.5        | Q(150.)        | 332.91     |
| LOGSTR          | -5.         | Q(75.)         | 167.43     |
| LOGSTR1         |             | Q(37.5)        | 84.73      |
| Isotope Correction | 0.     | Q(18.25)       | 43.41      |
| Minimum Energy  | 0. cm⁻¹    | Q(9.375)       | 22.80      |
| Dipoles:        |             |                |            |
| u(a)            | 3.0         | A =            |            |
| u(b)            |             | B = 56693.46   |            |
| u(c)            |             | C =            |            |

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

| Lines Listed | 437 |
| Max. Frequency | 9999 GHz |
| Max. J | 29.5 |
| LOGSTR | -9 |
| LOGSTR1 | 0 |
| Isotope Correction | 0. |
| Minimum Energy | 2068.7 cm⁻¹ |
| Dipoles: | |
| $u(a)$ | 3.0 |
| $u(b)$ | A |
| $u(c)$ | B = 56693.46 |
| | C = |

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

Lines Listed = 40
Max. Frequency = 3000. GHz
Max. J = 33
LOGSTR = -4
LOGSTR1 =
Isotope Correction = 0
Minimum Energy = 0 cm^{-1}
Dipoles: \mu(a) = 2.984 \ A
\mu(b) = B = 44315.975
\mu(c) = C =

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

Lines Listed = 33  Q(300) = 138.223
Max. Frequency = 3000. GHz  Q(225) = 103.801
Max. J = 34  Q(150) = 69.302
LOGSTR = -3  Q(75) = 34.814
LOGSTR1 =  Q(37.5) = 17.575
Isotope Correction = 0  Q(18.25) = 8.960
Minimum Energy = 0 cm⁻¹  Q(9.375) = 4.659
Dipoles:  

\[ \mu(a) = 2.699 \]
\[ \mu(b) = \]  \[ B = 45332. \]
\[ \mu(c) = \]  \[ C = \]

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

<table>
<thead>
<tr>
<th>Lines Listed</th>
<th>26</th>
<th>Q(300.) = 108.787</th>
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<tbody>
<tr>
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<td>3000. GHz</td>
<td>Q(225.) = 81.708</td>
</tr>
<tr>
<td>Max. J</td>
<td>26</td>
<td>Q(150.) = 54.581</td>
</tr>
<tr>
<td>LOGSTR</td>
<td>-5</td>
<td>Q(75.) = 27.454</td>
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<tr>
<td>LOGSTR1</td>
<td></td>
<td>Q(37.5) = 13.896</td>
</tr>
<tr>
<td>Isotope Correction</td>
<td>0</td>
<td>Q(18.25) = 7.122</td>
</tr>
<tr>
<td>Minimum Energy</td>
<td>0 cm⁻¹</td>
<td>Q(9.375) = 3.744</td>
</tr>
<tr>
<td>Dipole: µ(a)</td>
<td>0.1098 A</td>
<td>A =</td>
</tr>
<tr>
<td></td>
<td>µ(b) =</td>
<td>B = 57635.97</td>
</tr>
<tr>
<td></td>
<td>µ(c) =</td>
<td>C =</td>
</tr>
</tbody>
</table>


The dipole moment was measured by J. S. Muenter, 1975, J. Mol. Spect. 55, 490.
<table>
<thead>
<tr>
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<tbody>
<tr>
<td>Species Name:</td>
<td>HC-13-N</td>
</tr>
<tr>
<td>Version:</td>
<td>1</td>
</tr>
<tr>
<td>Date:</td>
<td>Dec 1979</td>
</tr>
<tr>
<td>Contributor:</td>
<td>R. L. Poynter</td>
</tr>
</tbody>
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<table>
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<td>Max. Frequency</td>
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<tr>
<td>Max. J</td>
<td>= 34</td>
</tr>
<tr>
<td>LOGSTR</td>
<td>= -4</td>
</tr>
<tr>
<td>LOGSTR1</td>
<td>=</td>
</tr>
<tr>
<td>Isotope Correction</td>
<td>= -1.955</td>
</tr>
<tr>
<td>Minimum Energy</td>
<td>= 0. cm⁻¹</td>
</tr>
<tr>
<td>Dipoles: μ(a)</td>
<td>= 2.984</td>
</tr>
<tr>
<td>μ(b)</td>
<td>=</td>
</tr>
<tr>
<td>μ(c)</td>
<td>=</td>
</tr>
</tbody>
</table>

Q(300.) = 435.38
Q(225.) = 326.93
Q(150.) = 218.26
Q(75.) = 109.62
Q(37.5) = 55.31
Q(18.25) = 28.17
Q(9.375) = 14.62


The dipole moment was assumed to be the same as the parent species.
Species Tag: 28003 Species Name: HCN-15
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
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<tbody>
<tr>
<td>Lines Listed</td>
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<tr>
<td>Max. Frequency</td>
<td>3000 GHz</td>
</tr>
<tr>
<td>Max. J</td>
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<td>LOGSTR</td>
<td>-2.6</td>
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<tr>
<td>Isotope Correction</td>
<td>-2.432</td>
</tr>
<tr>
<td>Minimum Energy</td>
<td>0 cm⁻¹</td>
</tr>
<tr>
<td>Dipole Moment</td>
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</tr>
<tr>
<td>μ(a)</td>
<td>2.984</td>
</tr>
<tr>
<td>μ(b)</td>
<td></td>
</tr>
<tr>
<td>μ(c)</td>
<td></td>
</tr>
<tr>
<td>Q(300.)</td>
<td>145.068</td>
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<tr>
<td>Q(225.)</td>
<td>109.337</td>
</tr>
<tr>
<td>Q(150.)</td>
<td>72.993</td>
</tr>
<tr>
<td>Q(75.)</td>
<td>36.660</td>
</tr>
<tr>
<td>Q(37.5)</td>
<td>18.498</td>
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<td>Q(18.25)</td>
<td>9.421</td>
</tr>
<tr>
<td>Q(9.375)</td>
<td>4.889</td>
</tr>
</tbody>
</table>


The dipole moment was assumed to be the same as the parent species.
<table>
<thead>
<tr>
<th>Species Tag: 28004</th>
<th>Species Name: DCN Hydrogen cyanide, deuterium isotope</th>
</tr>
</thead>
<tbody>
<tr>
<td>Version: 1</td>
<td></td>
</tr>
<tr>
<td>Date: Dec 1979</td>
<td></td>
</tr>
<tr>
<td>Contributor: R. L. Poynter</td>
<td></td>
</tr>
</tbody>
</table>

| Lines Listed = 54 | Q(300.) = 518.916 |
| Max. Frequency = 3000. GHz | Q(225.) = 389.604 |
| Max. J = 41 | Q(150.) = 260.036 |
| LOGSTR = -4.2 | Q(75.) = 130.504 |
| LOGSTR1 | Q(37.5) = 65.755 |
| Isotope Correction = -3.824 | Q(18.25) = 33.391 |
| Minimum Energy = 0. cm⁻¹ | Q(9.375) = 17.224 |
| Dipoles: | |
| μ(a) = 2.984 | A = 30207.46 |
| μ(b) | B = 30207.46 |
| μ(c) | C = 30207.46 |

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

| Lines Listed | 34 |
| Max. Frequency | 3000 GHz |
| Max. J | 35 |
| LOGSTR | -2.7 |
| LOGSTR1 | |
| Isotope Correction | -1.955 |
| Minimum Energy | 0 cm⁻¹ |
| Dipoles: | \( \mu(a) = 2.699 \) |
| | \( \mu(b) = \) |
| | \( \mu(c) = \) |

| Q(300.) | 143.880 |
| Q(225.) | 108.047 |
| Q(150.) | 72.132 |
| Q(75.) | 36.228 |
| Q(37.5) | 18.282 |

For the isotope correction, \( Q(18.25) = 9.313 \) and \( Q(9.375) = 4.835 \).

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

| Lines Listed | = 33 | Species Name: HN-15-C Hydrogen isocyanide, 15N isotope |
| Max. Frequency | = 3000. GHz | Q(300.) = 141.013 |
| Max. J | = 33 | Q(225.) = 105.893 |
| LGSTR | = -2.7 | Q(150.) = 70.697 |
| LOGSTR | = | Q(75.) = 35.511 |
| Isotope Correction | = -2.432 | Q(37.5) = 17.924 |
| Minimum Energy | = 0. cm\(^{-1}\) | Q(18.25) = 9.134 |

Dipoles:
\[
\begin{align*}
\mu(a) &= 2.699 \\
\mu(b) &= \\
\mu(c) &= 
\end{align*}
\]

A = 44433.04
B = C =

<table>
<thead>
<tr>
<th>Species Tag:</th>
<th>28007</th>
<th>Species Name:</th>
<th>DNC Hydrogen isocyanide, deuterium isotope</th>
</tr>
</thead>
<tbody>
<tr>
<td>Version:</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Date:</td>
<td>Dec 1979</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Contributor:</td>
<td>R. L. Poynter</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- Lines Listed = 39
- Max. Frequency = 3000 GHz
- Max. J = 39
- LOGSTR = -3
- LOGSTR1 =
- Isotope Correction = -3.824
- Minimum Energy = 0. cm⁻¹
- Dipoles:
  - $\mu(a) = 2.699$
  - $\mu(b) = 38152.995$
  - $\mu(c) = C$

Species Tag: 29001
Species Name: C-13-0 carbon monoxide, 13C isotope
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

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

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.
<table>
<thead>
<tr>
<th>Species Tag:</th>
<th>29002</th>
<th>Species Name:</th>
<th>HCU+ Formyl radical cation</th>
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</thead>
<tbody>
<tr>
<td>Version:</td>
<td>2</td>
<td>Date:</td>
<td>Jan 1984</td>
</tr>
<tr>
<td>Contributor:</td>
<td>R. L. Poynter</td>
<td>Lines Listed</td>
<td>33</td>
</tr>
<tr>
<td>Max. Frequency</td>
<td>3000. GHz</td>
<td>Q(300.) =</td>
<td>140.504</td>
</tr>
<tr>
<td>Max. J</td>
<td>33</td>
<td>Q(225.) =</td>
<td>105.506</td>
</tr>
<tr>
<td>LOGSTR</td>
<td>-3</td>
<td>Q(150.) =</td>
<td>70.440</td>
</tr>
<tr>
<td>LOGSTRI</td>
<td></td>
<td>Q(75.) =</td>
<td>35.384</td>
</tr>
<tr>
<td>Isotope Correction</td>
<td>0.</td>
<td>Q(37.5) =</td>
<td>17.860</td>
</tr>
<tr>
<td>Minimum Energy</td>
<td>0. cm⁻¹</td>
<td>Q(18.25) =</td>
<td>9.102</td>
</tr>
<tr>
<td>Dipoles:</td>
<td></td>
<td>Q(9.375) =</td>
<td>4.730</td>
</tr>
<tr>
<td>μ(a)</td>
<td>3.30</td>
<td>A =</td>
<td></td>
</tr>
<tr>
<td>μ(b)</td>
<td></td>
<td>B =</td>
<td>44594.419</td>
</tr>
<tr>
<td>μ(c)</td>
<td></td>
<td>C =</td>
<td></td>
</tr>
</tbody>
</table>

Species Tag: 29003  Species Name: CH₂NH  
Version: 2  Methyleneimine
Date: Jan 1981  
Contributor: R. L. Poynter

Lines Listed = 2957  
Q(300.) = 5892.86
Max. Frequency = 3000. GHz  
Q(225.) = 3800.14
Max. J = 33  
Q(150.) = 2084.97
LOGSTR = -8  
Q(75.) = 740.46
LOGSTR1 = -5 above 120 GHz  
Q(37.5) = 263.39
Isotope Correction = 0.  
Q(18.25) = 94.30
Minimum Energy = 0. cm⁻¹  
Q(9.375) = 34.20

Dipoles:  
μ(a) = 1.325  
μ(b) = 1.530  
μ(c) = 0.

Species Tag: 29004  
Species Name: HCO  
Version: 1  
Date: June 1983  
Contributor: H. M. Pickett and G. A. Blake  

Lines Listed = 2454  
Max. Frequency = 3000. CHz  
Max. J = 30  
LOGSTR = -8  
LOGSTRI = -8.  
Isotope Correction = 0.  
Minimum Energy = 0. cm-1  
Dipoles:  
\( \mu(a) = 1.3626 \)  
\( \mu(b) = 0.700 \)  
\( \mu(c) = 0 \)  

Species Tag: 29005  
Species Name: N$_2$H$^+$

Version: 1  
Date: Jan 1984  
Contributor: R. L. Poynter

Lines Listed = 34  
Max. Frequency = 3000 GHz  
Max. J = 32  
LOGSTR = -3  
LOGSTR1 =  
Isotope Correction = 0.  
Minimum Energy = 0. cm$^{-1}$  
Dipoles: $\mu(a) = 3.40$ cm$^{-1}$  
$\mu(b) = A$  
$\mu(c) = B = 46586.867$  
$\mu(c) = C$


The dipole moment was estimated theoretically by S. Green, J. A. Montgomery, Jr., and P. Thaddeus, (1974), Ap. J. (Lett), 193, L89.
Species Tag: 30001  Species Name: CO-18
Version: 1  Carbon monoxide, 18O isotope
Date: Dec 1979
Contributor: R. L. Poynter

Lines Listed = 27
Max. Frequency = 3000. GHz
Max. J = 27
LOGSTR = -5.1
LOGSTR1 =
Isotope Correction = -2.690
Minimum Energy = 0. cm⁻¹
Dipoles:  \( \mu(a) = 0.11 \)
         \( \mu(b) = \)
         \( \mu(c) = \)

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

The dipole moment was reported by W. L. Meerts, F. H. DeLeeuw, and A. Dymanus, 1977, Chem. Phys. 22, 319.
Species Tag: 30002  Species Name: HC-13-O+
Version: 2  Formyl radical cation, 13C isotope
Date: Dec 1983
Contributor: R. L. Poynter

Lines Listed = 34  Max. Frequency = 3000 GHz
Max. J = 34  Q(300.) = 144.486
LOGSTR = -2.7  Q(225.) = 108.459
LOGSTR1 = 0  Q(150.) = 72.407
Isotope Correction = -1.955  Q(125.) = 36.367
Minimum Energy = 0 cm⁻¹  Q(37.5) = 18.352
Dipoles: μ(a) = 3.3  Q(18.25) = 9.348
μ(b) = 4.367
μ(c) = 7

Only two lines of this molecule have been measured by R. C. Woods, R. J. Saykally, T. A. Dixon, P. G. Szanto and T. Anderson (1976), 31st Symposium on Molecular Spectroscopy, Columbus, Ohio, and by M. Bogey, C. Demuynck, and J. L. Destombes (1981), Mol. Physics 43, 1043. A least squares analysis cannot be done with this limited data. The catalogue entries are therefore just a simple calculation from the B and D rotational constants, and no error estimates can be given beyond the two measured lines. The dipole moment is assumed to be the same as for the parent species.
Species Tag: 30003  Species Name: DCO+
Version: 2
Date: Dec 1983
Contributor: R. L. Poynter

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

| Lines Listed | 611 |
| Max. Frequency | 3000. GHz |
| Max. J | 40 |
| LOGSTR | -20 |
| LOGSTH1 | |
| Isotope Correction | 0. |
| Minimum Energy | 0. cm⁻¹ |
| Dipoles: | |
| $\mu(a)$ | 2.331 |
| $\mu(b)$ | 0 |
| $\mu(c)$ | |

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:


Species Tag: 30005  
Species Name: C-13-H₂NH  
Version: 1  
Date: Jan 1980  
Contributor: R. L. Poynter

<table>
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<tr>
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<th>439</th>
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<tr>
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<td>3000 GHz</td>
</tr>
<tr>
<td>Max. J</td>
<td>10</td>
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<tr>
<td>LOGSTR</td>
<td>-8</td>
</tr>
<tr>
<td>LOGSTR1</td>
<td>0.</td>
</tr>
<tr>
<td>Isotope Correction</td>
<td>-1.955</td>
</tr>
<tr>
<td>Minimum Energy</td>
<td>0. cm⁻¹</td>
</tr>
<tr>
<td>Dipole (a)</td>
<td>1.325</td>
</tr>
<tr>
<td>Dipole (b)</td>
<td>1.530</td>
</tr>
<tr>
<td>Dipole (c)</td>
<td>0.</td>
</tr>
</tbody>
</table>

Q(300.) = 2012.45
Q(225.) = 1307.07
Q(150.) = 711.54
Q(75.) = 251.54
Q(37.5) = 88.94
Q(18.25) = 31.44
Q(9.375) = 11.12

The computational methods is the same as that used on the parent species, CH₂NH. The data are from R. Pearson, Jr. and F. J. Lovas, 1977, J. Chem. Phys. 66, 4149. The dipole moment has been assumed the same as for the parent species.
Species Tag: 30006  
Species Name: CH₂N-15-H  
Methylenimine,  
15N isotope  

Date: Jan 1980  
Contributor: R. L. Poynter

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

Q(300.) = 2015.79  
Q(225.) = 1309.18  
Q(150.) = 712.69  
Q(75.) = 251.97  
Q(37.5) = 89.09  
Q(18.25) = 31.50  
Q(9.375) = 11.14

The computational method is the same as that used on the parent species, CH₂NH. The data are from R. Pearson, Jr. and F. J. Lovas, 1977, J. Chem. Phys. 66, 4149. The dipole moment has been assumed the same as for the parent species.
Species Tag: 30007  
Species Name: CH₂ND

Version: 1  
Date: Feb 1981  
Contributor: R. L. Poynter

<table>
<thead>
<tr>
<th>Lines Listed</th>
<th>= 1834</th>
<th>Q(300.) = 7181.1</th>
</tr>
</thead>
<tbody>
<tr>
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<td>= 3000. GHz</td>
<td>Q(225.) = 4664.3</td>
</tr>
<tr>
<td>Max. J</td>
<td>= 14</td>
<td>Q(150.) = 2542.6</td>
</tr>
<tr>
<td>LOGSTR</td>
<td>= -5 above 120 GHz</td>
<td>Q(75.) = 811.7</td>
</tr>
<tr>
<td>LOGSTR1</td>
<td>=</td>
<td>Q(37.5) = 297.8</td>
</tr>
<tr>
<td>Isotope Correction</td>
<td>= -3.824</td>
<td>Q(18.25) = 92.62</td>
</tr>
<tr>
<td>Minimum Energy</td>
<td>= 0. cm⁻¹</td>
<td>Q(9.375) = 43.38</td>
</tr>
</tbody>
</table>

Dipoles:  
\[ \mu(a) = 1.325 \]  
\[ \mu(b) = 1.530 \]  
\[ \mu(c) = 0. \]

---

The computational method is the same as that used for the parent species, CH₂NH. The data are from R. Pearson, Jr. and F. J. Lovas, 1977, J. Chem. Phys. 66, 4149.

The dipole moment was assumed to be the same as for the parent species.
Species Tag: 30008
Species Name: NO
Version: 1
Date: Feb 1980
Contributor: H. M. Pickett

Nitric oxide, $^2\Pi$ ground states

Lines Listed = 1909
Max. Frequency = 3000. GHz
Max. J = 35.5
LOGSTR = -20
LOGSTR1 =
Isotope Correction = 0.
Minimum Energy = 0 cm$^{-1}$
Dipoles:
$\mu(a) = 0.15872$
$\mu(b) =$
$\mu(c) =$

The spectrum of NO was fit to the fine structure Hamiltonian described by C. Amiot, R. Bacis and G. Guelachvili, 1973, Can. J. Phys. 51, 251, along with the hyperfine Hamiltonian described by W. L. Meerts, 1976, Chem. Phys. 14, 421. The radio frequency lines are from W. L. Meerts and A. Dymanus, 1972, J. Mol. Spectroscopy, 44, 320. The millimeter lines were measured at JPL by H. M. Pickett and E. A. Cohen. The partition function was determined by a sum over states to J=71/2.
Species Tag:  30009  
Species Name:  \( \text{N}_2\text{D}^+ \)

Version:  1
Date:  Jan 1984
Contributor:  R. L. Poynter

Lines Listed  41
Max. Frequency  3000  GHz
Max. J  39
LOGSTR  -4
LOGSTR\(_1\)  =
Isotope Correction  -3.824
Minimum Energy  0.  cm\(^{-1}\)
Dipoles:  \( \mu(a) \)  3.40
\( \mu(b) \)  =
\( \mu(c) \)  =

Q(300.)  487.62
Q(225.)  365.939
Q(150.)  244.264
Q(75.)  122.626
Q(37.5)  61.813
Q(18.25)  31.421
Q(9.375)  16.241


The dipole moment was assumed the same as for the parent species.
Species Tag: 31001  Species Name: HCO-18+
Version: 2
Date: Dec 1983
Contributor: R. L. Poynter

Lines Listed = 34
Max. Frequency = 3000 GHz
Max. J = 34
LOGSTR = -2.7
Isotope Correction = -2.690
Minimum Energy = 0. cm⁻¹
Dipoles: u(a) = 3.30  A = 42581.21
        u(b) =  B =
        u(c) =  C =

Only two lines of this molecule have been measured, by C. Woods, R. J. Saykally, T. A. Dixon, P. G. Szanto and T. Anderson (1976), and by M. Bogey, C. Demuynck, and J. L. Destombes (1981), Mol. Physics 43, 1043. A least squares analysis cannot be done with this limited data. The catalogue entries are therefore just a simple calculation from the B and D rotational constants, and no error estimates can be given. The dipole moment is assumed to be the same as for the parent species.
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:


The dipole moment was assumed to be the same as the parent H\textsubscript{2}C\textsuperscript{12}CO.
Species Tag: 32001
Version: 2
Date: June 1980
Contributor: H. M. Pickett

| Lines Listed | Q(300.) = 2.8655 |
| Max. Frequency | 3000. GHz |
| Max. J | 60 |
| LOGSTR | -32 |
| Isotope Correction | 0 |
| Minimum Energy | 0 cm\(^{-1}\) |
| Dipoles: | \(\mu(a) = \text{magnetic}\) |
| | \(\mu(b) =\) |
| | \(\mu(c) =\) |

<table>
<thead>
<tr>
<th></th>
<th>A =</th>
<th>B =</th>
<th>C =</th>
</tr>
</thead>
<tbody>
<tr>
<td>Q(275)</td>
<td>200.426</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Q(250)</td>
<td>182.231</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Q(200)</td>
<td>145.919</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The measurements and calculational method are from T. Amano and E. Hirota, 1974. J. Mol. Spectroscopy 53, 346. The Raman lines of \(\text{O}_2\) (M. Loete and H. Berger, 1977, J. Mol. Spectroscopy 68, 317) were used with the millimeter wavelength measurements and the submillimeter-line of W. Steinbach and W. Wordy (1973, Phys. Rev. A 8, 1953) in a combined fit of the \(v = 0\) and \(v = 1\) transitions. The intensities of the magnetic dipole transitions have been calculated using the g values obtained from magnetic resonance by K. D. Bowers, R. A. Kamper and C. D. Lustig, 1959, Proc. Roy. Soc. (Lond.) A251, 565. The zero-frequency absorption is included but the frequency is set to a synthetic frequency of \(|g|J\) for the given level.
Species Tag: 32002 Species Name: O$_2$ V=1 state
Version: 3
Date: Dec. 1983
Contributor: H. M. Pickett

Lines Listed = 153
Max. Frequency = 3000 GHz
Max. J = 60
LOGSTR = -13.2
LOGSTRI
Isotope Correction = 0
Minimum Energy = 1556.33 cm$^{-1}$

Dipoles: $\mu(a)$ = magnetic $A = 42626.96$
$\mu(b) = B$
$\mu(c) = C$

The calculations are described for the ground state (Species 32001).
The vibrationally excited state, $v = 1$, is $1556.38 \pm 0.01$ cm$^{-1}$ above the ground state (M. Leote and H. Berger, 1977, J. Molec. Spectry. 68, 317).
Intensities were calculated using the ground state g values.
Species Tag: 32003
Version: 2
Date: Nov 1980
Contributor: H. M. Pickett

Species Name: CH$_3$OH
Methyl alcohol (methanol),
lowest A, E$_1$, and E$_2$
vibrational states

Lines Listed = 709
Max. Frequency = 3000. GHz
Max. J = 12
LOGSTR = -10
LOGSTR1 =
Isotope Correction = 0
Minimum Energy = 0. cm$^{-1}$

Dipoles: $\mu(a) = 0.885$
$\mu(b) = 1.440$
$\mu(c) = 0.$

Q(300.) = 6414.25
Q(225.) = 4165.82
Q(150.) = 2267.78
Q( 75.) =  801.68
Q( 37.5) =  283.47
Q(18.25) =  100.21
Q(9.375) =   39.35

The lines below 200 GHz are reported by R. M. Lees, F. J. Lovas, W. H. Kirchhoff, and D. R. Johnson, 1973, J. Phys. Chem. Ref. Data, 2, 205. Additional lines are referenced in F. J. Lovas, L. E. Snyder, and D. R. Johnson, 1979, Ap. J. Suppl., 41. The lines above 200 GHz were measured at JPL. Frequencies were predicted using energy polynomials in J (J + 1) for each value of K.

The $v$ quantum numbers in the catalogue are:

<table>
<thead>
<tr>
<th>$v$</th>
<th>species</th>
<th>asymmetric rotor correspondence</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>A$^+$</td>
<td>upper K state for K even, lower for K odd</td>
</tr>
<tr>
<td>2</td>
<td>A$^-$</td>
<td>K state for K odd, lower for K even</td>
</tr>
<tr>
<td>3</td>
<td>E$_1$</td>
<td>no direct correspondence</td>
</tr>
<tr>
<td>4</td>
<td>E$_2$</td>
<td>no direct correspondence</td>
</tr>
</tbody>
</table>

-66-
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:


The dipole moment was assumed to be the same as the parent species.
Species Tag: 33001  
Species Name: \( \text{HO}_2 \)

Version: 1  
Date: May 1983  
Contributor: H. M. Pickett

Lines Listed = 6174  
Max. Frequency = 3000 GHz  
Max. J = 30  
LOGSTR = -7.  
LOGSTR1 = -7.  
Isotope Correction = 0.  
Minimum Energy = 0. cm\(^{-1}\)  
Dipoles: \( \mu(a) = 1.412 \)  
\( \mu(b) = 1.541 \)  
\( \mu(c) = \)

\[ Q(300.) = 4344.6 \]  
\[ Q(225.) = 2837.8 \]  
\[ Q(150.) = 1547.0 \]  
\[ Q(75.) = 548.4 \]  
\[ Q(37.5) = 195.16 \]  
\[ Q(18.25) = 70.21 \]  
\[ Q(9.375) = 27.59 \]


The spectrum was computed using a full diagonalization of the spin-rotation Hamiltonian.
Species Tag: 340U1  
Species Name: 0-18-0  
Version: 2  
Date: Oct 1980  
Contributor: H. M. Pickett  

<table>
<thead>
<tr>
<th>Lines Listed</th>
<th>Max. Frequency</th>
<th>Max. J</th>
<th>LOGSTK</th>
<th>LOGSTR1</th>
<th>Isotope Correction</th>
<th>Minimum Energy</th>
<th>Dipole: μ(a)</th>
<th>μ(b)</th>
<th>μ(c)</th>
</tr>
</thead>
<tbody>
<tr>
<td>383</td>
<td>3000 JHz</td>
<td>60</td>
<td>-10.6</td>
<td></td>
<td>-2.389</td>
<td>0 cm⁻¹</td>
<td>magnetic</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Q(300.) = 462.32</td>
<td>Q(225.) = 346.96</td>
<td>Q(150.) = 231.67</td>
<td>Q(75.) = 116.45</td>
<td>Q(37.5) = 58.92</td>
<td>Q(18.25) = 30.26</td>
<td>A = 40708.</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The measurements and calculational method are from T. Amano and E. Hirota, 1974, J. Mol. Spectroscopy 53, 346. Intensities of magnetic dipole transitions have been calculated using the g values obtained from magnetic resonance by K. D. Bowers, R. A. Kamper and C. D. Lustig, 1959, Proc. Roy. Soc. (Lond.) A251, 565. The zero-frequency absorption is included but the frequency is set to a synthetic frequency of |g|J for the given level. The measured line at 233 GHz from W. Steinbach and W. Gordy, 1975, Phys. Rev. A11, 729 has been included in the catalogue.
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:


The dipole moment was reported by C. Huiszoon and A. Dymanus, 1965, Physica, 31, 1049.
Species Tag: 34003
Version: 2
Date: Aug 1983
Contributor: R. L. Poynter

Lines Listed = 142
Max. Frequency = 3000 GHz
Max. J = 19
LOGSTR = -17
LOGSTR1 =
Isotope Correction = 0.
Minimum Energy = 0. cm⁻¹

Dipoles:

\[ \mu(a) = 0.000072^* \]
\[ \mu(b) = \]
\[ \mu(c) = 0.574 \]

*centrifugally induced


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.
<table>
<thead>
<tr>
<th>Species Tag:</th>
<th>34004</th>
<th>Species Name:</th>
<th>H₂O₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>Version:</td>
<td>2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Date:</td>
<td>Oct 1980</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Contributor:</td>
<td>H. M. Pickett</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Lines Listed</td>
<td>883</td>
<td>Q(300.) = 7651.8</td>
<td></td>
</tr>
<tr>
<td>Max. Frequency</td>
<td>3000 GHz</td>
<td>Q(225.) = 4970.0</td>
<td></td>
</tr>
<tr>
<td>Max. J</td>
<td>23</td>
<td>Q(150.) = 2705.3</td>
<td></td>
</tr>
<tr>
<td>LOGSTR</td>
<td>-8</td>
<td>Q(75.) = 916.2</td>
<td></td>
</tr>
<tr>
<td>LOGSTR1</td>
<td></td>
<td>Q(37.5) = 288.7</td>
<td></td>
</tr>
<tr>
<td>Isotope Correction</td>
<td>0</td>
<td>Q(18.25) = 88.77</td>
<td></td>
</tr>
<tr>
<td>Minimum Energy</td>
<td>0 cm⁻¹</td>
<td>Q(9.375) = 26.64</td>
<td></td>
</tr>
<tr>
<td>Dipoles:</td>
<td>( \mu(a) = 0 )</td>
<td>A = 301878</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( \mu(b) = 0 )</td>
<td>B = 26211.9</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( \mu(c) = 1.5728 )</td>
<td>C = 25099.14</td>
<td></td>
</tr>
</tbody>
</table>


The quantum number designation is \( v = 0 \) for \( \tau = 1, 2 \) and \( v = 1 \) for \( \tau = 3, 4 \).
**Species Tag:** 35001  
**Species Name:** HDS  
**Version:** 1  
**Date:** Jan 1980  
**Contributor:** R. L. Poynter  

| Lines Listed | 1138 | Q(300.) = 430.90 |
| Max. Frequency | 3000 GHz | Q(225.) = 280.82 |
| Max. J | 20 | Q(150.) = 153.44 |
| LOGSTR | -11.4 | Q(75.) = 54.75 |
| LOGSTR1 |  | Q(37.5) = 19.758 |
| Isotope Correction | -3.523 | Q(18.25) = 7.291 |
| Minimum Energy | 0. cm⁻¹ | Q(9.375) = 2.829 |
| Dipoles: |  |
| \( \mu(a) \) | 0.470 A = 292351.302 |
| \( \mu(b) \) | 0.974 B = 147861.801 |
| \( \mu(c) \) | 0. C = 96704.120 |


The dipole moment was reported by R. E. Hillger and M. W. P. Strandberg, 1951, Phys. Rev. 83, 575.
Species Tag: 36001  
Species Name: HC135 
Version: 1  
Date: Feb 1980  
Contributor: R. L. Poynter and H. M. Pickett

<table>
<thead>
<tr>
<th>Lines Listed</th>
<th>Q(300.)</th>
<th>81.232</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max. Frequency</td>
<td>Q(225.)</td>
<td>60.924</td>
</tr>
<tr>
<td>Max. J</td>
<td>Q(150.)</td>
<td>40.616</td>
</tr>
<tr>
<td>LOGSTR</td>
<td>Q(75.)</td>
<td>21.249</td>
</tr>
<tr>
<td>LOGSTR1</td>
<td>Q(37.5)</td>
<td>11.437</td>
</tr>
<tr>
<td>Isotope Correction</td>
<td>Q(18.25)</td>
<td>6.583</td>
</tr>
<tr>
<td>Minimum Energy</td>
<td>Q(9.375)</td>
<td>4.488</td>
</tr>
<tr>
<td>Dipoles:</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
µ(a) = 1.109 | A = |
µ(b) = 0. | B = 312989.3 |
µ(c) = 0. | C = |

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

The dipole moment was measured by F. A. deLeeuw and A. Dymanus, 1971, Symposium on Molec. Spect., Columbus, Ohio.
Species Tag: 38001  
Species Name: HCl-37 hydrochloric acid, 37Cl isotope

Version: 1
Date: Feb 1980
Contributor: R. L. Poynter and H. M. Pickett

Lines Listed = 17
Max. Frequency = 3000. GHz
Max. J = 4
LOGSTR = -1.3
LOGSTR1 = -0.611
Isotope Correction = 0.611
Minimum Energy = 0. cm⁻¹
Dipoles: \( \mu(a) = 1.109 \)
\( \mu(b) = \)
\( \mu(c) = \)

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

The dipole moment was measured by F. A. DeLeeuw and A. Dymanus, 1971, Symposium on Molec. Spect., Columbus, Ohio.
Species Tag: 40001  
Species Name: CH₃CCH  
Version: 1  
Date: Dec 1979  
Contributor: R. L. Poynter

<table>
<thead>
<tr>
<th>Lines Listed</th>
<th>Q(300.)</th>
<th>5428.80</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max. Frequency</td>
<td>3000 GHz</td>
<td>Q(225.) = 3524.70</td>
</tr>
<tr>
<td>Max. J</td>
<td>79</td>
<td>Q(150.) = 1920.80</td>
</tr>
<tr>
<td>LOGSTR</td>
<td>-4.5 for J&gt;14</td>
<td>Q(75.) = 679.68</td>
</tr>
<tr>
<td>LOGSTR1</td>
<td>=</td>
<td>Q(37.5) = 241.25</td>
</tr>
<tr>
<td>Isotope Correction</td>
<td>= 0.</td>
<td>Q(18.25) = 88.27</td>
</tr>
<tr>
<td>Minimum Energy</td>
<td>= 0. cm⁻¹</td>
<td>Q(9.375) = 34.42</td>
</tr>
</tbody>
</table>

Dipoles:
- \( \mu(a) = 0.75 \)
- \( \mu(b) = 0. \)
- \( \mu(c) = 0. \)

The experimental measurements were obtained from A. Cuadrille, 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. Muenler and V. W. Laurie, 1966, J. Chem. Phys. 45, 855.

The dipole moment was reported by P. A. Steiner and W. Gordy, 1966, J. Mol. Spect. 21, 291.
Species Tag: 41002  
Species Name: CH$_3$CC-13-H propyne, $^{13}$C isotope on atom 1.

Date: Dec 1979  
Contributor: R. L. Poynter

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


The dipole moment was reported by P. A. Steiner and W. Gordy, 1966, J. Mol. Sptect. 21, 291.
Species Tag: 41003  
Species Name: CH$_3$C-13-CH$_3$ propyne, $^{13}$C isotope on atom 2.

Version: 1  
Date: Dec 1979  
Contributor: R. L. Poynter

Lines Listed = 813  
Max. Frequency = 3000 GHz  
Max. J = 79  
LOGSTR = -6.5 for J>14  
Isotope Correction = -1.955  
Minimum Energy = 0. cm$^{-1}$  
Dipoles:  
\[ \mu(a) = 0.75 \]  
\[ \mu(b) = \]  
\[ \mu(c) = \]

\[ Q(300.) = 5431.06 \]  
\[ Q(225.) = 3526.18 \]  
\[ Q(150.) = 1921.60 \]  
\[ Q(75.) = 679.96 \]  
\[ Q(37.5) = 241.35 \]  
\[ Q(18.25) = 88.31 \]  
\[ Q(9.375) = 34.44 \]


The dipole moment was reported by P. A. Steiner and W. Gordy, 1966, J. Mol. Spect. 21, 291.
Species Tag: 41004  
Species Name: H₃C-13-CCH propyne, ¹³C isotope on atom 3  
Version: 1  
Date: Dec 1979  
Contributor: R. L. Poynter  

Lines Listed = 821  
Max. Frequency = 3000 GHz  
Max. J = 80  
LOGSTR = -4.5 for J>14  
LOGSTR1 =  
Isotope Correction = -1.955  
Minimum Energy = 0. cm⁻¹  

Dipoles:  
μ(a) = 0.750  
μ(b) = 0.  
μ(c) = 0.  

The dipole moment was reported by P. A. Steiner and W. Gordy, 1966, J. Mol. Spect. 21, 291.
Species Tag: 41005  
Species Name: CH3CCD  
Version: 2  
Date: Jan 1984  
Contributor: R. L. Poynter  

<table>
<thead>
<tr>
<th>Lines Listed</th>
<th>822</th>
<th>Max. Frequency</th>
<th>405 GHz</th>
<th>Q(300.) = 17192.04</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max. J</td>
<td>40</td>
<td>Q(225.) = 11168.37</td>
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<td></td>
</tr>
<tr>
<td>LOGSTR</td>
<td>-7.8</td>
<td>Q(150.) = 6139.89</td>
<td></td>
<td></td>
</tr>
<tr>
<td>LOGSTR1</td>
<td></td>
<td>Q(75.) = 2243.60</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Isotope Correction</td>
<td>-3.824</td>
<td>Q(37.5) = 795.34</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Minimum Energy</td>
<td>0. cm⁻¹</td>
<td>Q(18.25) = 290.46</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Dipoles:  
μ(a) = .77  A = 158590.  
μ(b) =  B = 7788.170  
μ(c) =  C = B


The dipole moment was taken from Muenter and Laurie, above.
<table>
<thead>
<tr>
<th>Species Tag:</th>
<th>41006</th>
<th>Species Name:</th>
<th>CH$_2$DCCH</th>
</tr>
</thead>
<tbody>
<tr>
<td>Version:</td>
<td>2</td>
<td>prôpyne, deuterium</td>
<td></td>
</tr>
<tr>
<td>Date:</td>
<td>Aug 1983</td>
<td>isotope on methyl</td>
<td></td>
</tr>
<tr>
<td>Contributor:</td>
<td>R. L. Poynter</td>
<td>carbon atom</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Lines Listed</th>
<th>223</th>
<th>Q(300.) = 4428.44</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max. Frequency</td>
<td>3000 GHz</td>
<td>Q(225.) = 2875.21</td>
</tr>
<tr>
<td>Max. J</td>
<td>15</td>
<td>Q(150.) = 1633.43</td>
</tr>
<tr>
<td>LOGSTR</td>
<td>-10</td>
<td>Q(75.) = 904.90</td>
</tr>
<tr>
<td>LOGSTRI</td>
<td></td>
<td>Q(37.5) = 410.30</td>
</tr>
<tr>
<td>Isotope Correction</td>
<td>-3.347</td>
<td>Q(18.25) = 156.17</td>
</tr>
<tr>
<td>Minimum Energy</td>
<td>0 cm$^{-1}$</td>
<td>Q(9.375) = 55.87</td>
</tr>
<tr>
<td>Dipoles:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\mu(a)$</td>
<td>0.750</td>
<td>$A = 117744.370$</td>
</tr>
<tr>
<td>$\mu(b)$</td>
<td></td>
<td>$B = 8155.784$</td>
</tr>
<tr>
<td>$\mu(c)$</td>
<td></td>
<td>$C = 8025.577$</td>
</tr>
</tbody>
</table>


The dipole moment was assumed to be the same as the parent species for this calculation.
Species Tag: 42001  
Version: 1  
Date: Dec 1979  
Contributor: R. L. Poynter  
Species Name: CH$_3$CN-15, acetonitrile, $^{15}$N isotope  

| Lines Listed | = 2755 | Q(300.) = 5226.37 |
| Max. Frequency | = 3000 GHz | Q(225.) = 3394.69 |
| Max. J | = 99 | Q(150.) = 1847.57 |
| LOGSTR | = -5 for J>14 | Q(75.) = 653.73 |
| LOGSTR1 | | Q(37.5) = 232.06 |
| Isotope Correction | = -2.432 | Q(18.25) = 84.86 |
| Minimum Energy | = 0 cm$^{-1}$ | Q(9.375) = 33.08 |
| Dipoles: | $\mu(a)$ = 3.919 | A = 158290. |
| | $\mu(b)$ = | B = 9198.8993 |
| | $\mu(c)$ = | C = B |


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


The dipole moment was reported by Johnson (above) and E. Fabricant, et al. (above).
Species Tag: 43001  
Species Name: CHDCO, ketene, mono deuterium isotope  
Version: 1  
Date: Jan 1980  
Contributor: R. L. Poynter  

| Lines Listed | = 886 | Q(300.) = 6682.68 |
| Max. Frequency | = 3000 GHz | Q(225.) = 4340.53 |
| Max. J | = 29 | Q(150.) = 2344.00 |
| LOGSTR | = -23 | Q(75.) = 828.70 |
| LOGSTR1 |  | Q(37.5) = 295.80 |
| Isotope Correction | = -3.523 | Q(18.25) = 105.15 |
| Minimum Energy | = 0. cm\(^{-1}\) | Q(9.375) = 37.50 |
| Dipoles: \(\mu(a)\) | = 1.422 | A = 194313. |
| \(\mu(b)\) |  | B = 9647.396 |
| \(\mu(c)\) |  | C = 9174.975 |


The dipole moment was assumed the same as the parent species.
Species Name: CS, carbon monosulfide

Version: 2
Date: Jan 1984
Contributor: R. L. Poynter

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

The experimental data were taken from the following papers:

M. Bogey, C. Demuynck, and J. L. Destombes, 1982, J. Mol. Spect. 95, 35.

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

The dipole moment is from G. Winnewisser and H. L. Cook, 1968, J. Mol. Spect. 28, 266.
Species Tag: 44002  Species Name: $^{28}\text{SiO}$, silicon monoxide

Version: 2
Date: Jan 1984
Contributor: R. L. Poynter

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

The experimental data were taken from the following papers:


Species Tag: 44003  
Species Name: CH3CHO-A, acetaldehyde, ground vibrational state, A species.  
Version: 1  
Date: Jan 1980  
Contributor: R. L. Poynter  

Lines Listed = 1347  
Max. Frequency = 3000 GHz  
Max. J = 20  
LOGSTR = -9  
LOGSTR1 =  
Isotope Correction = 0.  
Minimum Energy = 0. cm^{-1}  
Dipoles: \mu(a) = 2.550  
\mu(b) = 0.870  
\mu(c) =  

Q(300.) = 12111.56  
Q(225.) = 7866.84  
Q(150.) = 4282.08  
Q(75.) = 1513.94  
Q(37.5) = 535.26  
Q(18.25) = 190.27  
Q(9.375) = 67.76  

\mu = (a) = 56609.474  
\mu = (b) = 10162.766  
\mu = (c) = 9100.412  

The data set used is referenced by A. Bauder, F. J. Lovas and D. R. Johnson 1976, J. Phys. Chem. Ref. Data 5, 53. The lines were fit to a rigid rotor with centrifugal distortion.
Species Tag: 44004  Species Name: N₂O
Version: 1
Date: Jan 1980
Contributor: R L. Poynter and H. M. Pickett

Lines Listed = 61  Q(300.) = 497.966
Max. Frequency = 3000 GHz  Q(225.) = 373.594
Max. J = 61  Q(150.) = 249.173
LOGSTR = 61  Q(75.) = 124.738
LOGSTR1 =  Q(37.5) = 62.546
Isotope Correction = 0.  Q(18.25) = 31.434
Minimum Energy = 0. cm⁻¹  Q(9.375) = 15.889
Dipoles: \( \mu(a) = 0.1608 \)  A = 
\( \mu(b) = \)  B = 12561.637
\( \mu(c) = \)  C =


The experimental lines of the lowest torsional state of E symmetry are listed in A. Bauder, F. J. Lovas, and D. R. Johnson, 1976, J. Chem. Phys. Ref. Data 5, 53. These lines were fit to a Hamiltonian which included terms up to sixth power in angular momentum as well as $P_a$, $P_a^2$, $P_a^4$, $P_a^3$, $P_a^5$, and $P_a^{3p^2}$ terms. The fit produced observed - calculated frequencies which were 3.5 times the experimental uncertainties in an rms sense. Calculated values of $\mu^2 S$ agree with those of Bauder et al. The reference energy is located at the J=0 level of the A state, but intensities are based on E state concentrations.
Species Tag: 45001  
Species Name: C-13-S  
Carbon monosulfide, T3C isotope  
Version: 2  
Date: Jan 1984  
Contributor: R. Poynter

Lines Listed = 29
Max. Frequency = 1340 GHz
Max. J = 28
LOGSTR = -4
LOGSTR1 =
Isotope Correction = -1.977
Minimum Energy = 0. cm⁻¹
Dipoles : u(a) = 1.957
u(b) =
u(c) =

The experimental measurements were reported by R. C. Mockler and G. R. Bird, 1955, Phys. Rev. 98, 1837, and by M. Bogey, C. Demuynck, and J. L. Destombes, 1982, J. Mol. Spect. 95, 35.

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

The maximum J and frequency were limited by the estimated uncertainty in the predicted lines.
Species Tag: 45002
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: $^{29}\text{SiO}$

silicon monoxide, $^{29}\text{Si}$ isotope

Lines Listed = 66
Q(300.) = 2.90870
Max. Frequency = 3000 GHz
Q(225.) = 219.180
Max. J = 66
Q(150.) = 146.184
LOGSTP = -6
Q(75.) = 73.2318
LOGSTRI =
Q(37.5) = 36.7790
Isotope Correction = -1.327
Q(18.25) = 18.5609
Minimum Energy = 0. cm$^{-1}$
Q(9.375) = 9.4515
Dipoles:
$\mu(a) = 3.098$
$\mu(\beta) = A$
$\mu(\gamma) = B = 21514.07$


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:


The dipole moment was reported in the paper by Kurland and Wilson.
The experimental measurements were reported by R. C. Mockler and G. R. Bird, 1955, Phys. Rev. 98, 1837, and by M. Bogey, C. Demuynck, and J. L. Destombes, 1982, J. Mol. Spect. 95, 35.

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

The maximum J and frequency were limited by the estimated uncertainty in the predicted lines.
Species Tag: 46002
Species Name: 30Si 0,
silicon monoxide,
30Si isotope
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Lines Listed = 67
Max. Frequency = 3000 GHz
Max. J = 67
LOGSTR = -6
LOGSTR1 = 
Isotope Correction = -1.506
Minimum Energy = 0. cm⁻¹

Dipoles: 
\[ \mu(a) = 3.098 \]
\[ \mu(b) = \]
\[ \mu(c) = \]

Q(300.) = 294.374
Q(225.) = 221.259
Q(150.) = 147.911
Q(75.) = 74.1139
Q(37.5) = 37.2220
Q(18.25) = 18.7759
\( \chi(9.375) = 9.5609 \)

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

The dipole moment was reported by J. W. Raymonda, J. S. Muenter, and
Species Tag: 46003  Species Name: \( \text{H}_2\text{CS} \), thioformaldehyde

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

Lines Listed = 517  
Max. Frequency = 3000 GHz  
Max. J = 27  
LOGSTR = -11  
LOGSTR1 =  
Isotope Correction = -0.022  
Minimum Energy = 0. cm\(^{-1}\)  
Dipoles:  
\[(a) = 1.649\]  
\[(b) =\]  
\[(c) =\]  

\[ \log Q(300.) = 5984.11 \]  
\[ \log Q(225.) = 3760.98 \]  
\[ \log Q(150.) = 2088.82 \]  
\[ \log Q(75.) = 750.067 \]  
\[ \log Q(37.5) = 265.644 \]  
\[ \log Q(18.25) = 91.1801 \]  
\[ \log Q(9.375) = 27.5233 \]  
\[ \log Q(1.875) = -0.022 \]

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333. The measurements were taken from D. R. Johnson, F. J. Lovas, and W. H. Kirchhoff, 1972, J. Phys. Chem. Ref. Data 1, 1011. Other references were taken from this paper.

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


Additional measurements were made by E. A. Cohen, 1979, private communication.

The dipole moment was reported by Takano, et al, above.
Species Tag: 46005  
Species Name: HCOOH  
Version: 1  
Date: Jan 1980  
Contributor: R. L. Poynter  

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

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


The dipole moment used in the present work was measured by H. Kim, R. Kelle, and W. D. Gwinn, 1962, J. Chem. Phys. 37, 2748, and was adjusted to the new OCS standard, (J. S. Muenter, 1968, J. Chem. Phys. 48, 4544). Improved values \([\mu_a = 1.4214(21)D\) and \(\mu_b = 0.2096(65)D\) have been recently reported by H. Kuze, T. Kuga, and T. Shimizu, 1982, J. Mol. Spect. 93, 248.
Species Tag: 46006  
Species Name: nitrogen dioxide, \( \text{NO}_2 \)

Version: 1  
Date: Feb 1980  
Contributor: R. L. Poynter

<table>
<thead>
<tr>
<th>Lines Listed</th>
<th>Q(300.) = 13402</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max. Frequency</td>
<td>Q(225.) = 8750</td>
</tr>
<tr>
<td>Max. J</td>
<td>Q(150.) = 4704</td>
</tr>
<tr>
<td>LOGSTR</td>
<td>Q(75.) = 1683</td>
</tr>
<tr>
<td>LOGSTR1</td>
<td>Q(37.5) = 596</td>
</tr>
<tr>
<td>Isotope Correction</td>
<td>Q(18.25) = 211.8</td>
</tr>
<tr>
<td>Minimum Energy</td>
<td>Q(9.375) = 75.7</td>
</tr>
<tr>
<td>Dipoles:</td>
<td></td>
</tr>
<tr>
<td>( \mu(a) = 239904 )</td>
<td>( A = 239904 )</td>
</tr>
<tr>
<td>( \mu(b) = 0.316 )</td>
<td>( B = 13002 )</td>
</tr>
<tr>
<td>( \mu(c) = 0 )</td>
<td>( C = 12305 )</td>
</tr>
</tbody>
</table>

The data are from W. C. Bowman and F. C. DeLucia, 1982, J. Chem. Phys. 77, 92. The spectra were calculated using a full diagonalization of the Hamiltonian.
Species Tag: 47001  
Species Name: $\text{H}_2^{13}\text{CS}$  
Version: 1  
Date: Jan 1980  
Contributor: R. L. Poynter

<table>
<thead>
<tr>
<th>Lines Listed</th>
<th>110</th>
<th>Q(300.) = 6220.14</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max. Frequency</td>
<td>335 GHz</td>
<td>Q(225.) = 4040.17</td>
</tr>
<tr>
<td>Max. J</td>
<td>10</td>
<td>Q(150.) = 2114.95</td>
</tr>
<tr>
<td>LOGSTR</td>
<td>-10</td>
<td>Q(75.) = 777.678</td>
</tr>
<tr>
<td>LOGSTR1</td>
<td></td>
<td>Q(37.5) = 264.363</td>
</tr>
<tr>
<td>Isotope Correction</td>
<td>-1.977</td>
<td>Q(18.25) = 94.2540</td>
</tr>
<tr>
<td>Minimum Energy</td>
<td>0. cm$^{-1}$</td>
<td>Q(9.375) = 28.6154</td>
</tr>
<tr>
<td>Dipoles</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\mu(a)$</td>
<td>1.649</td>
<td>A = 291660.0</td>
</tr>
<tr>
<td>$\mu(b)$</td>
<td></td>
<td>B = 16998.342</td>
</tr>
<tr>
<td>$\mu(c)$</td>
<td></td>
<td>C = 16030.791</td>
</tr>
</tbody>
</table>

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:


Other references were taken from this paper.

The dipole moment was assumed to be the same as the parent species.
Species Tag: 47002  
Species Name: H$_{13}$COOH

<table>
<thead>
<tr>
<th>Version:</th>
<th>1</th>
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</thead>
<tbody>
<tr>
<td>Date:</td>
<td>Jan 1980</td>
</tr>
<tr>
<td>Contributor:</td>
<td>R. L. Poynter</td>
</tr>
</tbody>
</table>

| Lines Listed | 1194 |
| Max. Frequency | 3000 GHz |
| Max. J | 20 |
| LOGSTR | -10 |
| LOGSTR1 | |
| Isotope Correction | -1.955 |
| Minimum Energy | 0 cm$^{-1}$ |
| Dipole moment: | |
| $\mu(a)$ | 1.396 |
| $\mu(b)$ | 0.260 |
| $\mu(c)$ | |

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


The dipole moment was assumed the same as the parent species, tag #46005.
Species Tag: 47003  
Species Name: DCOOH  
Version: 1  
Date: Jan 1980  
Contributor: R. L. Poynter  

| Lines Listed | 628 |
| Max. Frequency | 3000 GHz |
| Max. J | 20 |
| LOGSTR | -10 |
| Isotope Correction | -3.824 |
| Minimum Energy | 0 cm⁻¹ |
| Dipoles: μ(a) | 1.396 |
| μ(b) | 0.260 |
| μ(c) | |

Q(300.) = 10531.2
Q(225.) = 6840.2
Q(150.) = 3626.47
Q(75.) = 1251.4
Q(37.5) = 466.123
Q(18.25) = 165.882
Q(9.375) = 59.1562

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:


The dipole moment was assumed the same as the parent species, tag #46005.
Species Tag: 47004  
Species Name: HCOOD formic acid, deuterium isotope on O atom
Version: 1
Date: Jan 1980
Contributor: R. L. Poynter

| Lines Listed | 612 | Q(300.) = 9954.87 |
| Max. Frequency | 3000 GHz | Q(225.) = 6465.87 |
| Max. J | 20 | Q(150.) = 3519.57 |
| LOGSTR | -9 | Q(75.) = 1213.13 |
| LOGSTRI | | Q(37.5) = 440.555 |
| Isotope Correction | -3.824 | Q(18.25) = 156.82 |
| Minimum Energy | 0. cm⁻¹ | Q(9.375) = 55.9114 |
| Dipoles | | |
| μ(a) | 1.396 | A = 66100.14 |
| μ(b) | 0.260 | B = 11762.577 |
| μ(c) | | C = 9969.943 |

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


The dipole moment was assumed the same as the parent species, tag #46005.
Species Tag: 48001  
Species Name: $\text{SO}$, sulfur monoxide, $\Sigma$ ground state

Version: 1  
Date: Dec 1979  
Contributor: H. M. Pickett

Lines Listed = 330 $Q(300.) = 850.159$
Max. Frequency = 3000 GHz $Q(225.) = 632.266$
Max. J = 50 $Q(150.) = 414.277$
LOGSTR = -6 $Q(75.) = 197.515$
LOGSTRI = $Q(37.5) = 90.3441$
Isotope Correction = -0.022 $Q(18.25) = 38.8776$
Minimum Energy = 0. cm$^{-1}$ $Q(9.375) = 15.9038$
Dipoles: $\mu(a) = 1.55$  
$\mu(b) = A$
$\mu(c) = B = 21523.02$

The calculational method is described in T. Amano and E. Hirota, 1974, J. Molec. Spectroscopy 53, 346. The data used is from W. W. Clark and F. C. DeLucia, 1976, J. Molec. Spectroscopy 60, 332. Both electric dipole and magnetic dipole transitions are listed.
Species Tag: 48002  
Species Name: SO, sulfur monoxide

Version: 1  
Date: Dec 1979  
Contributor: H. M. Pickett

3^2 ground state, v=1 vibrational state

Lines Listed = 251  
Max. Frequency = 3000 GHz  
Max. J = 50  
LOGSTR = -8  
LOGSTR1 =  
Isotope Correction = -0.022  
Minimum Energy = 1111.5 cm^-1  

Dipoles:  
\( \mu(a) = 1.55 \)  
\( \mu(b) = \)  
\( \mu(c) = \)

\[ Q(300.) = 850.159 \]  
\[ Q(225.) = 632.266 \]  
\[ Q(150.) = 414.477 \]  
\[ Q(75.) = 197.515 \]  
\[ Q(0, 37.5) = 90.344 \]  
\[ \gamma(18, 25) = 38.8766 \]  
\[ \gamma(9, 37.5) = 15.9038 \]  
\[ A = \]  
\[ B = 21351.0 \]  
\[ C = \]

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 \( \gamma \). Morino, 1967, J. Phys. Soc. Japan 22, 399. All centrifugal distortion constants were fixed to their ground state values. Magnetic and electric dipole transitions are included.

This state is 1111.5 cm^-1 above v=0 (G. Herzberg, 1950, Spectra of Diatomic Molecules, Van Nostrand, New York).
Species Tag: 48003  
Species Name: H$_2$C$^{34}$S

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

34S isotope

<table>
<thead>
<tr>
<th>Lines Listed</th>
<th>Max. Frequency</th>
<th>Max. J</th>
<th>LOGSTR</th>
<th>LOGSTR1</th>
<th>Isotope Correction</th>
<th>Minimum Energy</th>
<th>Dipoles</th>
</tr>
</thead>
<tbody>
<tr>
<td>111</td>
<td>343 GHz</td>
<td>10</td>
<td>-9</td>
<td></td>
<td>-1.376</td>
<td>0. cm$^{-1}$</td>
<td>(a) = 1.647</td>
</tr>
</tbody>
</table>
<pre><code>                    | Q(300.) = 6084.16 | Q(225.) = 4563.52 | Q(150.) = 2150.80 | Q(75.) = 760.502 | Q(37.5) = 259.239 | Q(18.25) = 92.2997 | Q(9.375) = 28.0092 |
</code></pre>
<p>|              |                |        |        |          |                   |               | (b) =       |
|              |                |        |        |          |                   |               | (c) =       |</p>

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333. The measurements were taken from D. R. Johnson, F. J. Lovas and W. H. Kirchhoff, 1972, J. Phys. Chem. Ref. Data 1, 1011. Other references were taken from this paper.

The dipole moment was assumed to be the same as the parent species.
Species Tag: 48004  Species Name: $^{160}_3$ ozone

Version: 2
Date: Mar 1984
Contributor: H. M. Pickett

Lines Listed = 6471  Q(300.) = 3553.04
Max. Frequency = 10000 GHz  Q(225.) = 2263.60
Max. J = 80.  Q(150.) = 1198.67
LOGSTR = -10.  Q(75.) = 423.448
LOGSTRI = -10.  Q(37.5) = 150.037
Isotope Correction = 0.  Q(18.25) = 53.2967
Minimum Energy = 0. cm$^{-1}$  Q(9.375) = 19.0371

Dipoles: $\mu(a)$ = A = 106535.234
$\mu(b)$ = 0.5324  B = 13349.090
$\mu(c)$ = C = 11834.524

The catalog of the ozone lines is based on the work of M. J. C. Depannemaeker, B. Duterage, and M. J. Bellet, 1977, J. Quant. Spect. Radiat. Transfer 17, 519. Additional lines are cited in F. J. Lovas, 1978, J. Phys. Chem. Ref. Data 7, 1445. Further lines were measured at JPL by E. A. Cohen. The ground state lines were fit with the $v_1$ and $v_3$ lines and infrared lines in the 10$\mu$ region simultaneously. The maximum value of $K_a$ is 20.

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

The partition function includes contributions from all vibrational states.
<table>
<thead>
<tr>
<th>Species Tag:</th>
<th>48005</th>
<th>Species Name:</th>
<th>( \text{O}_3 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Version:</td>
<td>2</td>
<td>( v_2 )</td>
<td>vibrational</td>
</tr>
<tr>
<td>Date:</td>
<td>Mar 1984</td>
<td>state (010)</td>
<td></td>
</tr>
<tr>
<td>Contributor:</td>
<td>H. M. Pickett</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Lines Listed</td>
<td>4337</td>
<td>Q( (300.) = 3553.04 )</td>
<td></td>
</tr>
<tr>
<td>Max. Frequency</td>
<td>3000 GHz</td>
<td>Q( (225.) = 2263.60 )</td>
<td></td>
</tr>
<tr>
<td>Max. J</td>
<td>60</td>
<td>Q( (150.) = 1198.67 )</td>
<td></td>
</tr>
<tr>
<td>LOGSTR</td>
<td>-10.</td>
<td>Q( (75.) = 423.448 )</td>
<td></td>
</tr>
<tr>
<td>LOGSTR1</td>
<td>-10.</td>
<td>Q( (37.5) = 150.037 )</td>
<td></td>
</tr>
<tr>
<td>Isotope Correction</td>
<td>0.</td>
<td>Q( (18.25) = 53.2967 )</td>
<td></td>
</tr>
<tr>
<td>Minimum Energy</td>
<td>700.9 cm(^{-1})</td>
<td>Q( (9.375) = 19.0371 )</td>
<td></td>
</tr>
<tr>
<td>Dipoles: ( u(a) )</td>
<td>A = 108137.979</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( u(b) )</td>
<td>B = 13311.143</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( u(c) )</td>
<td>C = 11765.222</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The \( v_2 \) ozone lines were derived from a fit of the data given by M. J. C. Depannemaeker, B. Duterage, and M. J. Bellet, 1977, J. Quant. Spect. and Radiat. Transfer 17, 519. Additional lines are listed in F. J. Lovas, 1978, J. Phys. Chem. Ref. Data., 7, 1445. Further lines were measured at JPL by E. A. Cohen. The maximum valued \( K \) is 15.

The dipole moment was assumed to be the same as the parent species.
Species Tag: 48006  
Species Name: O₃  
Version: 2  
Date: Mar 1984  
Contributor: H. M. Pickett  

| Lines Listed | 9459 |  
| Max. Frequency | 10000 GHz |  
| Max. J | 80 |  
| LOGSTR | -10. |  
| MAXSTR1 | -10. |  
| Isotope Correction | 0. |  
| Minimum Energy | 1042 cm⁻¹ |  
| Dipole: μ(a) | | A = 104944. |  
| μ(b) | 0.5324 | B = 13229.7 |  
| μ(c) | | C = 11726.6 |  

The rotational lines were measured by T. Tanaka and Y. Morino, 1970, J. Mol. Spec. 33, 538 and A. Barbe, et al., 1977, J. Mol. Spec. 64, 343. The rotational lines of the ground, v₁ and v₃ states were fit along with infrared lines in the 10μ region simultaneously. The maximum value of K₃ is 20.

The (100) state has a vibrational label of 1, and the (001) state has a vibrational label of 3.
Species Tag: 48007  
Species Name: \( \text{O}_3 \nu_2 = 2 \) state \( \text{(0,2,0)} \)  
Version: 1  
Date: Mar 1984  
Contributor: H. M. Pickett  

| Lines Listed  | 1779 |  
| Max. Frequency | 9999 GHz |  
| Max. J | 50 |  
| LOGSTR | -10. |  
| LOGSTR1 | -10. |  
| Isotope Correction | -0 |  
| Minimum Energy | 1400. cm\(^{-1} \) |  
| Dipole (a) | A = 109796. |  
| Dipole (b) | 0.5324 |  
| Dipole (c) | B = 13273. |  

Data measured at JPL were combined with that of T. Tanaka and Y. Morino, 1970, J. Mol. Spectrosc. 33, 538.
| Species Tag: | 49001 | Species Name: | $^{16}O_{17}O_{016}$ | Ozone symmetric $^{17}O$ substitution |
| Version: | 1 | |
| Date: | Mar 1984 | |
| Contributor: | H. M. Pickett | |
| Lines Listed = | 13277 | Q(300.) = 19114.5 |
| Max. Frequency = | 999. GHz | Q(225.) = 13038.6 |
| Max. J = | 37 | Q(150.) = 7299.7 |
| LOGSTR = | -7.2 | Q(75.) = 2597.63 |
| LOGSTRI = | -7.2 | Q(37.5) = 920.348 |
| Isotope Correction = | -3.432 | Q(18.25) = 327.0 |
| Minimum Energy = | 0. cm$^{-1}$ | Q(9.375) = 116.8 |
| Dipoles : |  | |
| $\mu(a)$ = |  | A = 102351. |
| $\mu(b)$ = | 0.5324 | B = 13350.8 |
| $\mu(c)$ = |  | C = 11781.9 |

The spectra and calculation are from E. A. Cohen and H. M. Pickett, 1985, J. Molec. Str. 97, 97-100.
Species Tag: 49002
Species Name: 170-160-160
Ozone asymmetric
170 substitution

Version: 1
Date: Mar 1984
Contributor: H. M. Pickett

Lines Listed = 24138
Max. Frequency = 9999. GHz
Max. J = 37
LOGSTR = -7.5
LOGSTR1 = -7.5
Isotope Correction = -3.131
Minimum Energy = 0. cm^-1

Dipoles:
\[ \mu(a) = 0.0034 \]
\[ \mu(b) = 0.5324 \]
\[ \mu(c) = \]

Q(300.) = 40541.5
Q(225.) = 2732.5
Q(150.) = 14831.8
Q(75.) = 5257.0
Q(37.5) = 1862.4
Q(18.25) = 661.58
Q(9.375) = 236.21

\[ A = 105491. \]
\[ B = 12951. \]
\[ C = 11508. \]

The spectra and calculation are from E. A. Cohen and H. M. Pickett, 1983, J. Molec. Str. 97, 97-100. Additional lines have been measured by E. A. Cohen and K. Hillig. The calculation includes quadrupole interactions of \( \Delta N = 0, \pm 1, \pm 2 \).
Species Tag: 50001
Species Name: $^{34}\text{SO}$, sulfur monoxide,
Version: 1
$^{3\pi}$ ground state,
Date: Dec 1979
$^{34}\text{S}$ isotope
Contributor: H. M. Pickett

Lines Listed = 280
Max. Frequency = 3000 GHz
Max. J = 50
LOGSTR = -6
LOGSTR1 =
Isotope Correction = -1.376
Minimum Energy = 0 cm$^{-1}$
Dipoles: $\mu(a) = 1.55$
$\mu(b) =$
$\mu(c) =$

Q(300.) = 866.963
Q(225.) = 644.615
Q(150.) = 422.669
Q(75.) = 201.326
Q(37.5) = 92.0449
Q(18.25) = 39.5549
Q(9.375) = 16.1473

Species Tag: 50002  
Species Name: $^{32}$O, sulfur monoxide $^{3}$ ground state  
Version: 1  
Date: Dec 1979  
Contributor: H. M. Pickett  

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

The calculational method is described in T. Amano and E. Hirota, 1974, J. Molec. Spectroscopy 53, 346. The value of $\nu$ was fixed at -156.5 MHz and $\nu(1)$ was set to zero. Both electric dipole and magnetic dipole transitions are listed in the catalogue. The data used is listed in E. Tiemann, 1974, J. Phys. Chem. Ref. Data. 3, 259.
Species Tag: 50003  
Species Name: $^{160}$O$^{180}$O$^{160}$ ozone, ground state, symmetric $^{180}$ isotope

Date: Mar 1984  
Contributor: H. M. Pickett and R. L. Poynter

<table>
<thead>
<tr>
<th>Lines Listed</th>
<th>3184</th>
<th>(Q(300.) = 3525.34)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max. Frequency</td>
<td>9999. GHz</td>
<td>(Q(225.) = 2445.129)</td>
</tr>
<tr>
<td>Max. J</td>
<td>50</td>
<td>(Q(150.) = 1247.107)</td>
</tr>
<tr>
<td>LOGSTR</td>
<td>-9</td>
<td>(Q(75.) = 441.8769)</td>
</tr>
<tr>
<td>LOGSTR1</td>
<td>-9</td>
<td>(Q(37.5) = 156.5677)</td>
</tr>
<tr>
<td>Isotope Correction</td>
<td>-2.690</td>
<td>(Q(18.25) = 55.6161)</td>
</tr>
<tr>
<td>Minimum Energy</td>
<td>0. cm(^{-1})</td>
<td>(Q(9.375) = 19.8610)</td>
</tr>
</tbody>
</table>

Dipoles:
\(\mu(a) = 98646.687\)  
\(\mu(b) = 0.5324\)  
\(\mu(c) = 13352.732\)  
\(C = 11/31.767\)

The catalog of symmetric $^{180}$ ozone is based on the work of J. Depanlemäecker and J. Beilet (1977, J. Mol. Spectry. 66, 106). The dipole moment used is the \(^{160}_3\) value. The new version extends the calculation in frequency and J.
Species Tag: 50004  
Species Name: \( \text{H}_2\text{O}_2 \), asymmetric \( \text{O}_3 \) ozone, ground state

Version: 2  
Date: Mar 1984  
Contributor: H. M. Pickett and R. L. Poynter

Lines Listed = 7304  
Max. Frequency = 9999 GHz  
Max. J = 40  
LOGSTR = -9  
LOGSTRI = -9  
Isotope Correction = -2.389  
Minimum Energy = 0. cm\(^{-1}\)

Dipoles:  
\( u(\alpha) = 0.0068 \)  
\( u(\beta) = 0.5324 \)  
\( u(\gamma) = \) (missing)

The catalog of asymmetric \(^{180}\) ozone is based on the work of J. Depannemaecker and J. Bellet (1977, J. Mol. Spectry. 66, 106). The dipole moment used is the \(^{160}\) value rotated to the inertial axes of asymmetric \(^{180}\) ozone (based on the equilibrium structure). The new version extends the calculation in frequency and J.
Species Tag: 500005  
Species Name: $O_3$ symmetric $O^{18}$

Version: 1  
Date: Mar 1984  
Contributor: C. Chiu and E. A. Cohan

<table>
<thead>
<tr>
<th>Lines Listed</th>
<th>Max. Frequency</th>
<th>Max. J</th>
<th>LOGSTR</th>
<th>LOGSTR1</th>
<th>Isotope Correction</th>
<th>Minimum Energy</th>
<th>Dipoles: $\mu(a)$</th>
<th>$\mu(b)$</th>
<th>$\mu(c)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2387</td>
<td>9999 GHz</td>
<td>50</td>
<td>-8.9</td>
<td>-8.9</td>
<td>2.590</td>
<td>678 cm$^{-1}$</td>
<td>100177.</td>
<td>13316.</td>
<td>11659.</td>
</tr>
</tbody>
</table>

New spectra were measured at JPL and were fit to a Watson "S" set Hamiltonian. The assumed dipoles are based on the ground state. The vibrational energy is an assumed value.
Species: 5U006  Species Name: O$_3$ asymmetric  
Version: 1  
Date: Mar 1984  
Contributor: C. Chiu and E. A. Cohen  

Lines Listed = 42.3  
Max. Frequency = 9999 GHz  
Max. J = 50  
LOGSTR = -9.  
LOGSTRI = -9.  
Isotope Correction =  
Minimum Energy = 693 cm$^{-1}$  
Dipoles: $\mu(a) = 0.0068$  
$\mu(b) = 0.5324$  
$\mu(c) = \text{not listed}$  

New spectra were measured at JPL and were fit to a Watson "S" set Hamiltonian. The assumed dipoles are based on the ground state. The vibrational energy is an assumed value.
Species Tag: 51001  Species Name: HCCCN, cyanoacetylene
Version: 2
Date: Mar 1984
Contributor: R. L. Poynter

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

The set of experimental lines used in the calculation was obtained from the references in W. J. Lafferty and F. J. Lovas, 1978, J. Phys. Chem. Ref. Data, 7, 441.
Species Tag: 51002  
Species Name: $^{35}\text{ClO}$, chlorine monoxide

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

Lines Listed = 2610  
Max. Frequency = 3000 GHz  
Max. J = 87.5  
LOGSTR = -10  
LOGSTR1 =  
Isotope Correction = -0.122  
Minimum Energy = 0. cm$^{-1}$  
Dipoles: $\mu(a) = 1.239$, $\mu(b) =$, $\mu(c) =$

The experimental lines below 200 GHz are from R. K. Kakar, E. A. Cohen, and M. Geller, 1978, J. Mol. Spec. 70, 243. Lines above 200 GHz were measured at JPL by E. A. Cohen and H. M. Pickett. The lines were fit to a fine structure Hamiltonian which included $p_0$ and $q_0$ terms and centrifugal distortion on $B$ to sixth power in $J$. The hyperfine terms in the Hamiltonian included all off-diagonal matrix elements for $a$, $b$, $c$, $d$, $n_1$, $n_2$, and $n_3$. The partition function was determined by a sum over states to $F = 86$ for both the $\Omega =3/2$ and $\Omega =1/2$ states.
Species Tag: 52001  
Species Name: H$_{13}$CCCN  
Version: 1  
Date: Dec 1979  
Contributor: R. L. Poynter  

**Lines Listed** = 152  
**Max. Frequency** = 1000 GHz  
**Max. J** = 99  
**LOGSTR** = -7  
**LOGSTR1** = 0  
**Isotope Correction** = -1.955  
**Minimum Energy** = 0. cm$^{-1}$  
Dipoles: $u(a) = 3.724$  
$u(b) = 4530.198$  
$u(c) = 4530.198$

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 3.724 D.
<table>
<thead>
<tr>
<th>Species Tag:</th>
<th>52002</th>
<th>Species Name:</th>
<th>HCl$^1_3$CCN</th>
</tr>
</thead>
<tbody>
<tr>
<td>Version:</td>
<td>1</td>
<td>cyanoacetylene</td>
<td></td>
</tr>
<tr>
<td>Date:</td>
<td>Dec 1979</td>
<td>$^{13}$C isotope on</td>
<td></td>
</tr>
<tr>
<td>Contributor:</td>
<td>R. L. Poynter</td>
<td>atom 2</td>
<td></td>
</tr>
<tr>
<td>Lines Listed =</td>
<td>146</td>
<td>Q(300.) =</td>
<td>4140.95</td>
</tr>
<tr>
<td>Max. Frequency =</td>
<td>1000 GHz</td>
<td>Q(225.) =</td>
<td>3106.71</td>
</tr>
<tr>
<td>Max. $J$ =</td>
<td>99</td>
<td>Q(150.) =</td>
<td>2071.10</td>
</tr>
<tr>
<td>LOGSTR =</td>
<td>-7</td>
<td>Q( 75.) =</td>
<td>1036.10</td>
</tr>
<tr>
<td>LOGSTR1 =</td>
<td></td>
<td>Q( 37.5) =</td>
<td>518.561</td>
</tr>
<tr>
<td>Isotope Correction =</td>
<td>-1.955</td>
<td>Q(18.25) =</td>
<td>259.777</td>
</tr>
<tr>
<td>Minimum Energy =</td>
<td>0. cm$^{-1}$</td>
<td>Q(9.375) =</td>
<td>130.377</td>
</tr>
<tr>
<td>Dipoles: $\mu(a)$ =</td>
<td>3.724</td>
<td>$A =$</td>
<td></td>
</tr>
<tr>
<td>$\mu(b)$ =</td>
<td></td>
<td>$B =$</td>
<td>4529.76</td>
</tr>
<tr>
<td>$\mu(c)$ =</td>
<td></td>
<td>$C =$</td>
<td></td>
</tr>
</tbody>
</table>

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.
<table>
<thead>
<tr>
<th>Species Tag:</th>
<th>52003</th>
<th>Species Name:</th>
<th>H\textsuperscript{3}CCCN cyanoacetylene 13C isotope atom 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Version:</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Date:</td>
<td>Dec 1979</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Contributor:</td>
<td>R. L. Poynter</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

| Lines Listed      | 144                    | Q(300.)       | 4255.01                                                  |
| Max. Frequency    | 1000 GHz               | Q(225.)       | 3192.27                                                  |
| Max. J            | 99                     | Q(150.)       | 2128.14                                                  |
| LOGSTR            | -7                     | Q(75.)        | 1064.63                                                  |
| LOGSTR1           |                         | Q(37.5)       | 532.72                                                  |
| Isotope Correction| -1.955                 | Q(18.25)      | 266.870                                                  |
| Minimum Energy    | 0. cm\(^{-1}\)         | Q(9.375)      | 133.937                                                  |
| Dipoles:          |                        |               |                                                           |
| \(\mu(a)\)       | 3.724                  | A             |                                                           |
| \(\mu(b)\)       |                        | B             | 4408.44                                                  |
| \(\mu(c)\)       |                        | C             |                                                           |

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

The dipole moment was remeasured by the above authors as 3.724 D.
<table>
<thead>
<tr>
<th>Lines Listed</th>
<th>99</th>
<th>Q(300.) = 1415.47</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max. Frequency</td>
<td>1000 GHz</td>
<td>Q(225.) = 1061.94</td>
</tr>
<tr>
<td>Max. J</td>
<td>99</td>
<td>Q(150.) = 708.109</td>
</tr>
<tr>
<td>LOGSTR</td>
<td>-6</td>
<td>Q(75.) = 354.161</td>
</tr>
<tr>
<td>LOGSTR1</td>
<td></td>
<td>Q(37.5) = 177.256</td>
</tr>
<tr>
<td>Isotope Correction</td>
<td>-2.432</td>
<td>Q(18.25) = 83.7973</td>
</tr>
<tr>
<td>Minimum Energy</td>
<td>0 cm(^{-1})</td>
<td>Q(9.375) = 44.5656</td>
</tr>
</tbody>
</table>

Dipoles:
- \(\mu(a) = 3.724\), A =
- \(\mu(b) = \)
- \(\mu(c) = 4416.75\), 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.
Species Tag: 52005
Version: 1
Date: Dec. 1979
Contributor: R. L. Poynter

<table>
<thead>
<tr>
<th>Lines Listed</th>
<th>156</th>
<th>Q(300.)</th>
<th>4443.2393</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max. Frequency</td>
<td>1000 GHz</td>
<td>Q(225.)</td>
<td>3332.7310</td>
</tr>
<tr>
<td>Max. J</td>
<td>99</td>
<td>Q(150.)</td>
<td>2222.2842</td>
</tr>
<tr>
<td>LOGSTR</td>
<td>-7</td>
<td>Q(75.)</td>
<td>1111.7319</td>
</tr>
<tr>
<td>LOGSTR1</td>
<td></td>
<td>Q(37.5)</td>
<td>556.2878</td>
</tr>
<tr>
<td>Isotope Correction</td>
<td>-3.824</td>
<td>Q(18.25)</td>
<td>278.6121</td>
</tr>
<tr>
<td>Minimum Energy</td>
<td>0. cm⁻¹</td>
<td>Q(9.375)</td>
<td>139.8297</td>
</tr>
<tr>
<td>Dipoles:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>μ(a)</td>
<td>3.724</td>
<td>A</td>
<td></td>
</tr>
<tr>
<td>μ(b)</td>
<td>4221.58</td>
<td></td>
<td></td>
</tr>
<tr>
<td>μ(c)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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  
Species Name: HO$^{35}$Cl, hypochlorous acid

| Lines Listed | 3919 |  
| Max. Frequency | 10000 GHz |  
| Max. J | 60 |  
| LOGSTR | -8 |  
| LOGSTR1 | -8 |  
| Isotope Correction | -0.122 |  
| Minimum Energy | 0 cm$^{-1}$ |  
| Dipoles: |  
| \( u(a) \) | 0.3627 |  
| \( u(b) \) | 1.471 |  
| \( u(c) \) |  

The data and calculational method are given in H. E. Singbeil, et al. 1984, J. Molec. Spectr. 103, 466. Chlorine hyperfine structure is omitted in this version of the catalogue since the splittings are generally smaller than the width of lower stratospheric lines. Maximum value of \( K \) in the calculation is 20.
Species Tag: 53001 Species Name: C2H3CN, acrylonitrile
Version: 1
Date: Jan 1980
Contributor: R. L. Poynter

Lines Listed = 3697 Q(300.) = 26198.1
Max. Frequency = 3000 GHz Q(225.) = 17016.2
Max. J = 40 Q(150.) = 9262.4
LOGSTR = -9 Q(75.) = 3243.7
LOGSTR1 = Q(37.5) = 1159.8
Isotope Correction = 0 Q(18.25) = 410.9
Minimum Energy = 0. cm⁻¹ Q(9.375) = 145.8
Dipoles: μ(a) = 3.68 A = 49850.712
μ(b) = 1.25 B = 4971.0849
μ(c) = C = 4513.8005

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


Species Tag: 53002  Species Name: $^{37}$ClO,
Version: 2  chlorine monoxide,
Date: Oct 1980  $^{37}$Cl isotope
Contributor: H. M. Pickett

Lines Listed = 2649  Q(300.) = 3348.1118
Max. Frequency = 3000 GHz  Q(225.) = 2336.6826
Max. J = 85  Q(150.) = 1448.4390
LOGSTR = -10  Q(75.) = 700.9711
LOGSTRI = 0  Q(37.5) = 357.1905
Isotope Correction = -0.611  Q(18.25) = 186.3374
Minimum Energy = 0. cm$^{-1}$  Q(9.375) = 101.2744
Dipoles: $\mu$(a) = 1.239  A =
$\mu$(b) = B = 1828.70
$\mu$(c) = C =

The experimental lines below 200 GHz are from R. K. Kakar, E. A. Cohen, and M. Geller, 1978, J. Mol. Spec. 70, 243. Lines above 200 GHz were measured at JPL by E. A. Cohen and H. M. Pickett. The lines were fit to a fine structure Hamiltonian which included p$_D$ and q$_D$ terms and centrifugal distortion on B to sixth power in J. The hyperfine terms in the Hamiltonian included all off-diagonal matrix elements for a, b, c, d, n$_1$, n$_2$, and n$_3$. The partition function was determined by a sum over states to $F = 86$ for both the $\Omega = 1/2$ and $\Omega = 3/2$ states.
<table>
<thead>
<tr>
<th>Field</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Species Tag</td>
<td>54001</td>
</tr>
<tr>
<td>Species Name</td>
<td>CH\textsubscript{2}CH\textsuperscript{13}CN, acrylonitrile, \textsuperscript{13}C isotope on atom 1</td>
</tr>
<tr>
<td>Version</td>
<td>1</td>
</tr>
<tr>
<td>Date</td>
<td>Jan 1980</td>
</tr>
<tr>
<td>Contributor</td>
<td>R. L. Poynter</td>
</tr>
<tr>
<td>Lines Listed</td>
<td>118</td>
</tr>
<tr>
<td>Max. Frequency</td>
<td>3000 GHz</td>
</tr>
<tr>
<td>Max. J</td>
<td>10</td>
</tr>
<tr>
<td>LOGSTR</td>
<td>-9</td>
</tr>
<tr>
<td>Isotope Correction</td>
<td>-1.955</td>
</tr>
<tr>
<td>Minimum Energy</td>
<td>0. \text{ cm}^{-1}</td>
</tr>
<tr>
<td>Dipoles: ( \mu(a) )</td>
<td>3.68</td>
</tr>
<tr>
<td>Dipoles: ( \mu(b) )</td>
<td>1.25</td>
</tr>
<tr>
<td>Dipoles: ( \mu(c) )</td>
<td></td>
</tr>
<tr>
<td>Q(300.)</td>
<td>26332.9770</td>
</tr>
<tr>
<td>Q(225.)</td>
<td>17104.0740</td>
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<tr>
<td>Q(150.)</td>
<td>9311.0723</td>
</tr>
<tr>
<td>Q(75.)</td>
<td>3291.5420</td>
</tr>
<tr>
<td>Q(37.5)</td>
<td>1163.8567</td>
</tr>
<tr>
<td>Q(18.)</td>
<td>358.5091</td>
</tr>
<tr>
<td>Q(9.3)</td>
<td>138.3247</td>
</tr>
<tr>
<td>(\mu) (a)</td>
<td>49781.</td>
</tr>
<tr>
<td>(\mu) (b)</td>
<td>4948.153</td>
</tr>
<tr>
<td>(\mu) (c)</td>
<td>4494.485</td>
</tr>
</tbody>
</table>

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 G. P. Stoicheff, 1959, J. Chem. Phys. 30, 77.

The dipole moment was assumed to be the same as the parent species.
Species Tag: 54U02  Species Name: CH$_2^{13}$CHCN, acrylonitrile, $^{13}$C isotope on atom 2
Version: 1
Date: Jan 1980
Contributor: R. L. Poynter

<table>
<thead>
<tr>
<th>Lines Listed</th>
<th>Max. Frequency</th>
<th>Max. J</th>
<th>LOGSTR</th>
<th>LOGSTR1</th>
<th>Isotope Correction</th>
<th>Minimum Energy</th>
<th>Dipoles:</th>
<th>A</th>
<th>B</th>
<th>C</th>
</tr>
</thead>
<tbody>
<tr>
<td>117</td>
<td>3000 GHz</td>
<td>10</td>
<td>-9</td>
<td></td>
<td>-1.955</td>
<td>0. cm$^{-1}$</td>
<td>u(a) = 3.68</td>
<td>48645</td>
<td>4948700</td>
<td>4485.145</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>u(b) = 1.25</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>u(c)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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

The dipole moment was assumed to be the same as the parent species.
Species Tag: 54003
Species Name: $^{13}$CH$_2$CHCN,
13C isotope on
acrylonitrile,
atom 3

Date: Jan 1980
Contributor: R. L. Poynter

Lines Listed = 116
Max. Frequency = 178 GHz
Max. J = 10
LOGSTR = -9
LOGSTR1 =
Isotope Correction = -1.955
Minimum Energy = 0. cm$^{-1}$
Dipoles: $\mu(a) = 3.68$
$\mu(b) = 1.25$
$\mu(c) =$

Q(300.) = 27089.4530
Q(225.) = 26631.7500
Q(150.) = 9578.5527
Q(75.) = 3386.0991
Q(37.5) = 1197.2913
Q(18.25) = 366.8595
Q(9.375) = 141.7098

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

The dipole moment was assumed to be the same as the parent species.
Species Tag: 54004  
Species Name: CH₂COCN, acrylonitrile, deuterium isotope on atom 2  
Version: 1  
Date: Jan 1980  
Contributor: R. L. Pointer

| Lines Listed | 322 | Q(300.) = 29696.1490 |
| Max. Frequency | 300C GHz | Q(225.) = 19253.5940 |
| Max. J | 10 | Q(150.) = 10500.2640 |
| LOGSTR | -10 | Q(75.) = 3711.9375 |
| LOGSTR1 |  | Q(37.5) = 1312.5034 |
| Isotope Correction | -3.824 | Q(18.25) = 402.1610 |
| Minimum Energy | 0. cm⁻¹ | Q(9.375) = 155.4532 |

Dipoles:  
- \( \mu(a) = 3.68 \)  
- \( \mu(b) = 1.25 \)  
- \( \mu(c) = \)  

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

The dipole moment was assumed to be the same as the parent species.
Species Tag: 54005
Species Name: HO$^{37}$Cl, hypochlorous acid,
Version: 2
Date: Jan 1984
Contributor: H. M. Pickett

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

The data and calculational method are given in H. E. Singbeil, et al, 1984, J. Molec. Spectr. 103, 466. Chlorine hyperfine structure is omitted in this version of the catalogue since the splittings are generally smaller than the width of lower stratospheric lines. Maximum value of K in the calculation is 20.
Species Tag: 55001  
Species Name: C$_2$H$_5$CN, ethyl cyanide

Version: 2  
Date: Jan 1981  
Contributor: R. L. Poynter

Lines Listed = 3684  
Max. Frequency = 3000 GHz  
Max. J = 21  
LOGSTR = -5 above 160 GHz  
LOGSTRI = Q(18.25) = 1406.3713

Isotope Correction = 0  
Minimum Energy = 0 cm$^{-1}$  
Dipoles:  
$\mu(a) = 3.85$  
$\mu(b) = 1.23$  
$\mu(c) = 1.23$

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:


The dipole moment was taken from H. M. Heise, H. Lutz, and H. Dreizler, 1974, Z. Naturforsch. 29a, 1345.
Species Tag: 56001  
Species Name: CH$_2$CH$_2^{13}$CN, ethyl cyanide, $^{13}$C isotope on atom 1

Version: 2
Date: Jan 1981
Contributor: R. L. Poynter

| Lines Listed | 1183 |
| Max. Frequency | 3000 GHz |
| Max. J | 10 |
| LOGSTR | -5 above 160 GHz |
| LOGSTR1 | Q(37.5) = 4620.6172 |
| Isotope Correction | -1.955 |
| Minimum Energy | 0 cm$^{-1}$ |
| Dipole: | (a) = 3.84, A = 27634.94 |
| | (b) = 1.37, B = 4689.805 |
| | (c) = C = 4214.746 |


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

The dipole moment was assumed the same as in the parent species, tag #55001.
Species Tag: 56003  
Species Name: $^{13}\text{CH}_3\text{CH}_2\text{CN}$, ethyl cyanide, $^{13}\text{C}$ isotope on atom 3

Version: 2  
Date: Jan 1981

Contributor: R. L. Poynter

Lines Listed = 1183  
Max. Frequency = 3000 GHz  
Max. J = 10  
LOGSTR = -9 below 160 GHz  
LOGSTR1 = -5 above 160 GHz  
Isotope Correction = -1.955  
Minimum Energy = 0 cm$^{-1}$

Dipoles:

\[
\begin{align*}
\{(a)\} &= 3.84 \\
\{(b)\} &= 1.37 \\
\{(c)\} &= \_13.7
\end{align*}
\]

A = 27342.174  
B = 4597.939  
C = 4133.707


The dipole moment was assumed the same as in the parent species, tag #55001.
The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333. The measurements were taken from H. M. Heise, H. Mader, and H. Dreizler, 1976, Z. Naturforsch. 31a, 1228.

The dipole moment was assumed the same as in the parent species, tag #55001.
Species Tag: 56005  
Species Name: CH$_2$DCH$_2$CN-s, ethyl cyanide, deuterium isotope on methyl carbon trans to CN group  
Version: 2  
Date: Jan 1981  
Contributor: R. L. Poynter

Lines Listed = 1166  
Max. Frequency = 3000 GHz  
Max. J = 10  
LOGSTR = -9 below 160 GHz  
LOGSTR1 = -5 above 160 GHz  
Isotope Correction = -3.347  
Minimum Energy = 0 cm$^{-1}$  
Dipoles: $u(a) = 3.84$ cm$^{-1}$  
$u(b) = 1.37$  
$u(c) =$


The dipole moment was assumed to be the same as the parent species.
Species Tag: 56006  
Species Name: CH₂DCH₂CN-a, ethyl cyanide, deuterium isotope on methyl carbon gauche to the CN group

Version: 2
Date: Jan 1981
Contributor: R. L. Poynter

Lines Listed = 1286  
Max. Frequency = 3000 GHz  
Max. J = 10  
LOGSTR = -9 below 160 GHz  
LOGSTR1 = -5 above 160 GHz  
Isotope Correction = -3.347  
Minimum Energy = 0. cm⁻¹  
Dipoles: μ(a) = 3.84  
μ(b) = 1.37  
μ(c) =

Q(300.) = 121059.9  
Q(225.) = 76736.2  
Q(150.) = 42815.4  
Q(75.) = 15132.5  
Q(37.5) = 5350.1  
Q(18.25) = 1827.2  
Q(9.375) = 623.25  
A = 25022.568  
B = 4583.422  
C = 4110.245


The dipole moment was assumed to be the same as the parent species.
Species Tag: 60001
Species Name: OCS
Version: 2
Date: Jan 1981
Contributor: R. L. Poynter

Lines Listed = 99
Max. Frequency = 3000 GHz
Max. J = 99
LOGSTR = -7
LOGSTRI = -7
Isotope Correction = -0.022
Minimum Energy = 0. cm⁻¹
Dipoles: μ(a) = 0.715
μ(b) =
μ(c) =


Species Tag: 60002  
Species Name: $^{28}\text{Si}^{32}\text{S}$ silicon monosulfide  

Version: 1  
Date: Dec 1979  
Contributor: R. L. Poynter  

<table>
<thead>
<tr>
<th>Lines Listed</th>
<th>97</th>
<th>Q(300.)</th>
<th>688.9700</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max. Frequency</td>
<td>3000 GHz</td>
<td>Q(225.)</td>
<td>517.1307</td>
</tr>
<tr>
<td>Max. J</td>
<td>97</td>
<td>Q(150.)</td>
<td>344.8263</td>
</tr>
<tr>
<td>LOGSTR</td>
<td>-5</td>
<td>Q(75.)</td>
<td>172.5440</td>
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<tr>
<td>Isotope Correction</td>
<td>-0.057</td>
<td>Q(37.5)</td>
<td>86.4172</td>
</tr>
<tr>
<td>Minimum Energy</td>
<td>0. cm(^{-1})</td>
<td>Q(18.25)</td>
<td>43.3711</td>
</tr>
<tr>
<td>Dipoles:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\mu(a)$</td>
<td>1.730</td>
<td>A</td>
<td></td>
</tr>
<tr>
<td>$\mu(b)$</td>
<td></td>
<td>B</td>
<td>9077.45</td>
</tr>
<tr>
<td>$\mu(c)$</td>
<td></td>
<td>C</td>
<td></td>
</tr>
</tbody>
</table>


The dipole moment was assumed to be the same as the parent species.
Species Tag: 61002  Species Name: 29Si32S
Version: 1  silicon monoxide
Date: Dec 1979  29Si isotopic species
Contributor: R. L. Poynter

| Lines Listed | 98 | Q(300.) = 701.7784 |
| Max. Frequency | 3000 GHz | Q(225.) = 526.8662 |
| Max. J | 98 | Q(150.) = 351.2369 |
| LOGSTR | -5 | Q(75.) = 175.7521 |
| LOGSTR1 | | Q(37.5) = 88.0239 |
| Isotope Correction | -1.349 | Q(18.25) = 44.1774 |
| Minimum Energy | 0 cm⁻¹ | Q(9.375) = 22.2587 |
| Dipoles: | | |
| \( \mu(a) = 1.730 \) | A = | 8910.66 |
| \( \mu(b) = \) | B = | |
| \( \mu(c) = \) | C = | |


The dipole moment was assumed to be the same as the parent species.
<table>
<thead>
<tr>
<th>Lines Listed</th>
<th>Max. Frequency</th>
<th>Max. J</th>
<th>LOGSTIR</th>
<th>Isotope Correction</th>
<th>Minimum Energy</th>
<th>Dipoles: $\mu(a)$</th>
<th>$\mu(b)$</th>
<th>$\mu(c)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>99</td>
<td>3000 GHz</td>
<td>99</td>
<td>-6.4</td>
<td>-1.376</td>
<td>0. cm$^{-1}$</td>
<td>0.715</td>
<td>A</td>
<td>B = 5932.8338</td>
</tr>
</tbody>
</table>


The dipole moment was assumed to be the same as the parent species.
Species Tag: 62032  Species Name: $^{180}$OCS, carbonyl sulfide, $^{180}$O isotopic species
Version: 2  
Date: Jan 1981  
Contributor: R. L. Poynter

<table>
<thead>
<tr>
<th>Lines Listed</th>
<th>99</th>
<th>( Q(300.) = 1095.9731 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max. Frequency</td>
<td>3000 GHz</td>
<td>( Q(225.) = 822.4320 )</td>
</tr>
<tr>
<td>Max. J</td>
<td>99</td>
<td>( Q(150.) = 548.1509 )</td>
</tr>
<tr>
<td>LOGSTR</td>
<td>-6.4</td>
<td>( Q(75.) = 274.2837 )</td>
</tr>
<tr>
<td>LOGSTR1</td>
<td>( Q(37.5) = 137.3993 )</td>
<td></td>
</tr>
<tr>
<td>Isotope Correction</td>
<td>-2.712</td>
<td>( Q(18.25) = 68.8176 )</td>
</tr>
<tr>
<td>Minimum Energy</td>
<td>0 cm(^{-1})</td>
<td>( Q(9.375) = 34.5780 )</td>
</tr>
<tr>
<td>Dipoles: ( \mu(a) = 0.715 )</td>
<td>A =</td>
<td>5704.8574</td>
</tr>
<tr>
<td>( \mu(b) = )</td>
<td>B =</td>
<td></td>
</tr>
<tr>
<td>( \mu(c) = )</td>
<td>C =</td>
<td></td>
</tr>
</tbody>
</table>


The dipole moment was assumed to be the same as the parent species.
<table>
<thead>
<tr>
<th>Species Tag:</th>
<th>62003</th>
<th>Species Name:</th>
<th>$^{30}\text{Si}^{32}\text{S}$, silicon monosulfide, $^{30}\text{Si}$ isotopic species</th>
</tr>
</thead>
<tbody>
<tr>
<td>Version:</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Date:</td>
<td>Dec 1979</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Contributor:</td>
<td>R. L. Poynter</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Lines Listed</td>
<td>99</td>
<td>Q(300.) = 714.3315</td>
<td></td>
</tr>
<tr>
<td>Max. Frequency</td>
<td>3000 GHz</td>
<td>Q(225.) = 536.1669</td>
<td></td>
</tr>
<tr>
<td>Max. J</td>
<td>99</td>
<td>Q(150.) = 357.4372</td>
<td></td>
</tr>
<tr>
<td>LOGSTR</td>
<td>-5</td>
<td>Q(75.) = 178.8546</td>
<td></td>
</tr>
<tr>
<td>LOGSTRI</td>
<td></td>
<td>Q(37.5) = 89.5984</td>
<td></td>
</tr>
<tr>
<td>Isotope Correction</td>
<td>-1.528</td>
<td>Q(18.25) = 44.9573</td>
<td></td>
</tr>
<tr>
<td>Minimum Energy</td>
<td>0 cm$^{-1}$</td>
<td>Q(9.375) = 22.6465</td>
<td></td>
</tr>
<tr>
<td>Dipoles:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\mu(a)$</td>
<td>1.730</td>
<td>A =</td>
<td></td>
</tr>
<tr>
<td>$\mu(b)$</td>
<td></td>
<td>B = 8755.33</td>
<td></td>
</tr>
<tr>
<td>$\mu(c)$</td>
<td></td>
<td>C =</td>
<td></td>
</tr>
</tbody>
</table>


The dipole moment was assumed to be the same as the parent species.
### Silicon Monosulfide, $^{34}$S Isotopic Species

**Species Tag:** 62004  
**Species Name:** $^{28}$Si-$^{34}$S, silicon monosulfide, $^{34}$S isotopic species  
**Version:** 1  
**Date:** Dec 1979  
**Contributor:** R. L. Poynter  

<table>
<thead>
<tr>
<th>Lines Listed</th>
<th>Q(300.) = 708.2720</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max. Frequency</td>
<td>Q(225.) = 531.7408</td>
</tr>
<tr>
<td>Max. J</td>
<td>Q(150.) = 354.4869</td>
</tr>
<tr>
<td>LOGSTR</td>
<td>Q(75.) = 177.3781</td>
</tr>
<tr>
<td>LOGSTRI</td>
<td>Q(37.5) = 88.8383</td>
</tr>
<tr>
<td>Isotope Correction</td>
<td>Q(18.25) = 44.5862</td>
</tr>
<tr>
<td>Minimum Energy</td>
<td>Q(9.375) = 22.464/cm</td>
</tr>
<tr>
<td>Dipoles: $\mu(a)$</td>
<td>1.730</td>
</tr>
<tr>
<td>$\mu(b)$</td>
<td>B = 8828.86</td>
</tr>
</tbody>
</table>


The dipole moment was assumed to be the same as the parent species.
Species Tag: 63001
Species Name: HNO₃, nitric acid
Version: 2
Date: Jun 1983
Contributor: H. M. Pickett and R. L. Poynter

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


The dipole moment was taken from the remeasurements reported by A. P. Cox and J. M. Riveros, (1965), J. Chem. Phys. 42, 3106. Very small quadrupole splittings were resolvable for only the J = 1 + 0 transitions at dry ice temperatures. Because of the extremely large number of lines for this molecule, these splittings were not included in our predictions. Information on these quadrupole splittings can be found in D. J. Millen and J. R. Morton, (1960), J. Chem. Soc., 1523.
Species Tag: 64001  
Species Name: $S_2$, diatomic sulfur

**Version:** 1  
**Date:** Oct 1979  
**Contributor:** H. M. Pickett

| Lines Listed | 34 | $Q(300.) = 588.1659$ |
| Max. Frequency | 3000 GHz | $Q(225.) = 478.8508$ |
| Max. J | 3b | $Q(150.) = 340.0165$ |
| LOGSTR | -8.4 | $Q(75.) = 174.3814$ |
| LOGSTR1 | | $Q(37.5) = 87.7608$ |
| Isotope Correction | -0.044 | $Q(18.25) = 44.4836$ |
| Minimum Energy | 0. cm$^{-1}$ | $Q(9.375) = 22.9087$ |
| Dipoles: |  
| magnetic | $\mu(a) = A = 8831.2$ |
| | $\mu(b) = B$ |
| | $\mu(c) = C$ |

The experimentally measured lines are given in H. M. Pickett and T. L. Boyd, 1979, J. Mol. Spectry. 75, 53. The calculational method used is from T. Amano and E. Hirota, 1974, J. Mol. Spectry. 53, 346. For $S_2$, 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 $J = 50$. 

-150-
<table>
<thead>
<tr>
<th>Species Tag: 64002</th>
<th>Species Name: SO$_2$, sulfur dioxide</th>
</tr>
</thead>
<tbody>
<tr>
<td>Version: 2</td>
<td></td>
</tr>
<tr>
<td>Date: Jun 1983</td>
<td></td>
</tr>
<tr>
<td>Contributor: R. L. Poynter</td>
<td></td>
</tr>
</tbody>
</table>

- **Lines Listed**: 9622
- **Max. Frequency**: 10000 GHz
- **Max. J**: 74
- **LOGSTR**: -10
- **LOGSTR1**: -1
- **Isotope Correction**: -0.022
- **Minimum Energy**: 0 cm$^{-1}$

**Dipoles:**
- $\mu(a) = A = 60778.558$
- $\mu(b) = 1.633$
- $\mu(c) = B = 10317.913$
- $\mu(c) = C = 8799.652$


This version is a refit of all lines up through J = 74, using a new fitting program. The prediction only includes lines up through K=28.
Species Tag: 75001
Species Name: HC₅N, cyanodiacycetylene

Date: Dec 1979
Contributor: R. L. Poynter

Lines Listed = 99
Max. Frequency = 300 GHz
Max. J = 99
LOGSTR = -6.6
LOGSTRI = Q(37.5) = 587.2181
Isotope Correction = 0
Minimum Energy = 0 cm⁻¹
Dipoles: \( \mu(a) = 4.330 \) cm⁻¹
\( \mu(b) = 1331.33 \)
\( \mu(c) = \) cm⁻¹


The dipole moment was measured by the same authors.
Species Tag: 76001  
Version: 1  
Date: Dec 1979  
Contributor: R. L. Poynter  

Species Name: HCCCI$^3$CN, cyanodiacetylene, $^1$3C isotope on atom 1

Lines Listed = 99  
Max. Frequency = 300 GHz  
Max. J = 99  
LOGSTR = -6.6  
LOGSTRI = 99  
Q(300.) = 4742.4238  
Q(225.) = 3448.2642  
Q(150.) = 2336.6826  
Q(75.) = 1185.7676  
Q(37.5) = 593.0616  
Q(18.25) = 296.6880  
Q(9.375) = 148.5251

Isotope Correction = -1.933

Minimum Energy = 0. cm$^{-1}$

Dipoles: $\mu(a) = 4.330$ A  
$\mu(b) = 1318.18$  
$\mu(c) = c$


The dipole moment was assumed to be the same as the parent species.
Species Tag: 76002
Species Name: HCCCl^13CCN, cyanodiacyetylene, ^13C isotope
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Lines Listed = 99
Max. Frequency = 300 GHz
Max. J = 99
LOGSTR = -6.6
LOGSTR1 = -1.955
Isotope Correction = 0
Minimum Energy = cm^{-1}
Dipoles:
\(\mu(a) = 4.329\) A
\(\mu(b) = \) B = 1330.11
\(\mu(c) = \) C =


The dipole moment was assumed to be the same as the parent species.
Species Tag: 76003  Species Name: HCC$^{13}$CCCN, cyanodiacylene, $^{13}$C isotope on atom 3

Version: 1  Date: Dec 1979  Contributor: R. L. Poynter

Lines Listed = 99  Q(300.) = 4700.0195
Max. Frequency = 300 GHz  Q(225.) = 3417.4316
Max. J = 99  Q(150.) = 2317.3931
LOGSTR = -6.6  Q(75.) = 1175.1672
LOGSTR1 =  
Isotope Correction = -1.955  Q(37.5) = 587.8950
Minimum Energy = 0 cm$^{-1}$  Q(18.25) = 294.1033
Dipoles: $\mu(a) = 4.329$  A = 147.2313
$\mu(b) = \mu(c) = $  B = 1329.95


The dipole moment was assumed to be the same as the parent species.
<table>
<thead>
<tr>
<th>Species Tag:</th>
<th>76004</th>
<th>Species Name: HCl$_3$CCCCCN, cyanodiacetylene, $^{13}$C isotope on atom 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Version:</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Date:</td>
<td>Dec 1979</td>
<td></td>
</tr>
<tr>
<td>Contributor:</td>
<td>R. L. Poynter</td>
<td></td>
</tr>
<tr>
<td>Lines Listed</td>
<td>99</td>
<td>Q(300.) = 4744.6045</td>
</tr>
<tr>
<td>Max. Frequency</td>
<td>300 GHz</td>
<td>Q(225.) = 3449.8496</td>
</tr>
<tr>
<td>Max. J</td>
<td>99</td>
<td>Q(150.) = 2337.2217</td>
</tr>
<tr>
<td>LOGSTR</td>
<td>-6.6</td>
<td>Q(75.) = 1186.0413</td>
</tr>
<tr>
<td>LOGSTRI</td>
<td></td>
<td>Q(37.5) = 593.3350</td>
</tr>
<tr>
<td>Isotope Correction</td>
<td>-1.955</td>
<td>Q(18.25) = 296.8244</td>
</tr>
<tr>
<td>Minimum Energy</td>
<td>0 cm$^{-1}$</td>
<td>Q(9.375) = 148.5935</td>
</tr>
<tr>
<td>Dipoles:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\mu(a)$</td>
<td>4.329</td>
<td></td>
</tr>
<tr>
<td>$\mu(b)$</td>
<td></td>
<td>$A = 1$</td>
</tr>
<tr>
<td>$\mu(c)$</td>
<td></td>
<td>$B = 1317.689$</td>
</tr>
</tbody>
</table>


The dipole moment was assumed to be the same as the parent species.
Species Tag: 76005  
Species Name: $^{13}$C CCCCN, cyanodiacyetylene, $^{13}$C isotope on atom 5

<table>
<thead>
<tr>
<th>Lines Listed</th>
<th>99</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max. Frequency</td>
<td>300 GHz</td>
</tr>
<tr>
<td>Max. J</td>
<td>99</td>
</tr>
<tr>
<td>LOGSTR</td>
<td>-6.6</td>
</tr>
<tr>
<td>LOGSTR1</td>
<td></td>
</tr>
<tr>
<td>Isotope Correction</td>
<td>-1.955</td>
</tr>
<tr>
<td>Minimum Energy</td>
<td>0 cm$^{-1}$</td>
</tr>
<tr>
<td>Dipoles: $\mu(a)$</td>
<td>4.329</td>
</tr>
<tr>
<td>$\mu(b)$</td>
<td></td>
</tr>
<tr>
<td>$\mu(c)$</td>
<td></td>
</tr>
</tbody>
</table>

![Image](image-url)  


The dipole moment was assumed to be the same as the parent species.
<table>
<thead>
<tr>
<th>Species Tag:</th>
<th>76006</th>
<th>Species Name:</th>
<th>HC$_5^{15}$N, cyanodiacetylene, $^{15}$N isotopic species</th>
</tr>
</thead>
<tbody>
<tr>
<td>Version:</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Date:</td>
<td>Dec 1979</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Contributor:</td>
<td>R. L. Poynter</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Lines Listed</td>
<td>99</td>
<td>Q(300.) = 4813.9287</td>
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</tr>
<tr>
<td>Max. Frequency</td>
<td>300 GHz</td>
<td>Q(225.) = 3495.4258</td>
<td></td>
</tr>
<tr>
<td>Max. J</td>
<td>99</td>
<td>Q(150.) = 2369.7368</td>
<td></td>
</tr>
<tr>
<td>LOGSTR</td>
<td>-6.6</td>
<td>Q(75.) = 1203.3718</td>
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</tr>
<tr>
<td>LOGSTR1</td>
<td></td>
<td>Q(37.5) = 602.0048</td>
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</tr>
<tr>
<td>Isotope Correction</td>
<td>-2.432</td>
<td>Q(18.25) = 301.1616</td>
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</tr>
<tr>
<td>Minimum Energy</td>
<td>0 cm$^{-1}$</td>
<td>Q(9.375) = 150.7648</td>
<td></td>
</tr>
<tr>
<td>Dipoles:</td>
<td>μ(a) = 4.329</td>
<td>A = 1298.639</td>
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</tr>
<tr>
<td></td>
<td>μ(b)</td>
<td>B =</td>
<td></td>
</tr>
<tr>
<td></td>
<td>μ(c)</td>
<td>C =</td>
<td></td>
</tr>
</tbody>
</table>


The dipole moment was measured by the same authors.
Species Tag: 76007  Species Name: DC$_5$N, cyanodiacetylene,
Version: 1  D isotopic species
Date: Dec 1979
Contributor: R. L. Poynter

<table>
<thead>
<tr>
<th>Lines Listed</th>
<th>Max. Frequency</th>
<th>Max. J</th>
<th>LOGSTR</th>
<th>LOGSTRI</th>
<th>Isotope Correction</th>
<th>Minimum Energy</th>
<th>Dipoles: $\mu(a) = $</th>
<th>$\mu(b) = $</th>
<th>$\mu(c) =$</th>
</tr>
</thead>
<tbody>
<tr>
<td>99</td>
<td>300 GHz</td>
<td>99</td>
<td>-6.6</td>
<td>-3.821</td>
<td>-153.9927</td>
<td></td>
<td>4.329</td>
<td>1271.056</td>
<td></td>
</tr>
</tbody>
</table>


The dipole moment was assumed to be the same as the parent species.
Species Tag: 80001
Species Name: H\textsuperscript{79}Br,
Hydrogen Bromide,
\textsuperscript{79}Br isotopic species
Date: Feb 1980
Contributor: R. L. Poynter and H. M. Pickett

Lines Listed = 19
Max. Frequency = 10000 GHz
Max. J = 6
LOGSTR = -2.2
LOGSTR1 = 0.0
Isotope Correction = -2.95
Minimum Energy = 0 cm\textsuperscript{-1}
Dipoles: μ(a) = 0.828
μ(b) = 250357.6
μ(c) =

The experimental data were taken from F. A. Van Dijk and A. Dymanus.

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.
<table>
<thead>
<tr>
<th>Species Tag:</th>
<th>82001</th>
<th>Species Name:</th>
<th>$^8\text{H}^3\text{Br}$, Hydrogen Bromide, $^8\text{Br}$ isotopic species</th>
</tr>
</thead>
<tbody>
<tr>
<td>Version:</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Date:</td>
<td>Feb 1980</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Contributor:</td>
<td>R. L. Poynter and H. M. Pickett</td>
<td>species</td>
<td></td>
</tr>
<tr>
<td>Lines Listed</td>
<td>19</td>
<td>Q(300.) = 101.251</td>
<td></td>
</tr>
<tr>
<td>Max. Frequency</td>
<td>100000 GHz</td>
<td>Q(225.) = 73.3668</td>
<td></td>
</tr>
<tr>
<td>Max. J</td>
<td>6</td>
<td>Q(150.) = 50.3848</td>
<td></td>
</tr>
<tr>
<td>LOGSTR</td>
<td>-2.2</td>
<td>Q(75.) = 26.3573</td>
<td></td>
</tr>
<tr>
<td>LOGSTR1</td>
<td></td>
<td>Q(37.5) = 13.9155</td>
<td></td>
</tr>
<tr>
<td>Isotope Correction</td>
<td>-0.306</td>
<td>Q(8.25) = 7.7750</td>
<td></td>
</tr>
<tr>
<td>Minimum Energy</td>
<td>0. cm$^{-1}$</td>
<td>Q(9.375) = 4.9351</td>
<td></td>
</tr>
<tr>
<td>Dipoles:</td>
<td>[\mu(a) = 0.828 \text{ cm}^{-1}]</td>
<td>A =</td>
<td></td>
</tr>
<tr>
<td></td>
<td>[\mu(b) = ]</td>
<td>B = 250250.2</td>
<td></td>
</tr>
<tr>
<td></td>
<td>[\mu(c) = ]</td>
<td>C =</td>
<td></td>
</tr>
</tbody>
</table>

The experimental data were taken from F. A. Van Dijk and A. Dymanus, 1969, Chem. Phys. Lett. 4, 170.

The dipole moment was also reported by these same authors in a later publication, and updated in F. A. Van Dijk and A. Dymanus, 1971, 26th Symposium on Molecular Structure and Spectroscopy, Columbus, Ohio, R12, p. 80.
Species Tag: 95001  
Species Name: 79BrO,  
Version: 1  
Date: Feb 1980  
Contributor: H. M. Pickett

Bromine Monoxide,  
79Br isotopic species,  
2π3/2 state

Lines Listed = 850  
Q(300.) = 3897.6226  
Max. Frequency = 1300 GHz  
Q(225.) = 2938.3271  
Max. J = 49  
Q(150.) = 1965.1685  
LOGSTR = -9  
Q(75.) = 989.4642  
LOGSTR1 =  
Q(37.5) = 501.9954  
Isotope Correction = -0.296  
Q(18.25) = 259.5374  
Minimum Energy = 0 cm⁻¹  
Q(9.375) = 136.8043  
Dipoles:  
μ(a) = 1.765  
μ(b) =  
μ(c) = 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
Version: 1
Date: Feb 1980
Contributor: H. M. Pickett

Species Name: $^8\text{BrO}$, Bromine Monoxide,
$^8\text{Br}$ isotopic species, $^2\Pi_{3/2}$ state

Lines Listed = 850
Q(300.) = 3913.8101
Max. Frequency = 1500 GHz
Q(225.) = 2950.5308
Max. J = 49
Q(150.) = 1973.3323
LOGSTR = -9
Q(75.) = 993.5737
LOGSTR1 = 0
Q(37.5) = 503.9649
Isotope Correction = -0.306
Q(18.25) = 259.2984
Minimum Energy = 0 cm$^{-1}$
Q(9.375) = 137.2459
Dipoles:
$\mu(a) = 1.794$ cm$^{-1}$
$\mu(b) = \frac{A}{B} = 12777.08$
$\mu(c) = \frac{A}{C}$

The 63 GHz spectrum of BrO is referenced in F. J. Lovas and E. Tiemann, 1974, J. Phys. Chem. Ref. Data 3, 653. The other lines were measured at JPL by E. A. Cohen and H. M. Pickett, and a new fit was made which included these lines.
Species Tag: 97002  Species Name: $^{35}\text{ClNO}_3$
Version: 1  Chlorine nitrate
Date: Mar 1984  
Contributor: H. M. Pickett

Lines Listed = 4198
Max. Frequency = 3000 GHz
Max. J = 60
LOGSTR = -6
LOGSTR1 = -6
Isotope Correction = -0.122
Minimum Energy = 0 cm$^{-1}$

Dipoles: $\mu(a) = 0.72$  A = 12105.8
$\mu(b) = 0.28$  B = 2777.0
$\mu(c) = 0$  C = 2258.1

The data are taken from R. D. Suenram and F. J. Lovas, 1977, J. Molec. Spectrosc. 65, 239 (1977), and chlorine hyperfine structure is omitted in this version of the catalogue since the splittings are generally smaller than the width of lower stratospheric lines.
Species Tag: 99001
Species Name: $^{37}$ClNO$_3$
Chlorine nitrate

Version: 1
Date: Mar 1984
Contributor: H. M. Pickett

| Lines Listed | = 418Z
| Max. Frequency | = 3000 GHz
| Max. J | = 60
| LOGSTR | = -6
| LOGSTR1 | = -6
| Isotope Correction | = -0.611
| Minimum Energy | = 0 cm$^{-1}$
| Dipoles: | $\mu(a)$ = 0.72
| | $\mu(b)$ = 0.28
| | $\mu(c)$ = 0

Q(300.) = 103108.
Q(225.) = 66971.
Q(150.) = 36454.
Q(75.) = 12888.
Q(37.5) = 4561.
Q(18.25) = 1614.
Q(9.375) = 572.

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