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GX-11A
Schumann - Range Bands of $O_2$
GX-11B
Sulfur dioxide Cross Sections
GX-11C
Schumann Range Band of $O_2$ at 79K
GX-11D
Submillimeter , Millimeter and Microwave
Spectral line Catalog

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Table of Contents

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## 1. INTRODUCTION:

The documentation for this data set was originally on paper, kept in NSSDC's Data Set Catalogs (DSCs). The paper documentation in the Data Set Catalogs have been made into digital images, and then collected into a single PDF file for each Data Set Catalog. The inventory information in these DSCs is current as of July 1, 2004. This inventory information is now no longer maintained in the DSCs, but is now managed in the inventory part of the NSSDC information system. The information existing in the DSCs is now not needed for locating the data files, but we did not remove that inventory information.

The offline tape datasets have now been migrated from the original magnetic tape to Archival Information Packages (AIP’s).

A prior restoration may have been done on data sets, if a requestor of this data set has questions; they should send an inquiry to the request office to see if additional information exists.

## 2. ERRATA/CHANGE LOG:

NOTE: Changes are made in a text box, and will show up that way when displayed on screen with a PDF reader.

***When printing, special settings may be required to make the text box appear on the printed output.***

| Version | Date | Person | Page | Description of Change |
|---|---|---|---|---|
| 01 | | | | |
| 02 | | | | |

## 3 LINKS TO RELEVANT INFORMATION IN THE ONLINE NSSDC INFORMATION SYSTEM:

http://nssdc.gsfc.nasa.gov/nmc/

[NOTE: This link will take you to the main page of the NSSDC Master Catalog. There you will be able to perform searches to find additional information]

## 4. CATALOG MATERIALS:

a. Associated Documents    To find associated documents you will need to know the document ID number and then click here.
http://nssdcftp.gsfc.nasa.gov/miscellaneous/documents/

b. Core Catalog Materials

GX-11A ASXR-00082
Schumann - Range Bands of $O_2$

GX-11B ASXR-00083
Sulfur Dioxide Cross Sections

GX-11C ASXR-00084
Schumann Range Band of $O_2$ at 79K

GX-11D ASRA-00010
Submillimeter, Millimeter and Microwave
Spectral Line Catalogue

This dataset catalog contains of four datasets, each consisting of one tape each. Gx-11A,B and C are 9-track, 1600 BPI, ASCII and were created on an IBM 360 computer.

GX-11D consists of one tape. It is 9 track, 6250 BPI, written in files 11 format, and coded in ascii. The label name is GX_11D. This tape does not match the tape characteristics as documented in the publication documentation (JPL Publication 80-23,revision 2) for this data set. This tape has a logical record size of 76 bytes.
The tape was originally written on a DC600A Data Cartridge using a Sun work station. The data is written in stream line format, thus no inter-record gaps. The end of record may be noted by a hex 0A, which translates to a 'lf' meaning line feed.

| D # | C# | FILES | LABEL | DATA SET ID |
|---|---|---|---|---|
| D-51695 | C-22901 | 13 | N/A | GX-11A |
| D-65017 | C-25266 | 40 | N/A | GX-11B |
| D-76163 | C-26571 | 23 | N/A | GX-11C |
| D-84734 | C-28808 | 207 | GX_11D | GX-11D |

GX-11D

JPL PUBLICATION 80-23, REVISION 2

# 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

JPL PUBLICATION 80-23, REVISION 2

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

# ABSTRACT

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

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

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

# FOREWORD

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

New Species, Rev. 2 (18)

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

Revised Species, Rev. 2 (30)

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

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

New Species, Rev. 1 (9)

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

Revised Species, Rev. 1 (24)

| TAG | NAME | TAG | NAME | TAG | NAME |
|---|---|---|---|---|---|
| 17002 | NH3 | 34001 | 0-18-0 | 56002 | CH3C-13-H2CN |
| 18002 | N-15-H3 | 34002 | H2S | 56003 | C-13-H3CH2CN |
| 18003 | H20 | 34003 | PH3 | 56005 | CH2DCH2CN-S |
| 29003 | CH2NH | 45003 | NH2CHO | 56006 | CH2DCH2CN-A |
| 30007 | CH2ND | 51002 | CLO | 60001 | OCS |
| 32001 | 02 | 53002 | CL-37-0 | 61001 | OC-13-S |
| 32002 | 02-V1 | 55001 | C2H5CN | 62001 | OC-34-S |
| 32003 | CH30H | 56001 | CH3CH2C-13-N | 62002 | 0-18-CS |

# CONTENTS

## I. Introduction

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

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

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

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

## II. Format of Data Tape

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

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

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

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

The catalogue data tape also contains a second file with a species directory. Each element of this directory is an 80 character record with the following format:

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

NAME: an ASCII name for the species

NLINE: number of lines in catalogue

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

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

* Physical format of tape is different than doumentation, but logical format is correct.

Physical Format of Tape

Density: 800 or 1600 bytes/inch on 9 tracks

Encoding: ASCII

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

First file (catalogue):

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

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

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

Second file (directory):

Blocking: 80 characters per block

Length: 151 blocks followed by end of file mark

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

## III. Intensity Units and Conversions

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

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

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

where $\nu_{ba}$ is the line frequency, ${}^{x}S_{ba}$ 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 ${}^{x}S_{ba}$ and $Q_{rs}$ are determined with same state degeneracies. Note that with this definition the intensities are defined with respect to the total concentration of the vibration electronic state of the species. No vibrational partition function or vibrational Boltzmann factor is included. For the catalogue, Eq. (1) is evaluated for T=300K.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

in which g' is the degeneracy of the upper state. The value of g' is listed as part of the spectral line information in the catalogue. Values of $Q_{rs}$ are listed in Section VI.

## IV. General Comments on Precision

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

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

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

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

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 σ estimates to 3 σ estimates and are more usually "guesstimates". Unfortunately, many authors do not even report their experimental uncertainties. Therefore, the expected errors in predicted lines obtained from fits based on such data will usually reflect this ambiguity in laboratory uncertainties through Eq. (7) and (8). In some cases, the quality of the least squares fit of the parameters to the experimental lines can be a guide to the statistical nature of the experimental uncertainties. Whenever possible, the expected errors in this catalog will reflect an expected 95% confidence interval based on the model used to fit the data. However, the errors can be different from this design goal by factors of three just due to the quality of input error estimates. Lines with an expected error greater than 1 GHz have been dropped from the catalogue.

The expected errors can only be computed relative to the model used. There are at least two ways the model can be "wrong" for the predicted frequencies. First, higher-order centrifugal distortion terms may no longer be negligible for the predicted frequencies. This effect will generally be important for lines of higher J or K than the laboratory-determined data set. In a sense, the predictions are then a form of extrapolation rather than interpolation and are therefore more suspect. A second factor leading to discrepancies in the predicted frequencies comes from "resonances". These resonances come from a near overlap of energy states that are coupled by elements of the Hamiltonian matrix. Poor predictability comes when these elements are neglected in the model or are treated inadequately by some form of perturbation theory. Such a neglect of coupling elements is always necessary at some level in any practical calculation. A major contributing problem is that often the existing data set is not sensitive to the parameters which are needed to characterize the resonances.

Precision in the intensity estimates is generally less critical than precision in the frequency. Contributing to intensity uncertainty are errors in the dipole moment, errors in the line strength ${}^{x}S_{ba}$ and errors in the rotation-spin partition function. (The vibration-electronic partition function does not enter directly because the catalogue intensities are defined on the basis of concentrations of the given vibration-electronic state.) Dipole moment errors come directly from the experimental determination and indirectly from the J dependence of the dipole moment due to centrifugal mixing of vibrational states. Line strength errors can come from deficiencies in the model Hamiltonian and are particularly severe when resonances have been inadequately accounted for. Partition function errors are relatively benign but can become significant if the classical formulae are used at low temperatures for small molecules. With the exception of unanticipated resonances and poorly determined dipole moments, worst case errors in the intensity will generally be at the 1% level or lower.

There are many molecular models that are found in the literature. In principle, a very general model should be able to treat every possible case. In practice this is hardly ever done. A specific model is most frequently used for every case, mainly becasue every author starts with a different viewpoint of the problem. In our case, we have tried to develop a program that will treat a wide variety of problems with a minimum of adaptation. This saves a great deal of time in the initial set up, and provides a uniform output format for the final results. Most important, the basic treatment is the same for every molecule, regardless of the model used, so that a high degree of consistancy can be maintained, facilitating comparisons between different molecules. The particular model needed to analyze a specific problem is treated as a subroutine. For certain problems, this subroutine can be quite simple, which for others it is more complex.

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

Comments on specific models are given for the individual species.

## V. Format of Quantum Numbers

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

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

in which Q determines the type of molecule (see table below), H determines the coding of half integer quantum numbers, and NQN is the number of quantum numbers for each state. Q is defined so that MOD(Q,5) is the number of primary quantum numbers. If NQN is greater than the number of primary quantum numbers, the degeneracy is derived from the last quantum number. Otherwise the degeneracy is derived from the first quantum number. H is a 3 bit binary code for the existence of half integer quantum numbers for the <u>last three</u> 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 <u>up</u> to the next integer.

# TABLE I. QUANTUM NUMBER FORMATS

| type | Q | ITD | quantum order |
|---|---|---|---|
| atom | 0 | 0 | (J),(F),.... |
| linear - Σ | 1 | 2 | N,(J),($F_1$),($F_2$)(F) |
| linear - case b | 2 | 2 | N,Λ,($F_1$),($F_2$),(F) |
| linear - case a-2S+1 odd | 3 | 2 | J,Ω,Λ,($F_1$),($F_2$),(F) |
| linear - case a-2S+1 even | 8 | 2 | J+1/2,Ω+1/2,Λ,($F_1$),($F_2$),(F) |
| symmetric rotor | 2 | 3 | N,K,(J),($F_1$),($F_2$),(F) |
| symmetric rotor with vibration | 13 | 3 | N,K,v,(J),($F_1$),(F) |
| asymmetric rotor | 3 | 3 | N,$K_{-1}$,$K_{+1}$,(J),($F_1$),(F) |
| asymmetric rotor with vibration | 14 | 3 | N,$K_{-1}$,$K_{+1}$,v,(J),(F) |

conventions:

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

## VI. Documentation by Species

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

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

A blank entry for LOGSTR1 means that the second term was not included. THe partition functions listed (Q) include rotation and spin statistics but usually do not include vibrational corrections. (Exceptions are $H_2O$ and $O_3$.) Calculation of Q is based on a sum over states. At higher temperatures, the sum-over-states calculation is replaced by a classical calculation when the latter is larger due to a limited number of states in the catalogue. The spin statistics included are only a partial set but are consistent with the intensities in the catalogue.

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

## TABLE II. Assumed Relative Abundances of Isotopes for Catalogue Description

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

## Species List

| | |
|---|---|
| 1001 | H-ATOM |
| 2001 | D-ATOM |
| 3001 | HD |
| 12001 | C-ATOM |
| 13001 | C-13-ATOM |
| 13002 | CH |
| 14001 | N-ATOM |
| 14002 | N-ATOM-D-STATE |
| 16001 | 0-ATOM |
| 17001 | 0H |
| 17002 | NH3 |
| 17003 | CH3D |
| 17004 | NH3-V2 |
| 18001 | 0D |
| 18002 | N-15-H3 |
| 18003 | H20 |
| 18004 | NH2D |
| 18005 | H20-V2 |
| 19001 | H0-18 |
| 19002 | HD0 |
| 20001 | D20 |
| 25001 | CCH |
| 26001 | CN |
| 26002 | CN-V1 |
| 27001 | HCN |
| 27002 | HNC |
| 28001 | C0 |
| 28002 | HC-13-N |
| 28003 | HCN-15 |
| 28004 | DCN |
| 28005 | HNC-13 |
| 28006 | HN-15-C |
| 28007 | DNC |
| 29001 | C-13-0 |
| 29002 | HC0+ |
| 29003 | CH2NH |
| 29004 | HC0 |
| 29005 | NNH+ |
| 30001 | C0-18 |
| 30002 | HC-13-0+ |
| 30003 | DC0+ |
| 30004 | H2C0 |
| 30005 | C-13-H2NH |
| 30006 | CH2N-15-H |
| 30007 | CH2ND |
| 30008 | N0 |
| 30009 | NND+ |
| 31001 | HC0-18+ |
| 31002 | H2C-13-0 |
| 32001 | 02 |
| 32002 | 02-V1 |
| 32003 | CH30H |
| 32004 | H2C0-18 |
| 33001 | H02 |
| 34001 | 0-18-0 |
| 34002 | H2S |
| 34003 | PH3 |
| 34004 | H202 |
| 35001 | HDS |
| 36001 | HCl |
| 38001 | HCl-37 |
| 40001 | CH3CCH |
| 41001 | CH3CN |
| 41002 | CH3CC-13-H |
| 41003 | CH3C-13-CH |
| 41004 | C-13-H3CCH |
| 41005 | CH3CCD |
| 41006 | CH2DCCH |
| 42001 | CH3CN-15 |
| 42002 | CH2C0 |
| 43001 | CHDC0 |
| 44001 | CS |
| 44002 | SI0 |
| 44003 | CH3CH0-A |
| 44004 | N20 |
| 44005 | CH3CH0-E |
| 45001 | C-13-S |
| 45002 | SI-29-0 |
| 45003 | NH2CH0 |
| 46001 | CS-34 |
| 46002 | SI-30-0 |
| 46003 | H2CS |
| 46004 | C2H50H |
| 46005 | HC00H |
| 46006 | N02 |
| 47001 | H2C-13-S |
| 47002 | HC-13-00H |
| 47003 | DC00H |
| 47004 | HC00D |
| 48001 | S0 |
| 48002 | S0-V1 |
| 48003 | H2CS-34 |
| 48004 | 03 |
| 48005 | 03-V2 |
| 48006 | 03-V1,3 |
| 48007 | 03-2V2 |
| 49001 | 03-SYM-0-17 |
| 49002 | 03-ASYM-0-17 |
| 50001 | S-34-0 |
| 50002 | S0-18 |
| 50003 | 03-SYM-0-18 |
| 50004 | 03-ASYM-0-18 |
| 50005 | 03-S-018-V2 |
| 50006 | 03-A-018-V2 |
| 51001 | HCCCN |
| 51002 | CL0 |
| 52001 | HCCC-13-N |
| 52002 | HCC-13-CN |
| 52003 | HC-13-CCN |
| 52004 | HCCCN-15 |
| 52005 | DCCCN |
| 52006 | H0CL |
| 53001 | C2H3CN |
| 53002 | CL-37-0 |
| 54001 | CH2CHC-13-N |
| 54002 | CH2C-13-HCN |
| 54003 | C-13-H2CHCN |
| 54004 | CH2CDCN |
| 54005 | H0CL-37 |
| 55001 | C2H5CN |
| 56001 | CH3CH2C-13-N |
| 56002 | CH3C-13-H2CN |
| 56003 | C-13-H3CH2CN |
| 56004 | C2H5CN-15 |
| 56005 | CH2DCH2CN-S |
| 56006 | CH2DCH2CN-A |
| 60001 | 0CS |
| 60002 | SIS |
| 61001 | 0C-13-S |
| 61002 | SI-29-S |
| 62001 | 0C-34-S |
| 62002 | 0-18-CS |
| 62003 | SI-30-S |
| 62004 | SIS-34 |
| 63001 | HN03 |
| 64001 | S2 |
| 64002 | S02 |
| 75001 | HCCCCCN |
| 76001 | HCCCCC-13-N |
| 76002 | HCCCC-13-CN |
| 76003 | HCCC-13-CCN |
| 76004 | HCC-13-CCCN |
| 76005 | HC-13-CCCCN |
| 76006 | HCCCCCN-15 |
| 76007 | DCCCCCN |
| 80001 | HBR-79 |
| 82001 | HBR-81 |
| 95001 | BR-79-0 |
| 97001 | BR-81-0 |
| 97002 | CL-35-N03 |
| 99001 | CL-37-N03 |

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

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

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

Q( 300.) = 4.0
Q( 225.) = 4.0
Q( 150.) = 4.0
Q( 75.) = 4.0
Q( 37.5) = 3.99
Q(18.25) = 3.99
Q(9.375) = 3.98
A =
B =
C =

---

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

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

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

---

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

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

Species Name: HD
Mono-deuterated
molecular hydrogen

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

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

---

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

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

Species Name: Carbon atom
$^3P$ ground state

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

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

---

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

Species Tag: 13001
Version: 1
Date: Oct 1979
Contributor: H. M. Pickett

Species Name: Carbon atom
$^{13}$C isotope

Lines Listed = 7
Max. Frequency = 810. GHz
Max. J = 2
LOGSTR = -16.
LOGSTR1 =
Isotope Correction = -1.955
Minimum Energy = 0. $cm^{-1}$
Dipoles: $\mu(a)$ =
$\mu(b)$ =
$\mu(c)$ =

Q( 300.) = 15.666
Q( 225.) = 14.978
Q( 150.) = 13.720
Q( 75.) = 10.727
Q( 37.5) = 7.087
Q(18.25) = 4.060
Q(9.375) = 2.496
A =
B =
C =

---

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

Species Tag: 13002
Version: 1
Date: Feb 1984
Contributor: H. M. Pickett

Species Name: CH radical
$^2\Pi$ states

Lines Listed = 324
Max. Frequency = 10000 GHz
Max. F = 14
LOGSTR = -10.
LOGSTR1 = -7.
Isotope Correction = 0.
Minimum Energy = 0 $cm^{-1}$
Dipoles: $\mu(a)$ = 1.46
$\mu(b)$ =
$\mu(c)$ =

Q( 300.) = 120.840
Q( 225.) = 91.364
Q( 150.) = 61.997
Q( 75.) = 32.922
Q( 37.5) = 18.847
Q(18.25) = 12.200
Q(9.375) = 8.960
A =
B = 425472.8
C =

---

The laboratory spectra of C. R. Brazier and J. M. Brown, (1983) J. Chem. Phys. 78, 1608-1610 and M. Bogey, C. Demuynck and J. L. Destombes, (1983) Chem. Phys. Lett. 100, 105-109 were combined with the data of Rydbeck, et al, (1974) Astron. Astrophys. 34, 479 and the predictions of the rotational lines given by J. M. Brown and K. M. Evenson (1983) Ap. J. 268 L51 in a fit to a Hund's case b Hamiltonian with 8 fine structure parameters, B and D and 7 hyperfine parameters. Calculated values are given for the rotational transitions.

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

| | | | |
|---|---|---|---|
| Species Tag: | 14001 | Species Name: | N-atom<br>$^4S_{3/2}$ ground state |
| Version: | 1 | | |
| Date: | Oct 1979 | | |
| Contributor: | H. M. Pickett | | |
| Lines Listed | = 2 | Q( 300.) = | 12.0 |
| Max. Frequency | = 0.027 GHz | Q( 225.) = | 12.0 |
| Max. J | = 1.5 | Q( 150.) = | 12.0 |
| LOGSTR | = -13. | Q( 75.) = | 12.0 |
| LOGSTR1 | = | Q( 37.5) = | 12.0 |
| Isotope Correction | = 0. | Q(18.25) = | 12.0 |
| Minimum Energy | = 0. $cm^{-1}$ | Q(9.375) = | 12.0 |
| Dipoles: μ(a) | = | A = | |
| μ(b) | = | B = | |
| μ(c) | = | C = | |

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

| | | | | |
|---|---|---|---|---|
| Species Tag: | 14002 | | Species Name: | N-atom $^2$D state |
| Version: | 2 | | | |
| Date: | Aug 1983 | | | |
| Contributor: | H. M. Pickett | | | |
| Lines Listed | = 6 | | Q( 300.) = | 29.51 |
| Max. Frequency | = 261. | GHz | Q( 225.) = | 29.35 |
| Max. J | = 2.5 | | Q( 150.) = | 29.03 |
| LOGSTR | = -49. | | Q( 75.) = | 28.15 |
| LOGSTR1 | = | | Q( 37.5) = | 26.58 |
| Isotope Correction | = 0. | | Q(18.25) = | 24.13 |
| Minimum Energy | = 19223. | $cm^{-1}$ | Q(9.375) = | 21.12 |
| Dipoles: μ(a) | = | | A = | |
| μ(b) | = | | B = | |
| μ(c) | = | | C = | |

---

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

| | | | | |
|---|---|---|---|---|
| Species Tag: | 16001 | | Species Name: | O atom |
| Version: | 2 | | | $^3P$ ground state |
| Date: | Mar 1984 | | | |
| Contributor: | H. M. Pickett | | | |

| | | | | |
|---|---|---|---|---|
| Lines Listed = | 2 | | Q( 300.) = | 6.7407 |
| Max. Frequency = | 3000 | GHz | Q( 225.) = | 6.3243 |
| Max. J = | | | Q( 150.) = | 5.7705 |
| LOGSTR = | | | Q( 75.) = | 5.1568 |
| LOGSTR1 = | | | Q( 37.5) = | 5.0 |
| Isotope Correction = | | | Q(18.25) = | 5.015 |
| Minimum Energy = | | $cm^{-1}$ | Q(9.375) = | 5.000 |
| Dipoles: μ(a) = | | | A = | |
| μ(b) = | | | B = | |
| μ(c) = | | | C = | |

---

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

Species Tag: 17001
Version: 2
Date: May 1983
Contributor: H. M. Pickett

Species Name: OH
Hydroxyl radical

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

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

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

| | | | | |
|---|---|---|---|---|
| Species Tag: | 17002 | | Species Name: | NH$_3$<br>Ammonia |
| Version: | 3 | | | |
| Date: | Jan 1984 | | | |
| Contributor: | R. L. Poynter | | | |
| Lines Listed | = 446 | | Q( 300.) = | 578.98 |
| Max. Frequency | = 9500. | GHz | Q( 225.) = | 371.88 |
| Max. J | = 19 | | Q( 150.) = | 206.64 |
| LOGSTR | =-17. | | Q( 75.) = | 74.54 |
| LOGSTR1 | = 0 | | Q( 37.5) = | 26.608 |
| Isotope Correction | = 0. | | Q(18.25) = | 11.251 |
| Minimum Energy | = 0. | cm$^{-1}$ | Q(9.375) = | 5.398 |
| Dipoles: $\mu(a)$ | = 0 | | A = | B |
| $\mu(b)$ | = 0 | | B = | 298117.06 |
| $\mu(c)$ | = 1.476 | | C = | 186726.36 |

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

The rotational transitions and energy levels were taken from R. Poynter and J. S. Margolis, 1983, Mol. Phys. 48, 401. This analysis was based on a very extensive set of accurate $\nu_2$ measurements reported by R. Poynter and J. S. Margolis, 1984, Mol. Phys. 51, 393, and upon a series of "forbidden" transitions in the $\nu_4$ band, reported by E. A. Cohen, W. H. Weber, R. L. Poynter, and J. S. Margolis, 1983, Mol. Phys. 50, 727. The work of Cohen, et al. allowed the C, $D_K$, $H_K$, and $L_k$ constants to be determined, thus fixing the energy level scale. The $J = 1 \rightarrow 0$, $k = 0$ rotational transition was taken from P. Helminger, F. C. DeLucia, and W. Gordy, 1971, J. Mol. Spect. 39, 94. Becasuse of the important applications of these rotational lines, the upper frequency limit has been extended to 335 cm$^{-1}$ (9.5 THz). Hyperfine splittings have not been included.

Species Tag: 17003
Version: 1
Date: Feb 1980
Contributor: R. L. Poynter

Species Name: $CH_3D$
Mono deutero methane

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

Q( 300.) = 402.17
Q( 225.) = 315.14
Q( 150.) = 142.69
Q( 75.) = 51.09
Q( 37.5) = 18.47
Q(18.25) = 7.03
Q(9.375) = 2.98
A = 157412.
B = 116325.
C = B

---

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

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

Species Name: $NH_3$, $\nu_2$ - 010 state

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

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

---

The lines for this species were derived by combination differences from the $\nu_2$ - 010 lnes reported by R. L. Poynter and J. S. Margolis, 1984, Mol. Phys. 81, 393. Some measurements have been reported by F. Y. Chu and S. M. Freund, 1973, J. Mol. Spect. 48, 183, by S. Urban, et al., 1980, J. Mol. Spect. 79, 455, by E. N. Karyakin, et al., 1977, J. Mol. Spect. 66, 177, and by S. Urban, et al., 1981, J. Mol. Spect. 88, 274.

The transition dipole moment was reported by B. J. Orr and T. Oka, 1977, J. Mol. Spect. 66, 302.

Species Tag: 18001
Version: 1
Date: May 1983
Contributor: H. M. Pickett

Species Name: OD
Hydroxyl radical,
deuterium isotope

Lines Listed = 912
Max. Frequency = 10000. GHz
Max. J = 15.5
LOGSTR = -10.
LOGSTR1 = -10
Isotope Correction = -3.824
Minimum Energy = 0. $cm^{-1}$
Dipoles: $\mu(a)$ = 1.653
$\mu(b)$ = 0.
$\mu(c)$ = 0.

Q( 300.) = 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
A =
B = 296312.
C =

---

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

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

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

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

Q( 300.) = 575.84
Q( 225.) = 451.23
Q( 150.) = 206.21
Q( 75.) = 74.71
Q( 37.5) = 27.669
Q(18.25) = 11.277
Q(9.375) = 5.415
A = B
B = 297390.8
C = 186711.

---

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

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

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

Species Name: $H_2O$
water

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

Q( 300.) = 178.115
Q( 225.) = 116.017
Q( 150.) = 63.677
Q( 75.) = 23.170
Q( 37.5) = 8.580
Q(18.25) = 3.033
Q(9.375) = 1.257
A = 835840.29
B = 435351.72
C = 278138.70

---

The data set used in this new fit is based upon both the microwave and submillimeter lines reported by J. K. Messer, F. C. DeLucia and P. Helminger (1984), J. Mol. Spect. (in press), and on 720 ground state combination differences derived from the $\nu_2$ data of G. Guelachvilli (1983), J. Opt. Soc. Am. 73, 137. All of the submillimeter/microwave lines fit to within an 0.05 MHz RMS deviation, while the combination differences fit to within an RMS deviation of 0.00015 cm$^{-1}$ (4 MHz). Because of the importance of this molecule in many applications, the upper frequency limit of the predicted lines has been extended to 10. THz (300 cm$^{-1}$). The details of the analysis will be reported shortly. The dipole moment is from T. R. Dyke and J. S. Muenter, (1973), J. Chem. Phys. 59, 3125. Other references are given in F. C. DeLucia, P. Helminger and W. H. Kirchhoff, (1974), J. Phys. Chem. Ref. Data, 3, 211.

The partition function includes contributions from the $\nu_2$ state.

Species Tag: 18004
Version: 1
Date: Jan 1981
Contributor: H. M. Pickett

Species Name: $NH_2D$
Mono deutero
ammonia

Lines Listed = 5036
Max. Frequency = 3000. GHz
Max. J = 14
LOGSTR = -10
LOGSTR1 =
Isotope Correction = -3.347
Minimum Energy = 0. $cm^{-1}$
Dipoles: $\mu(a)$ = -0.18
$\mu(b)$ = 0
$\mu(c)$ = 1.463

Q( 300.) = 3790.
Q( 225.) = 2409.
Q( 150.) = 1293.
Q( 75.) = 434.4
Q( 37.5) = 137.0
Q(18.25) = 404.3
Q(9.375) = 13.24
A = 290124.
B = 192194.
C = 140797.

---

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

Species Tag: 18005
Version: 2
Date: Mar 1984
Contributor: H. M. Pickett

Species Name: $H_2O$-$\nu$2
excited bending
state (010)

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

Q( 300.) = 178.115
Q( 225.) = 116.017
Q( 150.) = 63.677
Q( 75.) = 23.170
Q( 37.5) = 8.580
Q(18.25) = 3.033
Q(9.375) = 1.257
A = 933052
B = 440318.
C = 273710.

---

The rotational lines were determined by M. Herman, J. W. C. Johns, and A. R. W. McKellar, 1979, Can. J. Phys. 57, 397, and H. Kuze, 1980, Ap. J. 239, 1131. Additional combination differences were obtained from the data of G. Guelachvili, 1983, J. Opt. Soc. Am. 73, 137.

The partition function is the same as that used for the ground state.

Species Tag: 19001
Version: 2
Date: May 1983
Contributor: H. M. Pickett

Species Name: HO-18
Hydroxyl radical

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

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

---

The microwave data are reported in R. A. Beaudet and R. L. Poynter, 1978, J. Phys. Chem. Ref. Data 7, 311. The fit involved constraining the constants by isotope relations to the mean of those for OH and OD, since only $\lambda$ doubling data is available.

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

Species Name: HDO
water, mono deuterium
isotope

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

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

---

The lines reported here were derived from a fit which included the microwave and submillimeter lines reported by J. K. Messer, F. C. DeLucia and P. Helminger (1984), J. Mol. Spect. (in press), and an extensive set of ground state energy levels obtained from new high resolution FTS measurements of the $\nu_2$ band reported by R. A. Toth, 1984 (private communication). The RMS deviations of the submillimeter lines is almost the same as that reported above by Messer, et al., while the RMS deviations for the fit of the ground state energy levels is 0.00015 cm$^{-1}$ (4 MHz). The dipole moment components are from S. A. Clough, Y. Beers, G. P. Klein and L. S. Rothman (1973), J. Chem. Phys. 59, 2254.

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

| | | | | |
|---|---|---|---|---|
| Species Tag: | 20001 | Species Name: | $D_2O$,<br>Water, fully substituted<br>with deuterium<br>deuterium oxide | |
| 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: μ(a) | = | | A = | 462278.8 |
| μ(b) | = 1.8545 | | B = | 218038.27 |
| μ(c) | = | | C = | 145258.00 |

---

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

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

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

H. Bluyssen, 1968, Thesis, Nijmegen

G. Eriandsson and J. Cox, 1956, J. Chem. Phys. 25, 778

C. K. Jen, D. R. Bianco, and J. T. Massey, 1953, J. Chem. Phys. 21, 520

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

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

G. Steenbeckeliers and J. Bellet, 1973, J. Mol. Spect. 45, 10

D. A. Stephenson and R. G. Strauch, 1970, J. Mol. Spect. 35, 494

J. Verhoeven, H. Bluyssen, and A. Dymanus, 1968, Phys. Letters 26A, 424

and on the infrared $\nu_2$ data of R. A. Toth, 1984, private communication.

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

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

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

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

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

---

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

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

Species Name: CN radical

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

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

---

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

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

Species Name: CN, v = 1

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: $\mu(a)$ = 3.0
$\mu(b)$ =
$\mu(c)$ =

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

---

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

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

Species Name: HCN
Hydrogen cyanide

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

Q( 300.) = 424.154
Q( 225.) = 318.504
Q( 150.) = 212.643
Q( 75.) = 106.811
Q( 37.5) = 53.910
Q(18.25) = 27.472
Q(9.375) = 14.272
A =
B = 44315.975
C =

---

The observed transitions are from F. C. DeLucia and W. Gordy (1969), Phys. Rev. 187, 58 and from F. C. Van den Heuvel, W. L. Meerts and A. Dymanus, (1982) Chem. Phys. Lett. 92, 215. The dipole moment is from G. Tomasevich, (1970), Thesis, Harvard Univ.

| | | | | |
|---|---|---|---|---|
| Species Tag: | 27002 | | Species Name: | HNC<br>Hydrogen isocyanide |
| Version: | 1 | | | |
| 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: μ(a) | = 2.699 | | A = | |
| μ(b) | = | | B = | 45332. |
| μ(c) | = | | C = | |

---

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

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

Species Name: CO
Carbon monoxide

Lines Listed = 26
Max. Frequency = 3000. GHz
Max. J = 26
LOGSTR = -5
LOGSTR1 =
Isotope Correction = 0
Minimum Energy = 0 $cm^{-1}$
Dipoles: $\mu(a)$ = 0.1098
$\mu(b)$ =
$\mu(c)$ =

Q( 300.) = 108.787
Q( 225.) = 81.708
Q( 150.) = 54.581
Q( 75.) = 27.454
Q( 37.5) = 13.896
Q(18.25) = 7.122
Q(9.375) = 3.744
A =
B = 57635.97
C =

---

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

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

Species Tag: 28002
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: HC-13-N
Hydrogen cyanide,
$^{13}$C isotope

Lines Listed = 45
Max. Frequency = 3000. GHz
Max. J = 34
LOGSTR = -4
LOGSTR1 =
Isotope Correction = -1.955
Minimum Energy = 0. cm$^{-1}$
Dipoles: μ(a) = 2.984
μ(b) =
μ(c) =

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
A =
B = 43170.137
C =

---

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

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

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

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

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

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

---

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

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

Species Tag: 28004
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: DCN
Hydrogen cyanide,
deuterium isotope

Lines Listed = 54
Max. Frequency = 3000. GHz
Max. J = 41
LOGSTR =-4.2
LOGSTR1 =
Isotope Correction = -3.824
Minimum Energy = 0. $cm^{-1}$
Dipoles: $\mu(a)$ = 2.984
$\mu(b)$ =
$\mu(c)$ =

Q( 300.) = 518.916
Q( 225.) = 389.604
Q( 150.) = 260.036
Q( 75.) = 130.504
Q( 37.5) = 65.755
Q(18.25) = 33.391
Q(9.375) = 17.224
A =
B = 36207.46
C =

---

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

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

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

Lines Listed = 34
Max. Frequency = 3000. GHz
Max. J = 35
LOGSTR =-2.7
LOGSTR1 =
Isotope Correction = -1.955
Minimum Energy = 0. $cm^{-1}$
Dipoles: $\mu(a)$ = 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
Q(18.25) = 9.313
Q(9.375) = 4.835
A =
B = 43545.61
C =

---

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

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

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

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

Q( 300.) = 141.013
Q( 225.) = 105.893
Q( 150.) = 70.697
Q( 75.) = 35.511
Q( 37.5) = 17.924
Q(18.25) = 9.134
Q(9.375) = 4.746
A =
B = 44433.04
C =

---

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

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

Species Name: DNC
Hydrogen isocyanide,
deuterium isotope

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

Q( 300.) = 164.169
Q( 225.) = 123.269
Q( 150.) = 82.279
Q( 75.) = 41.301
Q( 37.5) = 20.818
Q(18.25) = 10.580
Q(9.375) = 5.467
A =
B = 38152.995
C =

---

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

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

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

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

Q( 300.) = 113.776
Q( 225.) = 85.454
Q( 150.) = 57.077
Q( 75.) = 28.702
Q( 37.5) = 14.520
Q(18.25) = 7.434
Q(9.375) = 3.898
A =
B = 55101.02
C =

---

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

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

| | | | | |
|---|---|---|---|---|
| Species Tag: | 29002 | | Species Name: | HCO+<br>Formyl radical cation |
| Version: | 2 | | | |
| Date: | Jan 1984 | | | |
| Contributor: | R. L. Poynter | | | |

| | | | | |
|---|---|---|---|---|
| Lines Listed | = 33 | | Q( 300.) = | 140.504 |
| Max. Frequency | = 3000. | GHz | Q( 225.) = | 105.506 |
| Max. J | = 33 | | Q( 150.) = | 70.440 |
| LOGSTR | = -3 | | Q( 75.) = | 35.384 |
| LOGSTR1 | = | | Q( 37.5) = | 17.860 |
| Isotope Correction | = 0. | | Q(18.25) = | 9.102 |
| Minimum Energy | = 0. | $cm^{-1}$ | Q(9.375) = | 4.730 |
| Dipoles: μ(a) | = 3.30 | | A = | |
| μ(b) | = | | B = | 44594.419 |
| μ(c) | = | | C = | |

---

The observed lines are from R. C. Woods, T. A. Dixon, R. J. Saykally, and P. G. Szanto, (1975), Phys. Rev. Lett. 35, 1269, K. V. L. N. Sastry, E. Herbst and F. C. De Lucia, (1981), J. Chem. Phys. 75, 4169, and F. C. Van den Heuvel and A. Dymanus, (1982), Chem. Phys. Lett. 92, 219. The dipole moment was estimated theoretically by Woods, et al., above.

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

Species Name: $CH_2NH$
Methyleneimine

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

Q( 300.) = 5892.86
Q( 225.) = 3800.14
Q( 150.) = 2084.97
Q( 75.) = 740.46
Q( 37.5) = 263.39
Q(18.25) = 94.30
Q(9.375) = 34.20
A = 196211.045
B = 34532.395
C = 29352.232

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

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

Species Name: HCO
Formyl radical

Lines Listed = 2454
Max. Frequency = 3000. GHz
Max. J = 30
LOGSTR =-8
LOGSTR1 =-8.
Isotope Correction = 0.
Minimum Energy = 0. $cm^{-1}$
Dipoles: $\mu(a)$ = 1.3626
$\mu(b)$ = 0.700
$\mu(c)$ = 0

Q( 300.) = 3024.1
Q( 225.) = 1963.4
Q( 150.) = 1068.1
Q( 75.) = 378.4
Q( 37.5) = 134.8
Q(18.25) = 49.0
Q(9.375) = 20.3
A = 7829365.
B = 44788.
C = 41930.4

---

The data include some recently measured lines at Duke by G. A. Blake as well as those from S. Saito, 1972, Astrophys. J. 178, L95; J. A. Austin, et al., 1974, J. Chem. Phys. 60, 207; H. M. Pickett and T. L. Boyd, 1978, Chem. Phys. Lett. 58, 446.

Species Tag: 29005
Version: 1
Date: Jan 1984
Contributor: R. L. Poynter

Species Name: $N_2H^+$

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
$\mu(b)$ =
$\mu(c)$ =

Q( 300.) = 1210.8
Q( 225.) = 909.0
Q( 150.) = 607.0
Q( 75.) = 305.0
Q( 37.5) = 154.0
Q(18.25) = 78.6
Q(9.375) = 48.9
A =
B = 46586.867
C =

---

The experimental measurements were reported by R. J. Saykally, T. A. Dixon, T. G. Anderson, P. G. Szanto, and R. C. Woods, (1976), Ap. J. Lett. 205, L101, by K. V. L. N. Sastry, P. Helminger, E. Herbst, and F. C. DeLucia, (1981) Chem. Phys. Lett. 84, 286, and by F. C. Van den Heuvel and A. Dymanus, (1982), Chem. Phys. Lett. 92, 219.

The dipole moment was estimated theoretically by S. Green, J. A. Montgomery, Jr., and P. Thaddeus, (1974), Ap. J. (Lett), 193, L89.

Species Tag: 30001
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: CO-18
Carbon monoxide, $^{18}$O isotope

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
$\mu(b)$ =
$\mu(c)$ =

Q( 300.) = 114.210
Q( 225.) = 85.778
Q( 150.) = 57.294
Q( 75.) = 28.810
Q( 37.5) = 14.574
Q(18.25) = 7.461
Q(9.375) = 3.912
A =
B = 54891.425
C =

---

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

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

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

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

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

Q( 300.) = 144.486
Q( 225.) = 108.459
Q( 150.) = 72.407
Q( 75.) = 36.367
Q( 37.5) = 18.352
Q(18.25) = 9.348
Q(9.375) = 4.852
A =
B = 43377.32
C =

---

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

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

Species Name: DCO+
Formyl radical cation,
deuterium isotope

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

Q( 300.) = 173.872
Q( 225.) = 130.543
Q( 150.) = 87.129
Q( 75.) = 43.726
Q( 37.5) = 22.031
Q(18.25) = 11.186
Q(9.375) = 5.769
A =
B = 36019.76
C =

---

The observed lines are from R. C. Woods, R. J. Saykally, T. A. Dixon, P. G. Szanto, and T. Anderson (1976), 31st Symposium on Molecular Spectroscopy, Columbus, Ohio, M. Bogey, C. Demuynck, and J. L. Destombes, (1981), Mol. Phys. 43, 1043, and K. V. L. N. Sastry, E. Herbst, and F. C. DeLucia, (1981), J. Chem. Phys. 75, 4169. The dipole moment was assumed to be the same as the parent species.

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

Species Name: $H_2CO$
formaldehyde

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

Q( 300.) = 2876.7
Q( 225.) = 1868.2
Q( 150.) = 1019.7
Q( 75.) = 361.7
Q( 37.5) = 128.65
Q(18.25) = 44.68
Q(9.375) = 13.80
A = 281925.97
B = 38836.582
C = 34001.673

---

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

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

J. S. Chardon and D. Guichon, 1977, J. Phys. (Paris), 38, 113; 1975, J. Phys. (Paris), 34, 791.

F. Y. Chu, S. M. Freund, J. W. C. Johns, and T. Oka, 1973, J. Mol. Spect. 48, 328.

D. Dangoisse, E. Willemot, and J. Bellet, 1978, J. Mol. Spect. 71, 414.

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

A. F. Krupnov, L. I. Gershtein, V. G. Shustrov, and V. V. Polyakov, 1970, Opt. Spect. (USSR), 28, 257.

R. B. Lawrence and M. W. P. Strandberg, 1949, Phys. Rev. 75, 1774.

T. Oka, H. Hirakawa, and K. Shimoda, 1960, J. Phys. Soc. Japan, 15, 2265.

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

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

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

Species Name: C-13-$H_2$NH
Methylenimine,
$^{13}$C isotope

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

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

---

The computational methods is the same as that used on the parent species, $CH_2NH$. The data are from R. Pearson, Jr. and F. J. Lovas, 1977, J. Chem. Phys. 66, 4149. The dipole moment has been assumed the same as for the parent species.

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

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

Lines Listed = 440
Max. Frequency = 3000 GHz
Max. J = 10
LOGSTR = -8
LOGSTR1 =
Isotope Correction = -2.432
Minimum Energy = 0. $cm^{-1}$
Dipoles: $\mu$(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
A = 195738.07
B = 33736.10
C = 28688.61

---

The computational method is the same as that used on the parent species, $CH_2NH$. The data are from R. Pearson, Jr. and F. J. Lovas, 1977, J. Chem. Phys. 66, 4149. The dipole moment has been assumed the same as for the parent species.

| | | | |
|---|---|---|---|
| Species Tag: | 30007 | Species Name: | $CH_2ND$<br>Methylenimine,<br>deuterium isotope<br>on nitrogen atom |
| Version: | 1 | | |
| Date: | Feb 1981 | | |
| Contributor: | R. L. Poynter | | |

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

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The computational method is the same as that used for the parent species, $CH_2NH$. The data are from R. Pearson, Jr. and F. J. Lovas, 1977, J. Chem. Phys. 66, 4149.

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

Species Tag: 30008
Version: 1
Date: Feb 1980
Contributor: H. M. Pickett

Species Name: NO
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
$\mu(b)$ =
$\mu(c)$ =

Q( 300.) = 1159.46
Q( 225.) = 816.88
Q( 150.) = 492.32
Q( 75.) = 209.69
Q( 37.5) = 99.48
Q(18.25) = 51.99
Q(9.375) = 28.87
A =
B = 50849.06
C =

---

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

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

Species Name: $N_2D^+$

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

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

---

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

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

Species Tag: 31001
Version: 2
Date: Dec 1983
Contributor: R. L. Poynter

Species Name: HCO-18+
Formyl radical cation,
$^{18}O$ isotope

Lines Listed = 34
Max. Frequency = 3000 GHz
Max. J = 34
LOGSTR = -2.7
LOGSTR1 =
Isotope Correction = -2.690
Minimum Energy = 0. $cm^{-1}$
Dipoles: μ(a) = 3.30
μ(b) =
μ(c) =

Q( 300.) = 147.16
Q( 225.) = 110.47
Q( 150.) = 73.75
Q( 75.) = 37.04
Q( 37.5) = 18.68
Q(18.25) = 9.52
Q(9.375) = 4.94
A =
B = 42581.21
C =

---

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

Species Tag: 31002
Version: 1
Date: Jan 1980
Contributor: R. L. Poynter

Species Name: $H_2$C-13-O
Formaldehyde,
$^{13}$C isotope

Lines Listed = 601
Max. Frequency = 3000 GHz
Max. J = 40
LOGSTR = -9.3
LOGSTR1 =
Isotope Correction = -1.955
Minimum Energy = 0. $cm^{-1}$
Dipoles: $\mu(a)$ = 2.331
$\mu(b)$ = 0
$\mu(c)$ = 0

Q( 300.) = 2949.7
Q( 225.) = 1925.4
Q( 150.) = 1047.6
Q( 75.) = 370.9
Q( 37.5) = 131.9
Q(18.25) = 45.78
Q(9.375) = 14.13
A = 281930.85
B = 37811.92
C = 33213.19

---

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

D. Dangoisse, E. Willemot, and J. Bellet, 1978, J. Mol. Spect. 71, 414.

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

R. B. Lawrence and M. W. P. Strandberg, 1951, Phys. Rev. 83, 363.

R. Nerf, 1972, Ap. J., 174, 467.

T. Oka, H. Hirakawa, and K. Shimoda, 1960, J. Phys. Soc. Japan, 15, 2265.

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

K. D. Tucker, G. R. Tomasevich, and P. Thaddeus, 1972, Ap. J. 174, 463; 1971, Ap. J. 169, 429.

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

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

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

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

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

---

Q(275) = 200.426
Q(250) = 182.231
Q(200) = 145.919

The measurements and calculational method are from T. Amano and E. Hirota, 1974, J. Mol. Spectroscopy 53, 346. The Raman lines of $O_2$ (M. Loete and H. Berger, 1977, J. Mol. Spectroscopy 68, 317) were used with the millimeter wavelength measurements and the submillimeter-line of W. Steinbach and W. Gordy (1973, Phys. Rev A 8, 1953) in a combined fit of the v = 0 and v = 1 transitions. The intensities of the magnetic dipole transitions have been calculated using the g values obtained from magnetic resonance by K. D. Bowers, R. A. Kamper and C. D. Lustig, 1959, Proc. Roy. Soc. (Lond.) A251, 565. The zero-frequency absorption is included but the frequency is set to a synthetic frequency of |g|J for the given level.

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

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

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

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

---

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

Species Tag: 32003
Version: 2
Date: Nov 1980
Contributor: H. M. Pickett

Species Name: $CH_3OH$
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
A = 127484.
B = 24679.98
C = 23769.70

---

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

The v quantum numbers in the catalogue are:

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

Species Tag: 32004
Version: 1
Date: Feb 1980
Contributor: R. L. Poynter

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

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

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

---

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

D. Dangoisse, E. Willemot, and J. Bellet, 1978, J. Mol. Spect. 71, 414.

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

R. B. Lawrence and M. W. P. Strandberg, 1951, Phys. Rev. 83, 363.

T. Oka, H. Hirakawa, and K. Shimoda, 1960, J. Phys. Soc. Japan, 15, 2265.

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

R. D. Tucker, G. R. Tomasevich, and P. Thaddeus, 1972, Ap. J. 174, 463, 1971, Ap. J., 169, 429.

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

Species Tag: 33001
Version: 1
Date: May 1983
Contributor: H. M. Pickett

Species Name: $HO_2$
Hydroperoxyl radical

Lines Listed = 6174
Max. Frequency = 3000 GHz
Max. J = 30
LOGSTR = -7.
LOGSTR1 = -7.
Isotope Correction = 0.
Minimum Energy = 0. $cm^{-1}$
Dipoles: μ(a) = 1.412
μ(b) = 1.541
μ(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
A = 610273.
B = 33514.
C = 31672.

---

The data were obtained from A. Charo and F. C. DeLucia, 1982, J. Mol. Spectroscopy 94, 426; Y. Beers and C. J. Howard, 1975, J. Chem. Phys. 63, 4121; S. Saito, 1977, J. Mol. Spectrosc. 65, 229.

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

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

Species Name: 0-18-0
Molecular oxygen,
single substituted
$^{18}$O isotope

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

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

---

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

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

Species Name: $H_2S$
Hydrogen sulfide

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

Q( 300.) = 514.197
Q( 225.) = 333.981
Q( 150.) = 182.164
Q( 75.) = 65.525
Q( 37.5) = 23.865
Q(18.25) = 8.700
Q(9.375) = 2.911
A = 310182.24
B = 270884.05
C = 141705.88

---

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

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

P. Helminger, F. C. DeLucia, and W. H. Kirchhoff, 1973, J. Phys. Chem. Ref. Data 2, 213.

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

|  |  |  |  |  |
|---|---|---|---|---|
| Species Tag: | 34003 |  | Species Name: | $PH_3$<br>Phosphine |
| Version: | 2 |  |  |  |
| Date: | Aug 1983 |  |  |  |
| Contributor: | R. L. Poynter |  |  |  |
| Lines Listed | = 142 |  | Q( 300.) = | 405.64 |
| Max. Frequency | = 3000 | GHz | Q( 225.) = | 263.47 |
| Max. J | = 19 |  | Q( 150.) = | 143.41 |
| LOGSTR | = -17 |  | Q( 75.) = | 51.54 |
| LOGSTR1 | = |  | Q( 37.5) = | 18.59 |
| Isotope Correction | = 0. |  | Q(18.25) = | 6.958 |
| Minimum Energy | = 0. | $cm^{-1}$ | Q(9.375) = | 2.898 |
| Dipoles: $\mu(a)$ | = 0.000072* |  | A = | B |
| $\mu(b)$ | = |  | B = | 133480.22 |
| $\mu(c)$ | = 0.574 |  | C = | 117488.39 |

*centrifugally induced

The measured lines are taken from D. Helms and W. Gordy, 1971, J. Mol. Spect., 66, 206; F. Y. Chu and T. Oka, 1974, J. Chem. Phys. 60, 4612; P. B. Davies, R. M. Newman, S. C. Wofsy, and W. Klemperer, 1971, J. Chem. Phys. 55, 3564; A. F. Krupnov, A. A. Melnikov, and V. A. Skvortsov, 1979, Opt. Spectrosc. (USSR) 46, (5), 570; and H. M. Pickett, R. L. Poynter and E. A. Cohen, 1981, J. Quant. Spectrosc. and Radiat. Transfer, 26, 197.

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

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

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

Species Name: $H_2O_2$
Hydrogen peroxide,
ground torsional
states

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

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

---

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

Species Tag: 35001
Version: 1
Date: Jan 1980
Contributor: R. L. Poynter

Species Name: HDS
Hydrogen sulfide,
deuterium isotope

Lines Listed = 1138
Max. Frequency = 3000 GHz
Max. J = 20
LOGSTR = -11.4
LOGSTR1 =
Isotope Correction = -3.523
Minimum Energy = 0. $cm^{-1}$
Dipoles: $\mu(a)$ = 0.470
$\mu(b)$ = 0.974
$\mu(c)$ = 0.

Q( 300.) = 430.90
Q( 225.) = 280.92
Q( 150.) = 153.44
Q( 75.) = 54.75
Q( 37.5) = 19.758
Q(18.25) = 7.291
Q(9.375) = 2.829
A = 292351.302
B = 147861.801
C = 96704.120

---

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 40, 125. The experimental measurements were taken from R. E. Hillger and M. W. P. Strandberg, 1951, Phys. Rev. 83, 575; P. Thaddeus, L. C. Krisher, and J. H. N. Loubser, 1964, J. Chem. Phys. 40, 257; P. Helminger, R. L. Cook, and F. C. DeLucia, 1971, J. Mol. Spectrosc. 40, 125; P. Helminger, F. C. DeLucia, and W. H. Kirchhoff, 1973, J. Phys. Chem. Ref. Data 2, 215; and from G. Steenbeckeliers, quoted in F. J. Lovas, 1978, J. Phys. Chem. Ref. Data, 7, 1445.

The dipole moment was reported by R. E. Hillger and M. W. P. Strandberg, 1951, Phys. Rev. 83, 575.

Species Tag: 36001
Version: 1
Date: Feb 1980
Contributor: R. L. Poynter and H. M. Pickett

Species Name: HCl35
Hydrochloric acid,
$^{35}$Cl isotope

Lines Listed = 17
Max. Frequency = 3000 GHz
Max. J = 4
LOGSTR = -1.3
LOGSTR1 =
Isotope Correction = -0.122
Minimum Energy = 0. $cm^{-1}$
Dipoles: $\mu(a)$ = 1.109
$\mu(b)$ = 0.
$\mu(c)$ = 0.

Q( 300.) = 81.232
Q( 225.) = 60.924
Q( 150.) = 40.616
Q( 75.) = 21.249
Q( 37.5) = 11.437
Q(18.25) = 6.583
Q(9.375) = 4.488
A =
B = 312989.3
C =

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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<br>hydrochloric acid,<br>$^{37}$Cl isotope |
| Version: | 1 | | |
| Date: | Feb 1980 | | |
| Contributor: | R. L. Poynter and H. M. Pickett | | |

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

---

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

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

Species Tag: 40001
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: $CH_3CCH$
propyne

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

Q( 300.) = 5428.80
Q( 225.) = 3524.70
Q( 150.) = 1920.80
Q( 75.) = 679.68
Q( 37.5) = 241.25
Q(18.25) = 88.27
Q(9.375) = 34.42
A = 158590.
B = 8545.86
C = B

---

The experimental measurements were obtained from A. Dubrille, D. Boucher, J. Burie, and J. Demaison, 1978, J. Mol. Spect. 72, 158. The A moment was estimated from the structure.

The dipole moment was measured by J. S. Muenter and V. W. Laurie, 1966, J. Chem. Phys. 45, 855.

Species Tag: 41001
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: $CH_3CN$
acetonitrile

Lines Listed = 1441
Max. Frequency = 3000. GHz
Max. J = 82
LOGSTR = -4.5 for J>14
LOGSTR1 =
Isotope Correction = 0.
Minimum Energy = 0. $cm^{-1}$
Dipoles: μ(a) = 3.919
μ(b) = 0.
μ(c) = 0.

Q( 300.) = 15145.00
Q( 225.) = 9841.34
Q( 150.) = 5359.87
Q( 75.) = 1896.38
Q( 37.5) = 673.17
Q(18.25) = 246.34
Q(9.375) = 96.10
A = 158290.
B = 9198.9
C = B

---

The experimental measurements were taken from D. Boucher, J. Burie, J. Demaison, A. Dubrille, J. Legrand, and B. Segard, 1977, J. Mol. Spect. 64, 290; A. Bauer and S. Maes, 1969, J. Phys. 30, 169; S. G. Kukolich, D. J. Ruben, J. H. S. Wang, and J. R. Williams, 1973, J. Chem. Phys. 58, 3155.

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

Species Tag: 41002
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

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

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

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

---

The experimental measurements were taken from D. Boucher, J. Burie, J. Demaison, A. Dubrille, J. Legrand, and B. Segard, 1977, J. Mol. Spect. 64, 290; A. Bauer and S. Maes, 1969, J. Phys. 30, 169; S. G. Kukolich, D. J. Ruben, J. H. S. Wang, and J. R. Williams, 1973, J. Chem. Phys. 58, 3155.

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

Species Tag: 41003
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

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

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

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

---

The experimental measurements were taken from D. Boucher, J. Burie, J. Demaison, A. Dubrille, J. Legrand, and B. Segard, 1977, J. Mol. Spect. 64, 290; A. Bauer and S. Maes, 1969, J. Phys. 30, 169; S. G. Kukolich, D. J. Ruben, J. H. S. Wang, and J. R. Williams, 1973, J. Chem. Phys. 58, 3155.

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

Species Tag: 41004
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: $H_3$C-13-CCH propyne, $^{13}$C isotope on atom 3

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

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

---

The experimental measurements were taken from D. Boucher, J. Burie, J. Demaison, A. Dubrille, J. Legrand, and B. Segard, 1977, J. Mol. Spect. 64, 290; A. Bauer and S. Maes, 1969, J. Phys. 30, S. G. Kukolich, D. J. Ruben, J. H. S. Wang, and J. R. Williams, 1973, J. Chem. Phys. 58, 3155.

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

Species Tag: 41005
Version: 2
Date: Jan 1984
Contributor: R. L. Poynter

Species Name: $CH_3CCD$

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

Q( 300.) = 17192.04
Q( 225.) = 11168.37
Q( 150.) = 6139.89
Q( 75.) = 2243.60
Q( 37.5) = 795.34
Q(18.25) = 290.46
Q(9.375) = 113.17
A = 158590.
B = 7788.170
C = B

---

The experimental measurements are from J. S. Muenter and V. W. Laurie, (1966), J. Chem. Phys. 45, 855; L. F. Thomas, E. I. Sherrard, and J. Sheridan, (1955), Trans. Far. Soc. 51, 619; and C. D. Cogley, L. M. Tack, and S. G. Kukolich, (1982), J. Chem. Phys. 76, 5669.

The dipole moment was taken from Muenter and Laurie, above.

| | | | | |
|---|---|---|---|---|
| Species Tag: | 41006 | | Species Name: | $CH_2DCCH$<br>propyne, deuterium<br>isotope on methyl<br>carbon atom |
| Version: | 2 | | | |
| Date: | Aug 1983 | | | |
| Contributor: | R. L. Poynter | | | |

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

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

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

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

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

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

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

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

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

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

Species Name: $CH_2CO$, ketene

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

Q( 300.) = 10322.85
Q( 225.) = 6634.38
Q( 150.) = 3433.99
Q( 75.) = 1285.88
Q( 37.5) = 457.09
Q(18.25) = 157.22
Q(9.375) = 47.58
A = 282473.
B = 10293.80
C = 9916.38

---

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

B. Fabricant, D. Krieger, and J. S. Muenter, 1977, J. Chem. Phys. 67, 1576.

J. W. C. Johns, J.M. R. Stone, and G. Winnewisser, 1972, J. Mol. Spect. 42, 523.

H. R. Johnson and M. W. P. Strandberg, 1952, J. Chem. Phys. 20, 687.

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

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

Species Name: CHDCO, ketene,
mono deuterium isotope

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

Q( 300.) = 6682.68
Q( 225.) = 4340.53
Q( 150.) = 2344.00
Q( 75.) = 828.70
Q( 37.5) = 295.80
Q(18.25) = 105.15
Q(9.375) = 37.50
A = 194313.
B = 9647.396
C = 9174.975

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

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

Species Tag: 44001
Version: 2
Date: Jan 1984
Contributor: R. L. Poynter

Species Name: CS, carbon monosulfide

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

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

---

The experimental data were taken from the following papers:

R. Kewley, K. V. L. N. Sastry, M. Winnewisser, and W. Gordy, 1963, J. Chem. Phys. 39, 2856.

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

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

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

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

Species Tag: 44002

Version: 2

Date: Jan 1984

Contributor: R. L. Poynter

Species Name: $^{28}$SiO, silicon monoxide

Lines Listed = 31

Max. Frequency = 1350. GHz

Max. J = 30

LOGSTR = -4

LOGSTR1 =

Isotope Correction = -0.035

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

Dipoles : μ(a) = 3.098

μ(b) =

μ(c) =

Q( 300.) = 287.210

Q( 225.) = 215.874

Q( 150.) = 144.344

Q( 75.) = 72.327

Q( 37.5) = 36.325

Q(18.25) = 18.332

Q(9.375) = 9.339

A =

B = 21711.967

C =

---

The experimental data were taken from the following papers:

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

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

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

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

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

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
A = 56609.474
B = 10162.766
C = 9100.412

---

The data set used is referenced by A. Bauder, F. J. Lovas and D. R. Johnson 1976, J. Phys. Chem. Ref. Data 5, 53. The lines were fit to a rigid rotor with centrifugal distortion.

Species Tag: 44004
Species Name: $N_2O$
Version: 1
Date: Jan 1980
Contributor: R. L. Poynter and H. M. Pickett

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

Q( 300.) = 497.966
Q( 225.) = 373.594
Q( 150.) = 249.173
Q( 75.) = 124.738
Q( 37.5) = 62.546
Q(18.25) = 31.434
Q(9.375) = 15.889
A =
B = 12561.637
C =

---

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

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

| | | | |
|---|---|---|---|
| Species Tag: | 44005 | Species Name: | $CH_3CHO$-E<br>acetaldehyde,<br>E state |
| Version: | 1 | | |
| Date: | Dec 1980 | | |
| Contributor: | H. M. Pickett | | |

| | | | | |
|---|---|---|---|---|
| Lines Listed | = | 691 | Q( 300.) = | 12111.56 |
| Max. Frequency | = | 3000 GHz | Q( 225.) = | 7866.84 |
| Max. J | = | 15 | Q( 150.) = | 4282.08 |
| LOGSTR | = | -10 | Q( 75.) = | 1513.94 |
| LOGSTR1 | = | | Q( 37.5) = | 535.26 |
| Isotope Correction | = | 0. | Q(18.25) = | 189.46 |
| Minimum Energy | = | 0. $cm^{-1}$ | Q(9.375) = | 67.29 |
| Dipoles : $\mu(a)$ | = | 2.55 | A = | 56448.5 |
| $\mu(b)$ | = | 0.870 | B = | 10160.1 |
| $\mu(c)$ | = | | C = | 9101.3 |

---

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

Species Tag: 45001
Version: 2
Date: Jan 1984
Contributor: R. Poynter

Species Name: C-13-S
Carbon monosulfide, $^{13}$C isotope

Lines Listed = 29
Max. Frequency = 1340 GHz
Max. J = 28
LOGSTR = -4
LOGSTR1 =
Isotope Correction = -1.977
Minimum Energy = 0. cm$^{-1}$
Dipoles : $\mu(a)$ = 1.957
$\mu(b)$ =
$\mu(c)$ =

Q( 300.) = 270.65
Q( 225.) = 203.24
Q( 150.) = 135.550
Q( 75.) = 67.936
Q( 37.5) = 34.127
Q(18.25) = 17.235
Q(9.375) = 8.790
A =
B = 23123.856
C =

---

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

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

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

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

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

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

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

---

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

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

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

Species Name: Formamide
$NH_2CHO$

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

Q( 300.) = 29154.14
Q( 225.) = 18479.91
Q( 150.) = 10313.37
Q( 75.) = 3633.29
Q( 37.5) = 1293.30
Q(18.25) = 459.199
Q(9.375) = 163.719
A = 72716.954
B = 11373.453
C = 9833.903

---

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

C. C. Costain and J. M. Dowling, 1960, J. Chem. Phys. 32, 290.

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

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

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

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

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

Species Tag: 46001
Version: 2
Date: Jan 1984
Contributor: R. L. Poynter

Species Name: $C^{34}S$, carbon monosulfide $^{34}S$ isotope

Lines Listed = 34
Max. Frequency = 1640 GHz
Max. J = 33
LOGSTR = -4
LOGSTR1 =
Isotope Correction = -1.376
Minimum Energy = 0. $cm^{-1}$
Dipoles : $\mu(a)$ = 1.957
$\mu(b)$ =
$\mu(c)$ =

Q( 300.) = 259.657
Q( 225.) = 194.939
Q( 150.) = 130.047
Q( 75.) = 65.1779
Q( 37.5) = 32.7567
Q(18.25) = 16.5463
Q(9.375) = 8.4470
A =
B = 24103.541
C =

---

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

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

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

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

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

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

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

---

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

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

Species Tag: 46003

Species Name: $H_2CS$, thioformaldehyde

Version: 1

Date: Jan 1980

Contributor: R. L. Poynter

Lines Listed = 517

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) =

Q( 300.) = 5984.11

Q( 225.) = 3760.98

Q( 150.) = 2088.82

Q( 75.) = 750.067

Q( 37.5) = 265.644

Q(18.25) = 91.1801

Q(9.375) = 27.5233

A = 291291.641

B = 17699.628

C = 16651.830

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

The dipole moment was taken from B. Fabricant, D. Krieger, and J. S. Muenter, 1977, J. Chem. Phys. 67, 1576.

| | | | |
|---|---|---|---|
| Species Tag: | 46004 | Species Name: | $C_2H_5OH$<br>ethyl alcohol,<br>ground trans state |
| Version: | 1 | | |
| Date: | Jan 1980 | | |
| Contributor: | R. L. Poynter | | |

| | | | |
|---|---|---|---|
| Lines Listed = | 1236 | Q( 300.) = | 17009.8 |
| Max. Frequency = | 3000 GHz | Q( 225.) = | 11048.4 |
| Max. J = | 20 | Q( 150.) = | 6013.13 |
| LOGSTR = | -11 | Q( 75.) = | 2020.23 |
| LOGSTR1 = | | Q( 37.5) = | 747.653 |
| Isotope Correction = | 0. | Q(18.25) = | 267.547 |
| Minimum Energy = | 0. cm$^{-1}$ | Q(9.375) = | 95.2357 |
| Dipoles : $\mu(a)$ = | 0.046 | A = | 34891.75 |
| $\mu(b)$ = | 1.438 | B = | 9350.635 |
| $\mu(c)$ = | | C = | 8135.236 |

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

J. Michielson-Effinger, 1969, J. de Phys. 30, 333.

Y. Sasada, M. Takano, and T. Satoh, 1971, J. Mol. Spect. 38, 33.

H. Takano, Y. Sasada, and T. Satoh, 1968, J. Mol. Spect. 26, 157.

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

The dipole moment was reported by Takano, et al, above.

Species Tag: 46005
Version: 1
Date: Jan 1980
Contributor: R. L. Poynter

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

Species Name: HCOOH
formic acid
ground trans state

Q( 300.) = 8883.82
Q( 225.) = 5770.32
Q( 150.) = 3141.23
Q( 75.) = 1085.67
Q( 37.5) = 393.460
Q(18.25) = 139.991
Q(9.375) = 49.9344
A = 77512.25
B = 12055.11
C = 10416.12

---

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

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

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

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

The dipole moment used in the present work was measured by H. Kim, R. Keller, and W. D. Gwinn, 1962, J. Chem. Phys. 37, 2748, and was adjusted to the new OCS standard, (J. S. Muenter, 1968, J. Chem. Phys. 48, 4544). Inproved values [$\mu_a$ = 1.4214(21)D and $\mu_b$ = 0.2096(65)D] have been recently reported by H. Kuze, T. Kuga, and T. Shimizu, 1982, J. Mol. Spect. 93, 248.

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

Species Name: nitrogen dioxide, $NO_2$

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

Q( 300.) = 13402.
Q( 225.) = 8750.
Q( 150.) = 4764.
Q( 75.) = 1683.
Q( 37.5) = 596.
Q(18.25) = 211.8
Q(9.375) = 75.7
A = 239904.
B = 13002.
C = 12305.

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

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

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

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

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

---

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

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

Other references were taken from this paper.

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

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

| | | | |
|---|---|---|---|
| Lines Listed = | 1194 | Q( 300.) = | 8896.12 |
| Max. Frequency = | 3000 GHz | Q( 225.) = | 6672.68 |
| Max. J = | 20 | Q( 150.) = | 3144.85 |
| LOGSTR = | -10 | Q( 75.) = | 1094.21 |
| LOGSTR1 = | | Q( 37.5) = | 399.209 |
| Isotope Correction = | -1.955 | Q(18.25) = | 142.037 |
| Minimum Energy = | 0. $cm^{-1}$ | Q(9.375) = | 50.6640 |
| Dipoles : $\mu(a)$ = | 1.396 | A = | 77580.494 |
| $\mu(b)$ = | 0.260 | B = | 12053.567 |
| $\mu(c)$ = | | C = | 10378.997 |

---

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

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

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

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

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

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

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

Q( 300.) = 10531.2
Q( 225.) = 6840.2
Q( 150.) = 3626.47
Q( 75.) = 1251.4
Q( 37.5) = 466.123
Q(18.25) = 165.882
Q(9.375) = 59.1562
A = 57709.33
B = 12055.971
C = 9955.609

---

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

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

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

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

Species Tag: 47004
Version: 1
Date: Jan 1980
Contributor: R. L. Poynter

Lines Listed = 612
Max. Frequency = 3000 GHz
Max. J = 20
LOGSTR = -9
LOGSTR1 =
Isotope Correction = -3.824
Minimum Energy = 0. cm$^{-1}$
Dipoles : $\mu(a)$ = 1.396
$\mu(b)$ = 0.260
$\mu(c)$ =

Species Name: HCOOD
formic acid,
deuterium isotope
on O atom

Q( 300.) = 9954.87
Q( 225.) = 6465.87
Q( 150.) = 3519.57
Q( 75.) = 1213.13
Q( 37.5) = 440.555
Q(18.25) = 156.820
Q(9.375) = 55.9114
A = 66100.14
B = 11762.577
C = 9969.943

---

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

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

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

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

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

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

Lines Listed = 330
Max. Frequency = 3000 GHz
Max. J = 50
LOGSTR = -6
LOGSTR1 =
Isotope Correction = -0.022
Minimum Energy = 0. $cm^{-1}$
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( 37.5) = 90.3441
Q(18.25) = 38.8776
Q(9.375) = 15.9038
A =
B = 21523.02
C =

---

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

Species Tag: 48002
Version: 1
Date: Dec 1979
Contributor: H. M. Pickett

Species Name: SO, sulfur monoxide
$^3\Sigma$ ground state,
v=1 vibrational state

Lines Listed = 261
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( 37.5) = 90.3441
Q(18.25) = 38.8776
Q(9.375) = 15.9038
A =
B = 21351.0
C =

---

The calculational method is described in T. Amano and E. Hirota, 1974, J. Molec. Spectroscopy <u>53</u>, 346. The data are from T. Amano, E. Hirota, and Y. Morino, 1967, J. Phys. Soc. Japan <u>22</u>, 399. All centrifugal distortion constants were fixed to their ground state values. Magnetic and electric dipole transitions are included.

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

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

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

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

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

---

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

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

Species Tag: 48004
Version: 2
Date: Mar 1984
Contributor: H. M. Pickett

Species Name: $^{16}O_3$, ozone

Lines Listed = 6471
Max. Frequency = 10000 GHz
Max. J = 80.
LOGSTR = -10.
LOGSTR1 = -10.
Isotope Correction = 0.
Minimum Energy = 0. $cm^{-1}$
Dipoles : $\mu(a)$ =
$\mu(b)$ = 0.5324
$\mu(c)$ =

Q( 300.) = 3553.04
Q( 225.) = 2263.60
Q( 150.) = 1198.67
Q( 75.) = 423.448
Q( 37.5) = 150.037
Q(18.25) = 53.2967
Q(9.375) = 19.0371
A = 106535.234
B = 13349.090
C = 11834.524

---

The catalog of the ozone lines is based on the work of M. J. C. Depannemaecker, B. Duterage, and M. J. Bellet, 1977, J. Quant. Spect. Radiat. Transfer 17, 519. Additional lines are cited in F. J. Lovas, 1978, J. Phys. Chem. Ref. Data 7, 1445. Further lines were measured at JPL by E. A. Cohen. The ground state lines were fit with the $\nu_1$ and $\nu_3$ lines and infrared lines in the 10μ region simultaneously. The maximum value of $K_a$ is 20.

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

The partition function includes contributions from all vibrational states.

Species Tag: 48005
Version: 2
Date: Mar 1984
Contributor: H. M. Pickett

Species Name: $O_3$ $\nu_2$ vibrational state (010)

Lines Listed = 4337
Max. Frequency = 3000 GHz
Max. J = 60
LOGSTR = -10.
LOGSTR1 = -10.
Isotope Correction = 0.
Minimum Energy = 700.9 $cm^{-1}$
Dipoles : μ(a) =
μ(b) = 0.5324
μ(c) =

Q( 300.) = 3553.04
Q( 225.) = 2263.60
Q( 150.) = 1198.67
Q( 75.) = 423.448
Q( 37.5) = 150.037
Q(18.25) = 53.2967
Q(9.375) = 19.0371
A = 108137.979
B = 13311.143
C = 11765.222

---

The $\nu_2$ ozone lines were derived from a fit of the data given by M. J. C. Depannemaecker, B. Duterage, and M. J. Bellet, 1977, J. Quant. Spect. and Radiat. Transfer 17, 519. Additional lines are listed in F. J. Lovas, 1978, J. Phys. Chem. Ref. Data., 7, 1445. Further lines were measured at JPL by E. A. Cohen. The maximum valued K is 15.

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

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

Species Name: $O_3$
$\nu_1$, $\nu_3$ vibrational
states (100)
and (001)

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

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

---

The rotational lines were measured by T. Tanaka and Y. Morino, 1970, J. Mol. Spec. 33, 538 and A. Barbe, *et al*., 1977, J. Mol. Spec. 64, 343. The rotational lines of the ground, $\nu_1$ and $\nu_3$ states were fit along with infrared lines in the 10$\mu$ region simultaneously. The maximum value of $K_a$ is 20.

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

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

Species Name: $O_3$ $\nu_2$ = 2 state
(0,2,0)

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

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

---

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

Species Tag: 49001

Version: 1

Date: Mar 1984

Contributor: H. M. Pickett

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

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

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

---

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

Species Tag: 49002
Version: 1
Date: Mar 1984
Contributor: H. M. Pickett

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

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 : μ(a) = 0.0034
μ(b) = 0.5324
μ(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. <u>97</u>, 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
Version: 1
Date: Dec 1979
Contributor: H. M. Pickett

Species Name: $^{34}$SO, sulfur monoxide,
$^{3}\Sigma$ ground state,
$^{34}$S isotope

Lines Listed = 280
Max. Frequency = 3000 GHz
Max. J = 50
LOGSTR = -6
LOGSTR1 =
Isotope Correction = -1.376
Minimum Energy = 0 $\text{cm}^{-1}$
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
A =
B = 21102.72
C =

---

The calculational method is described in T. Amano and E. Hirota, 1974, J. Molec. Spectroscopy 53, 346. The data used is reported in E. Tiemann, 1974, J. Phys. Chem. Ref. Data 3, 259. Both electric dipole and magnetic dipole transitions are listed in the catalogue.

Species Tag: 50002
Version: 1
Date: Dec 1979
Contributor: H. M. Pickett

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

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

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

---

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

Species Tag: 50003
Version: 2
Date: Mar 1984
Contributor: H. M. Pickett and R. L. Poynter

Species Name: $^{16}O^{18}O^{16}O$
ozone, ground state,
symmetric $^{18}O$ isotope

Lines Listed = 3184
Max. Frequency = 9999. GHz
Max. J = 50
LOGSTR = -9
LOGSTR1 = -9
Isotope Correction = -2.690
Minimum Energy = 0. $cm^{-1}$
Dipoles : $\mu(a)$ =
$\mu(b)$ = 0.5324
$\mu(c)$ =

Q( 300.) = 3525.34
Q( 225.) = 2445.129
Q( 150.) = 1247.107
Q( 75.) = 441.8769
Q( 37.5) = 156.5677
Q(18.25) = 55.6161
Q(9.375) = 19.8610
A = 98646.687
B = 13352.732
C = 11731.767

---

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

Species Tag: 50004
Version: 2
Date: Mar 1984
Contributor: H. M. Pickett and R. L. Poynter

Species Name: $^{18}O^{16}O^{16}O$, asymmetric $^{18}O$ ozone, ground state

Lines Listed = 7304
Max. Frequency = 9999 GHz
Max. J = 40
LOGSTR = -9
LOGSTR1 = -9
Isotope Correction = -2.389
Minimum Energy = 0. $cm^{-1}$
Dipoles : $\mu(a)$ = 0.0068
$\mu(b)$ = 0.5324
$\mu(c)$ =

Q( 300.) = 7214.414
Q( 225.) = 4994.599
Q( 150.) = 2549.761
Q( 75.) = 904.0679
Q( 37.5) = 320.2580
Q(18.25) = 113.7639
Q(9.375) = 40.6069
A = 104573.161
B = 12591.48
C = 11212.5057

---

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

| | | | |
|---|---|---|---|
| Species Tag: | 52006 | Species Name: | HO$^{35}$Cl,<br>hypochlorous acid |
| Version: | 2 | | |
| Date: | Jan 1984 | | |
| Contributor: | H. M. Pickett | | |

| | | | |
|---|---|---|---|
| Lines Listed = | 3919 | Q( 300.) = | 2380.4 |
| Max. Frequency = | 10000 GHz | Q( 225.) = | 1545.4 |
| Max. J = | 60 | Q( 150.) = | 840.9 |
| LOGSTR = | -8 | Q( 75.) = | 297.5 |
| LOGSTR1 = | -8 | Q( 37.5) = | 105.5 |
| Isotope Correction = | -0.122 | Q(18.25) = | 37.66 |
| Minimum Energy = | 0. $cm^{-1}$ | Q(9.375) = | 14.59 |
| Dipoles: $\mu(a)$ = | 0.3627 | A = | 613483.8 |
| $\mu(b)$ = | 1.471 | B = | 15116.795 |
| $\mu(c)$ = | | C = | 14725.78 |

---

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

Species Tag: 52005
Version: 1
Date: Dec. 1979
Contributor: R. L. Poynter

Species Name: DCCCN,
cyanoacetylene,
deuterium isotope

Lines Listed = 156
Max. Frequency = 1000 GHz
Max. J = 99
LOGSTR = -7
LOGSTR1 =
Isotope Correction = -3.824
Minimum Energy = 0. $cm^{-1}$
Dipoles: $\mu(a)$ = 3.724
$\mu(b)$ =
$\mu(c)$ =

Q( 300.) = 4443.2393
Q( 225.) = 3332.7310
Q( 150.) = 2222.2842
Q( 75.) = 1111.7319
Q( 37.5) = 556.2878
Q(18.25) = 278.6121
Q(9.375) = 139.8297
A =
B = 4221.58
C =

---

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

| | | | |
|---|---|---|---|
| Species Tag: | 53001 | Species Name: | $C_2H_3CN$,<br>acrylonitrile |
| Version: | 1 | | |
| Date: | Jan 1980 | | |
| Contributor: | R. L. Poynter | | |

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

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

C. C. Costain and B. P. Stoicheff, 1959, J. Chem. Phys. 30, 777.

M. C. L. Gerry and G. Winnewisser, 1973, J. Mol. Spect. 48, 1.

M. C. L. Gerry, K. Yamada, and G. Winnewisser, 1979, J. Phys. Chem. Ref. Data 8, 107.

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

Species Tag: 53002
Version: 2
Date: Oct 1980
Contributor: H. M. Pickett

Species Name: $^{37}$ClO,
chlorine monoxide,
$^{37}$Cl isotope

Lines Listed = 2649
Max. Frequency = 3000 GHz
Max. J = 85
LOGSTR = -10
LOGSTR1 =
Isotope Correction = -0.611
Minimum Energy = 0. cm$^{-1}$
Dipoles: $\mu(a)$ = 1.239
$\mu(b)$ =
$\mu(c)$ =

Q( 300.) = 3348.1118
Q( 225.) = 2336.6826
Q( 150.) = 1448.4390
Q( 75.) = 700.9711
Q( 37.5) = 357.1905
Q(18.25) = 186.3374
Q(9.375) = 101.2744
A =
B = 1828.70
C =

---

The experimental lines below 200 GHz are from R. K. Kakar, E. A. Cohen, and M. Geller, 1978, J. Mol. Spec. 70, 243. Lines above 200 GHz were measured at JPL by E. A. Cohen and H. M. Pickett. The lines were fit to a fine structure Hamiltonian which included $p_D$ and $q_D$ terms and centrifugal distortion on B to sixth power in J. The hyperfine terms in the Hamiltonian included all off-diagonal matrix elements for a, b, c, d, $\eta_1$, $\eta_2$, and $\eta_3$. The partition function was determined by a sum over states to F = 86 for both the $\Omega = 1/2$ and $\Omega = 3/2$ states.

| | | | |
|---|---|---|---|
| Species Tag: | 54001 | Species Name: | $CH_2CH^{13}CN$,<br>acrylonitrile,<br>$^{13}C$ isotope on<br>atom 1 |
| Version: | 1 | | |
| Date: | Jan 1980 | | |
| Contributor: | R. L. Poynter | | |
| Lines Listed = | 118 | Q( 300.) = | 26332.9770 |
| Max. Frequency = | 3000 GHz | Q( 225.) = | 17104.0740 |
| Max. J = | 10 | Q( 150.) = | 9311.0723 |
| LOGSTR = | -9 | Q( 75.) = | 3291.5420 |
| LOGSTR1 = | | Q( 37.5) = | 1163.8567 |
| Isotope Correction = | -1.955 | Q(18.25) = | 358.5091 |
| Minimum Energy = | 0. $cm^{-1}$ | Q(9.375) = | 138.3247 |
| Dipoles: $\mu(a)$ = | 3.68 | A = | 49781. |
| $\mu(b)$ = | 1.25 | B = | 4948.153 |
| $\mu(c)$ = | | C = | 4494.485 |

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

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

Species Tag: 54002
Version: 1
Date: Jan 1980
Contributor: R. L. Poynter

Species Name: $CH_2{}^{13}CHCN$,
acrylonitrile,
$^{13}C$ isotope on
atom 2

Lines Listed = 117
Max. Frequency = 3000 GHz
Max. J = 10
LOGSTR = -9
LOGSTR1 =
Isotope Correction = -1.955
Minimum Energy = 0. $cm^{-1}$
Dipoles: μ(a) = 3.68
μ(b) = 1.25
μ(c) =

Q( 300.) = 26662.4960
Q( 225.) = 17318.0740
Q( 150.) = 9427.5684
Q( 75.) = 3332.7310
Q( 37.5) = 1178.4197
Q(18.25) = 362.9110
Q(9.375) = 140.0232
A = 48645.
B = 4948.700
C = 4485.145

---

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

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

Species Tag: 54003
Version: 1
Date: Jan 1980
Contributor: R. L. Poynter

Species Name: $^{13}CH_2CHCN$, acrylonitrile, $^{13}C$ isotope on atom 3

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
A = 49180.
B = 4837.34
C = 4398.07

---

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

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

Species Tag: 54004
Version: 1
Date: Jan 1980
Contributor: R. L. Poynter

Species Name: $CH_2CDCN$,
acrylonitrile,
deuterium isotope
on atom 2

Lines Listed = 322
Max. Frequency = 3000 GHz
Max. J = 10
LOGSTR = -10
LOGSTR1 =
Isotope Correction = -3.824
Minimum Energy = 0. $cm^{-1}$
Dipoles: $\mu(a)$ = 3.68
$\mu(b)$ = 1.25
$\mu(c)$ =

Q( 300.) = 29696.1680
Q( 225.) = 19288.5940
Q( 150.) = 10500.2640
Q( 75.) = 3711.9375
Q( 37.5) = 1312.5034
Q(18.25) = 402.1610
Q(9.375) = 155.4532
A = 40198.6
B = 4934.35
C = 4388.41

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

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

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

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

$^{37}Cl$ isotope

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

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

---

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

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

Species Name: $C_2H_5CN$,
ethyl cyanide

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

Q( 300.) = 111840.8900
Q( 225.) = 70892.5160
Q( 150.) = 39554.9140
Q( 75.) = 12589.2560
Q( 37.5) = 4595.1553
Q(18.25) = 1406.3713
Q(9.375) = 650.8787
A = 27663.66
B = 4714.144
C = 4235.041

---

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

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

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

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

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

| | | | |
|---|---|---|---|
| Species Tag: | 56001 | Species Name: | $CH_3CH_2{}^{13}CN$,<br>ethyl cyanide,<br>$^{13}C$ isotope on<br>atom 1 |
| Version: | 2 | | |
| Date: | Jan 1981 | | |
| Contributor: | R. L. Poynter | | |
| Lines Listed = | 1183 | Q( 300.) = | 112460.3700 |
| Max. Frequency = | 3000 GHz | Q( 225.) = | 71285.1870 |
| Max. J = | 10 | Q( 150.) = | 39774.0860 |
| LOGSTR = | -5 above 160 GHz | Q( 75.) = | 12659.0120 |
| LOGSTR1 = | | Q( 37.5) = | 4620.6172 |
| Isotope Correction = | -1.955 | Q(18.25) = | 1414.1650 |
| Minimum Energy = | 0 $cm^{-1}$ | Q(9.375) = | 654.4858 |
| Dipoles: (a) = | 3.84 | A = | 27634.94 |
| (b) = | 1.37 | B = | 4689.805 |
| (c) = | | C = | 4214.746 |

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333 and W. H. Kirchhoff and D. R. Johnson, 1973, J. Mol. Spect. 45, 159. The measurements were taken from H. M. Heise, H. Lutz, and H. Dreizler, 1973, Z. Naturforsch. 29a, 1345.

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

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

Species Name: $CH_3{}^{13}CH_2CN$, $^{13}C$ isotope on atom 2

Lines Listed = 1252
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: (a) = 3.84
(b) = 1.37
(c) =

Q( 300.) = 113684.2800
Q( 225.) = 72060.9840
Q( 150.) = 40206.7970
Q( 75.) = 12796.7320
Q( 37.5) = 4670.8945
Q(18.25) = 1429.5522
Q(9.375) = 661.6073
A = 27045.40
B = 4697.868
C = 4207.046

---

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333 and W. H. Kirchhoff and D. R. Johnson, 1973, J. Mol. Spect. 45, 159. The measurements were taken from H. M. Heise, H. Lutz and H. Dreizler, 1973, Z. Naturforsch. 29a, 1345.

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

| | | | |
|---|---|---|---|
| Species Tag: | 56003 | Species Name: | $^{13}CH_3CH_2CN$,<br>ethyl cyanide,<br>$^{13}C$ isotope on<br>atom 3 |
| Version: | 2 | | |
| Date: | Jan 1981 | | |
| Contributor: | R. L. Poynter | | |

| | | | |
|---|---|---|---|
| Lines Listed = | 1183 | Q( 300.) = | 115292.3300 |
| Max. Frequency = | 3000 GHz | Q( 225.) = | 73080.2660 |
| Max. J = | 10 | Q( 150.) = | 40775.6020 |
| LOGSTR = | -9 below 160 GHz | Q( 75.) = | 12977.7660 |
| LOGSTR1 = | -5 above 160 GHz | Q( 37.5) = | 4736.9639 |
| Isotope Correction = | -1.955 | Q(18.25) = | 1449.4407 |
| Minimum Energy = | 0 $cm^{-1}$ | Q(9.375) = | 670.9657 |
| Dipoles: (a) = | 3.84 | A = | 27342.174 |
| (b) = | 1.37 | B = | 4597.939 |
| (c) = | | C = | 4133.707 |

---

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333 and W. H. Kirchhoff and D. R. Johnson, 1973, J. Mol. Spect. 45, 159. The measurements were taken from H. M. Heise, H. Lutz, and H. Dreizler, 1973, Z. Naturforsch. 29a, 1345.

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

Species Tag: 56004
Version: 1
Date: Jan 1980
Contributor: R. L. Poynter

Species Name: $CH_3CH_2C^{15}N$,
ethyl cyanide,
$^{15}N$ isotope

Lines Listed = 1621
Max. Frequency = 3000 GHz
Max. J = 20
LOGSTR = -9
LOGSTR1 =
Isotope Correction = -2.432
Minimum Energy = 0 $cm^{-1}$
Dipoles: $\mu(a)$ = 3.84
$\mu(b)$ = 1.37
$\mu(c)$ =

Q( 300.) = 38458.0
Q( 225.) = 24980.4
Q( 150.) = 13598.7
Q( 75.) = 3966.4
Q( 37.5) = 1542.4
Q(18.25) = 598.1
Q(9.375) = 213.9
A = 27541.953
B = 4574.771
C = 4119.430

---

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333. The measurements were taken from H. M. Heise, H. Mader, and H. Dreizler, 1976, Z. Naturforsch. 31a, 1228.

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

| | | | |
|---|---|---|---|
| Species Tag: | 56005 | Species Name: | $CH_2DCH_2CN$-s, ethyl cyanide, deuterium isotope on methyl carbon trans to CN group |
| Version: | 2 | | |
| Date: | Jan 1981 | | |
| Contributor: | R. L. Poynter | | |
| Lines Listed = | 1166 | Q( 300.) = | 118795. |
| Max. Frequency = | 3000 GHz | Q( 225.) = | 75300. |
| Max. J = | 10 | Q( 150.) = | 42000. |
| LOGSTR = | -9 below 160 GHz | Q( 75.) = | 14849. |
| LOGSTR1 = | -5 above 160 GHz | Q( 37.5) = | 5250. |
| Isotope Correction = | -3.347 | Q(18.25) = | 1787.8 |
| Minimum Energy = | 0 $cm^{-1}$ | Q(9.375) = | 607.95 |
| Dipoles: $\mu(a)$ = | 3.84 | A = | 27650.795 |
| $\mu(b)$ = | 1.37 | B = | 4425.061 |
| $\mu(c)$ = | | C = | 4000.763 |

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The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333 and W. H. Kirchhoff and D. R. Johnson, 1973, J. Mol. Spect. 45, 159. The measurements were taken from H. Mader, H. M. Heise, and H. Dreizler, 1973, Z. Naturforsch. 29a, 164.

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

Species Tag: 56006
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: $\mu(a)$ = 3.84
$\mu(b)$ = 1.37
$\mu(c)$ =

Species Name: $CH_2DCH_2CN$-a, ethyl cyanide, deuterium isotope on methyl carbon gauche to the CN group

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

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The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. 41, 333 and W. H. Kirchhoff and D. R. Johnson, 1973, J. Mol. Spect. 45, 159. The measurements were taken from H. Mader, H. M. Heise, and H. Dreizler, 1973, Z. Naturforsch. 29a, 164.

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

Species Tag: 60001
Version: 2
Date: Jan 1981
Contributor: R. L. Poynter

Species Name: OCS
carbonyl sulfide

Lines Listed = 99
Max. Frequency = 3000 GHz
Max. J = 99
LOGSTR = -7
LOGSTR1 =
Isotope Correction = -0.022
Minimum Energy = 0. $cm^{-1}$
Dipoles: $\mu(a)$ = 0.715
$\mu(b)$ =
$\mu(c)$ =

Q( 300.) = 1028.2539
Q( 225.) = 771.6135
Q( 150.) = 514.3989
Q( 75.) = 257.2764
Q( 37.5) = 128.8250
Q(18.25) = 64.5803
Q(9.375) = 32.4565
A =
B = 6081.4921
C =

---

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

The dipole moment has been remeasured by J.M.L.J. Reinartz and A. Dymanus, 1974, Chem. Phys. Lett., 24, 346.

| | | | |
|---|---|---|---|
| Species Tag: | 60002 | Species Name: | $^{28}\mathrm{Si}^{32}\mathrm{S}$<br>silicon monosulfide |
| Version: | 1 | | |
| Date: | Dec 1979 | | |
| Contributor: | R. L. Poynter | | |

| | | | |
|---|---|---|---|
| Lines Listed = | 97 | Q( 300.) = | 688.9700 |
| Max. Frequency = | 3000 GHz | Q( 225.) = | 517.1307 |
| Max. J = | 97 | Q( 150.) = | 344.8263 |
| LOGSTR = | -5 | Q( 75.) = | 172.5440 |
| LOGSTR1 = | | Q( 37.5) = | 86.4172 |
| Isotope Correction = | -0.057 | Q(18.25) = | 43.3711 |
| Minimum Energy = | 0. $\mathrm{cm}^{-1}$ | Q(9.375) = | 21.8575 |
| Dipoles: $\mu(a)$ = | 1.730 | A = | |
| $\mu(b)$ = | | B = | 9077.45 |
| $\mu(c)$ = | | C = | |

---

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

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

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

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

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

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

---

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

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

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

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

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

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

---

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

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

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

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

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

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

---

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

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

Species Tag: 62002
Version: 2
Date: Jan 1981
Contributor: R. L. Poynter

Species Name: $^{18}$OCS,
carbonyl sulfide,
$^{18}$O isotopic species

Lines Listed = 99
Max. Frequency = 3000 GHz
Max. J = 99
LOGSTR = -6.4
LOGSTR1 =
Isotope Correction = -2.712
Minimum Energy = 0 cm$^{-1}$
Dipoles: $\mu$(a) = 0.715
$\mu$(b) =
$\mu$(c) =

Q( 300.) = 1095.9731
Q( 225.) = 822.4320
Q( 150.) = 548.1509
Q( 75.) = 274.2837
Q( 37.5) = 137.3093
Q(18.25) = 68.8176
Q(9.375) = 34.5780
A =
B = 5704.8574
C =

---

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

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

Species Tag: 62003
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

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

Lines Listed = 99
Max. Frequency = 3000 GHz
Max. J = 99
LOGSTR = -5
LOGSTR1 =
Isotope Correction = -1.528
Minimum Energy = 0 $cm^{-1}$
Dipoles: $\mu(a)$ = 1.730
$\mu(b)$ =
$\mu(c)$ =

Q( 300.) = 714.3315
Q( 225.) = 536.1669
Q( 150.) = 357.4372
Q( 75.) = 178.8546
Q( 37.5) = 89.5984
Q(18.25) = 44.9573
Q(9.375) = 22.6465
A =
B = 8755.33
C =

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

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

Species Tag: 62004
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: $^{28}Si^{34}S$,
silicon monosulfide,
$^{34}S$ isotopic species

Lines Listed = 99
Max. Frequency = 3000 GHz
Max. J = 99
LOGSTR = -5
LOGSTR1 =
Isotope Correction = 1.411
Minimum Energy = 0. $cm^{-1}$
Dipoles: $\mu(a)$ = 1.730
$\mu(b)$ =
$\mu(c)$ =

Q( 300.) = 708.2720
Q( 225.) = 531.7408
Q( 150.) = 354.4869
Q( 75.) = 177.3781
Q( 37.5) = 88.8383
Q(18.25) = 44.5862
Q(9.375) = 22.4647
A =
B = 8828.86
C =

---

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

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

| | | | |
|---|---|---|---|
| Species Tag: | 63001 | Species Name: | $HNO_3$,<br>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 data set used in this fit includes the microwave and submillimeter lines reported by G. Cazzoli and F. C. DeLucia, (1979), J. Mol. Spectrosc. 76, 131, by W. C. Bowman, F. C. DeLucia, and P. Helminger, (1981), J. Mol. Spectrosc. 88, 431, by P. N. Ghosh, C. E. Blom, and A. Bauder, (1981), J. Mol. Spectrosc. 89, 159, and the far infrared lines measured by K. M. Evenson, (1983), private communication. Inclusion of the data from this last source produces a more reliable prediction of the far infrared transitions.

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

Species Tag: 64001
Version: 1
Date: Oct 1979
Contributor: H. M. Pickett

Species Name: $S_2$ , diatomic sulfur
v=0, $^3\Sigma_g^-$
ground state

Lines Listed = 34
Max. Frequency = 3000 GHz
Max. J = 35
LOGSTR = -8.4
LOGSTR1 =
Isotope Correction = -0.044
Minimum Energy = 0. $cm^{-1}$
Dipoles: magnetic $\mu$(a) =
$\mu$(b) =
$\mu$(c) =

Q( 300.) = 588.1659
Q( 225.) = 478.8508
Q( 150.) = 340.0165
Q( 75.) = 174.3814
Q( 37.5) = 87.7608
Q(18.25) = 44.4836
Q(9.375) = 22.9087
A =
B = 8831.2
C =

---

The experimentally measured lines are given in H. M. Pickett and T. L. Boyd, 1979, J. Mol. Specty. 75, 53. The calculational method used is from T. Amano and E. Hirota, 1974, J. Mol. Specty. 53, 346. For $S_2$, the parameter $\mu$(1) is assumed to be zero. Only transitions between states with J = N and J = N - 1 are listed because the energies of the J = N + 1 states are uncertain by more than 1 GHz. All the neglected transitions from J = N + 1 states lie above 450 GHz for J < 35.

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

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

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

Species Name: HCCC$^{15}$N
cyanoacetylene
$^{15}$N isotope

Lines Listed = 99
Max. Frequency = 1000 GHz
Max. J = 99
LOGSTR = -6
LOGSTR1 =
Isotope Correction = -2.432
Minimum Energy = 0. cm$^{-1}$
Dipoles: $\mu(a)$ = 3.724
$\mu(b)$ =
$\mu(c)$ =

Q( 300.) = 1415.47
Q( 225.) = 1061.94
Q( 150.) = 708.109
Q( 75.) = 354.161
Q( 37.5) = 177.256
Q(18.25) = 88.7973
Q(9.375) = 44.5656
A =
B = 4416.75
C =

---

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

The dipole moment was remeasured by the above authors as 3.724D.

Species Tag: 52003
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: $H^{13}CCCN$
cyanoacetylene
$^{13}C$ isotope atom 3

Lines Listed = 144
Max. Frequency = 1000 GHz
Max. J = 99
LOGSTR = -7
LOGSTR1 =
Isotope Correction = -1.955
Minimum Energy = 0. $cm^{-1}$
Dipoles: $\mu(a)$ = 3.724
$\mu(b)$ =
$\mu(c)$ =

Q( 300.) = 4255.01
Q( 225.) = 3192.27
Q( 150.) = 2128.14
Q( 75.) = 1064.63
Q( 37.5) = 532.721
Q(18.25) = 266.870
Q(9.375) = 133.937
A =
B = 4408.44
C =

---

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

The dipole moment was remeasured by the above authors as 3.724D.

Species Tag: 52002
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: $HC^{13}CCN$
cyanoacetylene
$^{13}C$ isotope on
atom 2

Lines Listed = 146
Max. Frequency = 1000 GHz
Max. J = 99
LOGSTR = -7
LOGSTR1 =
Isotope Correction = -1.955
Minimum Energy = 0. $cm^{-1}$
Dipoles : μ(a) = 3.724
μ(b) =
μ(c) =

Q( 300.) = 4140.95
Q( 225.) = 3106.71
Q( 150.) = 2071.10
Q( 75.) = 1036.10
Q( 37.5) = 518.561
Q(18.25) = 259.777
Q(9.375) = 130.377
A =
B = 4529.76
C =

---

The set of experimental lines used in the calculation was obtained from the references in W. J. Lafferty and F. J. Lovas, 1978, J. Phys. Chem. Ref. Data, _7_, 441.

The dipole moment was remeasured by the above authors as 3.724D.

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

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

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

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

---

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

The dipole moment was remeasured by the above authors as 3.724D.

Species Tag: 51002
Version: 2
Date: Oct 1980
Contributor: H. M. Pickett

Species Name: $^{35}$ClO, chlorine monoxide
$^{2}\Pi$ states, $\nu = 0$

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
$\mu(b)$ =
$\mu(c)$ =

Q( 300.) = 3291.54
Q( 225.) = 2297.20
Q( 150.) = 1424.30
Q( 75.) = 689.287
Q( 37.5) = 351.318
Q(18.25) = 183.316
Q(9.375) = 99.7011
A =
B = 18602.865
C =

---

The experimental lines below 200 GHz are from R. K. Kakar, E. A. Cohen, and M. Geller, 1978, J. Mol. Spec. 70, 243. Lines above 200 GHz were measured at JPL by E. A. Cohen and H. M. Pickett. The lines were fit to a fine structure Hamiltonian which included $p_D$ and $q_D$ terms and centrifugal distortion on B to sixth power in J. The hyperfine terms in the Hamiltonian included all off-diagonal matrix elements for a, b, c, d, $\eta_1$, $\eta_2$, and $\eta_3$. The partition function was determined by a sum over states to F = 86 for both the $\Omega = 3/2$ and $\Omega = 1/2$ states.

Species Tag: 51001
Version: 2
Date: Mar 1984
Contributor: R. L. Poynter

Species Name: HCCCN, cyanoacetylene

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

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

---

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

Species: 50006  
Species Name: $O_3$ asymmetric $^{18}O$ $\nu_2 = 1$  
Version: 1  
Date: Mar 1984  
Contributor: C. Chiu and E. A. Cohen

Lines Listed = 4213  
Max. Frequency = 9999 GHz  
Max. J = 50  
LOGSTR = -9.  
LOGSTR1 = -9.  
Isotope Correction =  
Minimum Energy = 693 $cm^{-1}$  
Dipoles : $\mu(a)$ = 0.0068  
$\mu(b)$ = 0.5324  
$\mu(c)$ =

Q( 300.) = 7214.414  
Q( 225.) = 4994.599  
Q( 150.) = 2549.761  
Q( 75.) = 904.0679  
Q( 37.5) = 320.2580  
Q(18.25) = 113.7639  
Q(9.375) = 40.6069  
A = 106071.8  
B = 12556.0  
C = 11150.6

---

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

Species Tag: 50005

Version: 1

Date: Mar 1984

Contributor: C. Chiu and E. A. Cohen

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

Lines Listed = 2387
Max. Frequency = 9999 GHz
Max. J = 50
LOGSTR = -8.9
LOGSTR1 = -8.9
Isotope Correction = 2.690
Minimum Energy = 678. $cm^{-1}$
Dipoles : $\mu(a)$ =
$\mu(b)$ = 0.5324
$\mu(c)$ =

Q( 300.) = 3525.34
Q( 225.) = 2445.129
Q( 150.) = 1247.107
Q( 75.) = 441.8769
Q( 37.5) = 156.5677
Q(18.25) = 55.6161
Q(9.375) = 19.8610
A = 100177.
B = 13316.
C = 11659.

---

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

| | | | |
|---|---|---|---|
| Species Tag: | 64002 | Species Name: | $SO_2$ ,<br>sulfur dioxide |
| Version: | 2 | | |
| Date: | Jun 1983 | | |
| Contributor: | R. L. Poynter | | |
| Lines Listed = | 9622 | Q( 300.) = | 5899.2969 |
| Max. Frequency = | 10000 GHz | Q( 225.) = | 3765.3037 |
| Max. J = | 74 | Q( 150.) = | 2075.8706 |
| LOGSTR = | -10 | Q( 75.) = | 738.9240 |
| LOGSTR1 = | -10 | Q( 37.5) = | 261.6373 |
| Isotope Correction = | -0.022 | Q(18.25) = | 92.8325 |
| Minimum Energy = | 0 $cm^{-1}$ | Q(9.375) = | 33.0674 |
| Dipoles: μ(a) = | | A = | 60778.558 |
| μ(b) = | 1.633 | B = | 10317.913 |
| μ(c) = | | C = | 8799.652 |

---

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

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

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

Species Tag: 75001
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: HC$_5$N , cyanodiacetylene

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

Q( 300.) = 4695.6914
Q( 225.) = 3315.8906
Q( 150.) = 2314.7271
Q( 75.) = 1174.0852
Q( 37.5) = 587.2181
Q(18.25) = 293.7650
Q(9.375) = 147.0618
A =
B = 1331.33
C =

---

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

The dipole moment was measured by the same authors.

| | | | |
|---|---|---|---|
| Species Tag: | 76001 | Species Name: | HCCCC$^{13}$CN, cyanodiacetylene, $^{13}$C isotope on atom 1 |
| Version: | 1 | | |
| Date: | Dec 1979 | | |
| Contributor: | R. L. Poynter | | |

| | | | |
|---|---|---|---|
| Lines Listed = | 99 | Q( 300.) = | 4742.4238 |
| Max. Frequency = | 300 GHz | Q( 225.) = | 3448.2642 |
| Max. J = | 99 | Q( 150.) = | 2336.6826 |
| LOGSTR = | -6.6 | Q( 75.) = | 1185.7676 |
| LOGSTR1 = | | Q( 37.5) = | 593.0616 |
| Isotope Correction = | -1.933 | Q(18.25) = | 296.6880 |
| Minimum Energy = | 0. cm$^{-1}$ | Q(9.375) = | 148.5251 |
| Dipoles: $\mu(a)$ = | 4.330 | A = | |
| $\mu(b)$ = | | B = | 1318.18 |
| $\mu(c)$ = | | C = | |

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

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

Species Tag: 76002
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: HCCC$^{13}$CCN,
cyanodiacetylene,
$^{13}$C isotope
on atom 2

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
$\mu(b)$ =
$\mu(c)$ =

Q( 300.) = 4700.0195
Q( 225.) = 3417.4316
Q( 150.) = 2316.8604
Q( 75.) = 1174.8972
Q( 37.5) = 587.7594
Q(18.25) = 294.0357
Q(9.375) = 147.1974
A =
B = 1330.11
C =

---

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

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

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

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

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

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

---

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

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

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

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

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

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

---

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

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

Species Tag: 76005
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: $H^{13}CCCCCN$,
cyanodiacetylene,
$^{13}C$ isotope
on atom 5

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

Q( 300.) = 4820.5898
Q( 225.) = 3500.2559
Q( 150.) = 2372.4639
Q( 75.) = 1205.3130
Q( 37.5) = 602.9758
Q(18.25) = 301.6474
Q(9.375) = 150.9731
A =
B = 1296.88
C =

---

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

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

Species Tag: 76006
Version: 1
Date: Dec 1979
Contributor: R. L. Poynter

Species Name: $HC_5{}^{15}N$, cyanodiacetylene, $^{15}N$ isotopic species

Lines Listed = 99
Max. Frequency = 300 GHz
Max. J = 99
LOGSTR = -6.6
LOGSTR1 =
Isotope Correction = -2.432
Minimum Energy = 0 $cm^{-1}$
Dipoles: μ(a) = 4.329
μ(b) =
μ(c) =

Q( 300.) = 4813.9287
Q( 225.) = 3495.4258
Q( 150.) = 2369.7368
Q( 75.) = 1203.3718
Q( 37.5) = 602.0048
Q(18.25) = 301.1616
Q(9.375) = 150.7648
A =
B = 1298.639
C =

---

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

The dipole moment was measured by the same authors.

| | | | |
|---|---|---|---|
| Species Tag: | 76007 | Species Name: | $DC_5N$,<br>cyanodiacetylene,<br>D isotopic species |
| Version: | 1 | | |
| Date: | Dec 1979 | | |
| Contributor: | R. L. Poynter | | |

| | | | |
|---|---|---|---|
| Lines Listed = | 99 | Q( 300.) = | 4918.1348 |
| Max. Frequency = | 300 GHz | Q( 225.) = | 3564.5166 |
| Max. J = | 99 | Q( 150.) = | 2417.1284 |
| LOGSTR = | -6.6 | Q( 75.) = | 1229.4199 |
| LOGSTR1 = | | Q( 37.5) = | 615.0352 |
| Isotope Correction = | -3.824 | Q(18.25) = | 307.6805 |
| Minimum Energy = | 0 $cm^{-1}$ | Q(9.375) = | 153.9927 |
| Dipoles: $\mu(a)$ = | 4.329 | A = | |
| $\mu(b)$ = | | B = | 1271.056 |
| $\mu(c)$ = | | C = | |

---

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

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

Species Tag: 80001
Version: 1
Date: Feb 1980
Contributor: R. L. Poynter and H. M. Pickett

Species Name: $H^{79}Br$ ,
Hydrogen Bromide,
$^{79}Br$ isotopic species

Lines Listed = 19
Max. Frequency = 10000 GHz
Max. J = 6
LOGSTR = -2.2
LOGSTR1 =
Isotope Correction = -2.96
Minimum Energy = 0 $cm^{-1}$
Dipoles: $\mu(a)$ = 0.828
$\mu(b)$ =
$\mu(c)$ =

Q( 300.) = 101.2045
Q( 225.) = 73.3500
Q( 150.) = 50.3732
Q( 75.) = 26.3512
Q( 37.5) = 13.9123
Q(18.25) = 7.7732
Q(9.375) = 4.9340
A =
B = 250357.6
C =

---

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

The dipole moment was also reported by these same authors in a later publication, and updated in F. A. Van Dijk and A. Dymanus, 1971, 26th Symposium on Molecular Structure and Spectroscopy, Columbus, Ohio, R12, p. 80.

Species Tag: 82001
Version: 1
Date: Feb 1980
Contributor: R. L. Poynter and H. M. Pickett

Species Name: $H^{81}Br$ ,
Hydrogen Bromide,
$^{81}Br$ isotopic
species

Lines Listed = 19
Max. Frequency = 10000 GHz
Max. J = 6
LOGSTR = -2.2
LOGSTR1 =
Isotope Correction = -0.306
Minimum Energy = 0. $cm^{-1}$
Dipoles: $\mu(a)$ = 0.828
$\mu(b)$ =
$\mu(c)$ =

Q( 300.) = 101.2511
Q( 225.) = 73.3668
Q( 150.) = 50.3848
Q( 75.) = 26.3573
Q( 37.5) = 13.9155
Q(18.25) = 7.7750
Q(9.375) = 4.9351
A =
B = 250250.2
C =

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

The dipole moment was also reported by these same authors in a later publication, and updated in F. A. Van Dijk and A. Dymanus, 1971, 26th Symposium on Molecular Structure and Spectroscopy, Columbus, Ohio, R12, p. 80.

Species Tag: 95001
Version: 1
Date: Feb 1980
Contributor: H. M. Pickett

Species Name: $^{79}$BrO ,
Bromine Monoxide,
$^{79}$Br isotopic species,
$^{2}\Pi_{3/2}$ state

Lines Listed = 850
Max. Frequency = 1300 GHz
Max. J = 49
LOGSTR = -9
LOGSTR1 =
Isotope Correction = -0.296
Minimum Energy = 0 $cm^{-1}$
Dipoles: $\mu(a)$ = 1.765
$\mu(b)$ =
$\mu(c)$ =

Q( 300.) = 3897.6226
Q( 225.) = 2938.3271
Q( 150.) = 1965.1685
Q( 75.) = 989.4642
Q( 37.5) = 501.9954
Q(18.25) = 259.5374
Q(9.375) = 136.8043
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: $^{81}$BrO ,
Bromine Monoxide,
$^{81}$Br isotopic species,
$^{2}\Pi_{3/2}$ state

Lines Listed = 850
Max. Frequency = 1500 GHz
Max. J = 49
LOGSTR = -9
LOGSTR1 =
Isotope Correction = -0.306
Minimum Energy = 0 $\mathrm{cm}^{-1}$
Dipoles: $\mu(a)$ = 1.794
$\mu(b)$ =
$\mu(c)$ =

Q( 300.) = 3913.8101
Q( 225.) = 2950.5308
Q( 150.) = 1973.3323
Q( 75.) = 993.5737
Q( 37.5) = 503.9649
Q(18.25) = 259.2984
Q(9.375) = 137.2459
A =
B = 12777.08
C =

---

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

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

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

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

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

---

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

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

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

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

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

---

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

GX-11D

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44008 HNC-13-O       4332 3.8722 3.7016 3.4466 2.9974 2.5478 2.1126 1.7510 1*
44009 N2O-v2          146 2.6972 2.5724 2.3965 2.0960 1.7962 1.4974 1.2011 1*
45001 C-13-S           29 2.4324 2.3080 2.1321 1.8321 1.5331 1.2364 0.9440 2
45002 Si-29-O          66 2.4637 2.3408 2.1649 1.8647 1.5656 1.2686 0.9755 1
45003 NH2CHO         3476 4.4647 4.2667 4.0134 3.5603 3.1117 2.6620 2.2141 2
45005 HCS+             64 2.4676 2.3427 2.1669 1.8668 1.5677 1.2706 0.9775 1*
45006 HNCO-18        4929 3.9097 3.7316 3.4713 3.0208 2.5712 2.1359 1.7741 1*
45007 NN-15-O          85 2.6974 2.5725 2.3966 2.0961 1.7962 1.4975 1.2011 1*
45008 N-15-NO          87 2.7123 2.5874 2.4114 2.1109 1.8110 1.5122 1.2157 1*
46001 CS-34            34 2.4144 2.2899 2.1141 1.8141 1.5153 1.2187 0.9267 2
46002 Si-30-O          67 2.4689 2.3449 2.1700 1.8699 1.5708 1.2736 0.9805 1
46003 H2CS            517 3.7770 3.5753 3.3199 2.8751 2.4243 1.9599 1.4397 1
46004 C2H5OH         1236 4.2307 4.0433 3.7791 3.3054 2.8737 2.4274 1.9788 1
46005 HCOOH          1888 3.9486 3.7612 3.4971 3.0357 2.5949 2.1461 1.6984 1
46006 NO2           16444 4.1306 3.9426 3.6780 3.2263 2.7755 2.3260 1.8791 2*
46007 N2O-18           88 2.7224 2.5975 2.4215 2.1210 1.8210 1.5222 1.2256 1*
47001 H2C-13-s        110 3.7938 3.6064 3.3253 2.8908 2.4222 1.9743 1.4566 1
47002 HC-13-OOH      1194 3.9492 3.8243 3.4976 3.0391 2.6012 2.1524 1.7047 1
47003 DCOOH           628 4.0224 3.8351 3.5595 3.0974 2.6685 2.2198 1.7720 1
47004 HCOOD           612 3.9980 3.8106 3.5465 3.0839 2.6440 2.1954 1.7475 1
48001 SO              330 2.9295 2.8009 2.6175 2.2956 1.9559 1.5897 1.2015 1
48002 SO-v1           261 2.9295 2.8009 2.6175 2.2956 1.9559 1.5897 1.2015 1
48003 H2CS-34         111 3.7842 3.6593 3.3326 2.8811 2.4137 1.9652 1.4473 1
```

GAUD CATDIR

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  1001 H-atom                  1 0.6021 0.6021 0.6021 0.6021 0.6021 0.6021 0.6021 1
  2001 D-atom                  1 0.7782 0.7782 0.7782 0.7782 0.7782 0.7782 0.7782 1
  3001 HD                      1 0.7004 0.5864 0.4315 0.1962 0.0406 0.0014 0.0001 2*
  4001 H2D+                   19 1.8682 1.6944 1.4398 0.9880 0.4916 0.0845 0.0016 1*
 12001 C-atom                  2 0.8939 0.8744 0.8363 0.7295 0.5494 0.3075 0.0962 2*
 13001 C-13-atom               7 1.1950 1.1754 1.1374 1.0305 0.8504 0.6085 0.3972 2*
 13002 CH                    324 2.0822 1.9608 1.7924 1.5175 1.2752 1.0864 0.9523 1
 14001 N-atom                  2 1.0792 1.0792 1.0792 1.0792 1.0792 1.0792 1.0792 1
 14002 N-atom-D-state          6 1.4700 1.4676 1.4629 1.4495 1.4246 1.3827 1.3247 3*
 16001 O-atom                  2 0.8287 0.8010 0.7612 0.7123 0.6996 0.6990 0.6990 2
 17001 OH                    788 1.9111 1.7803 1.6036 1.3570 1.2313 1.2042 1.2022 3*
 17002 NH3                   446 2.7627 2.5780 2.3162 1.8725 1.4410 1.0512 0.7322 3
 17003 CH3D                   80 2.6044 2.4985 2.1544 1.7083 1.2664 0.8469 0.4742 1
 17004 NH3-v2                442 2.7627 2.5780 2.3162 1.8725 1.4410 1.0512 0.7322 1
 18001 OD                    912 2.3272 2.1858 1.9889 1.6899 1.4899 1.3983 1.3804 1
 18002 N-15-H3               235 2.7603 2.6544 2.3143 1.8734 1.4420 1.0522 0.7336 2
 18003 H2O                   783 2.2507 2.0645 1.8040 1.3649 0.9335 0.4819 0.0994 4*
 18004 NH2D                 5036 3.5787 3.3818 3.1117 2.6378 2.1367 1.6068 1.1219 1
 18005 H2O-v2                292 2.2507 2.0645 1.8040 1.3649 0.9335 0.4819 0.0994 2
 19001 HO-18                 295 1.9135 1.7826 1.6056 1.3584 1.2318 1.2043 1.2022 2
 19002 HDO                  1401 2.1669 1.9803 1.7185 1.2753 0.8421 0.4332 0.1252 3*
 19003 H2O-17                404 2.2524 2.0664 1.8059 1.3668 0.9353 0.4835 0.0999 1*
 20001 D2O                  1137 3.0190 2.8322 2.5696 2.1242 1.6863 1.2685 0.9367 2*
 20002 HF                      8 1.0213 0.9009 0.7343 0.4622 0.2212 0.0524 0.0024 1*
 20003 H2O-18                726 2.2544 2.0682 1.8076 1.3685 0.9369 0.4849 0.1004 1*
 21001 HDO-18                952 2.1724 1.9858 1.7239 1.2806 0.8472 0.4378 0.1274 1*
 21002 DF                     20 1.2917 1.1691 0.9978 0.7118 0.4416 0.2043 0.0443 1*
 25001 CCH                   114 2.7591 2.6344 2.4589 2.1598 1.8628 1.5699 1.2852 1
 26001 CN                    385 2.8221 2.6976 2.5223 2.2238 1.9280 1.6376 1.3579 1
 26002 CN-v1                 437 2.8221 2.6976 2.5223 2.2238 1.9280 1.6376 1.3579 1
 27001 HCN                    40 2.6277 2.5031 2.3276 2.0286 1.7317 1.4389 1.1545 2
 27002 HNC                    33 2.1406 2.0162 1.8407 1.5418 1.2449 0.9523 0.6683 1
 27003 HCN-v2                132 2.1506 2.0260 1.8505 1.5515 1.2546 0.9618 0.6774 1*
 28001 CO                     91 2.0369 1.9123 1.7370 1.4386 1.1429 0.8526 0.5733 2*
 28002 HC-13-N                45 2.6389 2.5145 2.3390 2.0399 1.7428 1.4498 1.1650 1
 28003 HCN-15                 35 2.1634 2.0388 1.8633 1.5642 1.2671 0.9741 0.6892 1
 28004 DCN                    54 2.7151 2.5906 2.4150 2.1156 1.8179 1.5236 1.2361 1
 28005 HNC-13                 34 2.1580 2.0336 1.8581 1.5590 1.2620 0.9691 0.6844 1
 28006 HN-15-C                33 2.1494 2.0249 1.8494 1.5504 1.2534 0.9607 0.6763 1
 28007 DNC                    39 2.2153 2.0908 1.9153 1.6160 1.3184 1.0245 0.7377 1
 29001 C-13-O                 27 2.0560 1.9317 1.7565 1.4579 1.1612 0.8712 0.5909 1
 29002 HCO+                   33 2.1477 2.0233 1.8478 1.5488 1.2519 0.9591 0.6748 2
 29003 CH2NH                2957 3.7703 3.5798 3.3191 2.8695 2.4206 1.9745 1.5341 2
 29004 HCO                  2454 3.4806 3.2930 3.0286 2.5779 2.1298 1.6901 1.3077 1
 29005 NNH+                   34 3.0831 2.9586 2.7832 2.4842 2.1875 1.8952 1.6116 1
 30001 CO-18                  27 2.0577 1.9334 1.7581 1.4595 1.1636 0.8728 0.5924 1
 30002 HC-13-O+               34 2.1597 2.0353 1.8598 1.5607 1.2637 0.9707 0.6859 2
 30003 DCO+                   41 2.7176 2.5929 2.4173 2.1179 1.8201 1.5258 1.2382 2
 30004 H2CO                  611 3.4589 3.2714 3.0085 2.5584 2.1094 1.6501 1.1399 1
 30005 C-13-H2NH             439 3.3037 3.1163 2.8522 2.4006 1.9491 1.4975 1.0460 1
 30006 CH2N-15-H             440 3.3044 3.1170 2.8529 2.4013 1.9498 1.4982 1.0467 1
 30007 CH2ND                1834 3.8562 3.6688 3.4053 2.9094 2.4740 1.9667 1.6373 1
 30008 NO                   1909 3.0643 2.9122 2.6922 2.3216 1.9977 1.7160 1.4604 1
 30009 NND+                   41 2.6881 2.5634 2.3878 2.0886 1.7911 1.4972 1.2106 1
 31001 HCO-18+                34 2.1678 2.0432 1.8677 1.5686 1.2716 0.9784 0.6934 2
 31002 H2C-13-O              601 3.4698 3.2845 3.0202 2.5693 2.1201 1.6607 1.1501 1
 32001 O2                    237 2.3398 2.2152 2.0398 1.7419 1.4477 1.1618 0.8960 3*
 32002 O2-v1                 237 2.3398 2.2152 2.0398 1.7419 1.4477 1.1618 0.8960 4*
 32003 CH3OH                 709 3.8071 3.6197 3.3556 2.9040 2.4525 2.0009 1.5494 2
 32004 H2CO-18               449 3.4796 3.2922 3.0281 2.5789 2.1299 1.6703 1.1596 1
```

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48004 O3                 7089 3.5506 3.3484 3.0787 2.6268 2.1762 1.7267 1.2796 3*
48005 O3-v2              4947 3.5506 3.3484 3.0787 2.6268 2.1762 1.7267 1.2796 3*
48006 O3-v1,3            9685 3.5506 3.3484 3.0787 2.6268 2.1762 1.7267 1.2796 3*
48007 O3-2v2             3031 3.5506 3.3484 3.0787 2.6268 2.1762 1.7267 1.2796 2*
48008 O3-v1,3+v2        10912 3.5506 3.3484 3.0787 2.6268 2.1762 1.7267 1.2796 1*
49001 O3-sym-O-17       13267 4.2814 4.1152 3.8633 3.4145 2.9640 2.5145 2.0673 1
49002 O3-asym-O-17      24138 4.6079 4.4366 4.1712 3.7207 3.2701 2.8206 2.3733 1
50001 S-34-O              280 2.9380 2.8093 2.6260 2.3039 1.9640 1.5972 1.2081 1
50002 SO-18               179 2.9626 2.8296 2.6500 2.3280 1.9873 1.6191 1.2275 1
50003 O3-sym-O-18        3184 3.5472 3.3599 3.0959 2.6453 2.1947 1.7452 1.2980 2
50004 O3-asym-O-18       7304 3.8582 3.6708 3.4065 2.9562 2.5055 2.0560 1.6086 2
50005 O3-s-O18-v2        2387 3.5472 3.3883 3.0959 2.6453 2.1947 1.7452 1.2980 1
50006 O3-a-O18-v2        4213 3.8582 3.6985 3.4065 2.9562 2.5055 2.0560 1.6086 1
50007 CH3Cl-35           6372 4.4505 4.2630 3.9990 3.5482 3.0822 2.6511 2.2519 1*
51001 HCCCN               154 3.6152 3.4904 3.3144 3.0135 2.7130 2.4127 2.1134 2
51002 ClO                2585 3.5250 3.3632 3.1537 2.8384 2.5457 2.2632 1.9987 3
51003 ClO-v1             2112 3.5250 3.3632 3.1537 2.8384 2.5457 2.2632 1.9987 1*
52001 HCCC-13-N           152 3.6170 3.4922 3.3162 3.0153 2.7147 2.4145 2.1152 1
52002 HCC-13-CN           146 3.6171 3.4923 3.3162 3.0154 2.7148 2.4146 2.1152 1
52003 HC-13-CCN           144 3.6289 3.5041 3.3280 3.0272 2.7265 2.4263 2.1269 1
52004 HCCCN-15             99 3.1509 3.0261 2.8501 2.5492 2.2486 1.9484 1.6490 1
52005 DCCCN               156 3.6477 3.5228 3.3468 3.0460 2.7453 2.4450 2.1456 1
52006 HOCl               6929 3.9787 3.7911 3.5268 3.0756 2.6252 2.1779 1.7662 3*
52007 SiCC                224 3.4214 3.3265 3.1628 2.8016 2.3700 1.9213 1.4738 1*
52008 CCCO                 51 3.1132 2.9888 2.8129 2.5121 2.2115 1.9114 1.6121 1*
52009 CH3Cl-37           6403 4.4567 4.2696 4.0052 3.5544 3.0891 2.6579 2.2585 1*
52010 CH2F2             11942 4.7435 4.5317 4.2551 3.8010 3.3502 2.9003 2.4522 1*
52011 CH2F2-v4           7808 4.7435 4.5317 4.2551 3.8010 3.3502 2.9003 2.4522 1*
53001 C2H3CN             3697 4.4183 4.2309 3.9667 3.5110 3.0644 2.6138 2.1638 1
53002 Cl-37-O            2624 3.5327 3.3706 3.1611 2.8457 2.5528 2.2700 2.0049 3
53003 C-13-CCO             99 3.1304 3.0054 2.8294 2.5285 2.2279 1.9277 1.6284 1*
53004 CC-13-CO             99 3.1164 2.9915 2.8154 2.5146 2.2139 1.9138 1.6145 1*
53005 CCC-13-O             99 3.1152 2.9902 2.8142 2.5133 2.2127 1.9126 1.6133 1*
53006 Cl-37-O-v1         2132 3.5327 3.3706 3.1611 2.8457 2.5528 2.2700 2.0049 1*
54001 CH2CHC-13-N         118 4.4205 4.2331 3.9690 3.5174 3.0659 2.5545 2.1409 1
54002 CH2C-13-HCN         117 4.4259 4.2385 3.9744 3.5228 3.0713 2.5598 2.1462 1
54003 C-13-H2CHCN         116 4.4328 4.4254 3.9813 3.5297 3.0782 2.5645 2.1514 1
54004 CH2CDCN             322 4.4727 4.2853 4.0212 3.5696 3.1181 2.6044 2.1916 1
54005 HOCl-37            6925 3.9863 3.7987 3.5344 3.0832 2.6328 2.1854 1.7736 3*
54006 CCCO-18              99 3.1361 3.0112 2.8351 2.5342 2.2336 1.9334 1.6341 1*
55001 C2H5CN             3684 5.0486 4.8506 4.5972 4.1000 3.6623 3.1481 2.8135 2
56001 CH3CH2C-13-N       1183 5.0510 4.8530 4.5996 4.1024 3.6647 3.1505 2.8159 2
56002 CH3C-13-H2CN       1252 5.0557 4.8577 4.6043 4.1071 3.6694 3.1552 2.8206 2
56003 C-13-H3CH2CN       1183 5.0618 4.8638 4.6104 4.1132 3.6755 3.1612 2.8267 2
56004 C2H5CN-15          1621 4.5850 4.3976 4.1335 3.5984 3.1882 2.7768 2.3302 1
56005 CH2DCH2CN-s        1166 5.0748 4.8768 4.6232 4.1717 3.7202 3.2523 2.7839 2
56006 CH2DCH2CN-a        1286 5.0830 4.8850 4.6316 4.1799 3.7284 3.2618 2.7947 2
60001 OCS                  99 3.0121 2.8874 2.7113 2.4104 2.1100 1.8101 1.5113 2
60002 SiS                  97 2.8382 2.7136 2.5376 2.2369 1.9366 1.6372 1.3396 1
61001 OC-13-S              99 3.0135 2.8887 2.7126 2.4119 2.1114 1.8115 1.5127 2
61002 Si-29-S              98 2.8462 2.7217 2.5456 2.2449 1.9446 1.6452 1.3475 1
62001 OC-34-S              99 3.0228 2.8908 2.7220 2.4212 2.1207 1.8208 1.5219 2
62002 O-18-CS              99 3.0398 2.9151 2.7389 2.4382 2.1377 1.8377 1.5388 2
62003 Si-30-S              99 2.8539 2.7293 2.5532 2.2525 1.9523 1.6528 1.3550 1
62004 SiS-34               99 2.8502 2.7257 2.5496 2.2489 1.9486 1.6492 1.3515 1
63001 HNO3              36551 4.4462 4.2589 3.9947 3.5433 3.0923 2.6418 2.1926 3*
63002 HNO3-v7           16478 4.4462 4.2589 3.9947 3.5433 3.0923 2.6418 2.1926 1*
63003 HNO3-v9           32404 4.7472 4.6599 4.2957 3.8443 3.3933 2.9428 2.4936 1*
63004 HNO3-v6           15704 4.4462 4.2589 3.9947 3.5433 3.0923 2.6418 2.1926 1*
63005 HNO3-v8           14537 4.4462 4.2589 3.9947 3.5433 3.0923 2.6418 2.1926 1*
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 63006 HNO3-v5         13269 4.4462 4.2589 3.9947 3.5433 3.0923 2.6418 2.1926 1*
 64001 S2                174 2.9954 2.8607 2.6651 2.3091 1.9145 1.4876 1.0947 2*
 64002 SO2             10654 3.7721 3.5845 3.3202 2.8686 2.4177 1.9677 1.5194 3*
 66001 COF2            23090 4.7883 4.6008 4.3366 3.8852 3.4341 2.9836 2.5342 1*
 67001 OCl-35-O        20815 4.7134 4.5365 4.2762 3.8250 3.3739 2.9238 2.4754 1*
 68001 CCCS               99 3.3309 3.2093 3.0341 2.7332 2.4325 2.1320 1.8320 1*
 69001 OCl-37-O        20799 4.7195 4.5429 4.2827 3.8315 3.3805 2.9304 2.4819 1*
 70001 CCCS-34            99 3.3410 3.2198 3.0448 2.7439 2.4431 2.1426 1.8426 1*
 75001 HCCCCCN            99 3.6717 3.5206 3.3645 3.0697 2.7688 2.4680 2.1675 1
 76001 HCCCCC-13-N        99 3.6760 3.5376 3.3686 3.0740 2.7731 2.4723 2.1718 1
 76002 HCCCC-13-CN        99 3.6721 3.5337 3.3649 3.0700 2.7692 2.4684 2.1679 1
 76003 HCCC-13-CCN        99 3.6721 3.5337 3.3650 3.0701 2.7693 2.4685 2.1680 1
 76004 HCC-13-CCCN        99 3.6762 3.5378 3.3687 3.0741 2.7733 2.4725 2.1720 1
 76005 HC-13-CCCCN        99 3.6831 3.5441 3.3752 3.0811 2.7803 2.4795 2.1789 1
 76006 HCCCCCN-15         99 3.6825 3.5435 3.3747 3.0804 2.7796 2.4788 2.1783 1
 76007 DCCCCCN            99 3.6918 3.5520 3.3833 3.0897 2.7889 2.4881 2.1875 1
 79001 HOONO2          50775 5.0793 4.9375 4.6972 4.2216 3.7512 3.2982 2.8469 1*
 80001 HBr-79             19 2.0052 1.8654 1.7022 1.4208 1.1434 0.8906 0.6932 1
 82001 HBr-81             19 2.0054 1.8655 1.7023 1.4209 1.1435 0.8907 0.6933 1
 95001 Br-79-O           850 3.5908 3.4681 3.2934 2.9954 2.7007 2.4142 2.1361 1
 97001 Br-81-O           850 3.5926 3.4699 3.2952 2.9972 2.7024 2.4138 2.1375 1
 97002 Cl-35-NO3        4198 5.0023 4.8149 4.5508 4.0992 3.6481 3.1970 2.7459 1
 98001 H2SO4            2359 4.7402 4.6164 4.4325 4.1029 3.7492 3.3603 2.9340 1*
 99001 Cl-37-NO3        4182 5.0133 4.8259 4.5617 4.1102 3.6590 3.2080 2.7572 1
102001 ClOOCl          17266 5.6303 5.4429 5.1793 4.7274 4.2757 3.8244 3.3735 1*
104001 Cl-37-OOCl      17482 5.6427 5.4552 5.1915 4.7398 4.2880 3.8367 3.3858 1*
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CC04001.ED4

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 648336.8741194.0012 -2.3558 3  354.4029  7    4001 303 3 2 1 0      3 2 2 0
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1370146.0000    .2000 -1.2773 3      .0000  3   -4001 303 1 0 1 0      0 0 0 0
2161102.9860 40.9063 -1.1604 3  254.1041 21    4001 303 3 1 2 0      3 1 3 0
2363138.4675 22.1220  -.3086 3   60.0642 15    4001 303 2 1 2 0      1 1 1 0
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4493777.1278 42.3293   .1663 3  254.1041 27    4001 303 4 1 4 0      3 1 3 0
4503394.0360 33.8792   .1782 3  175.9737 21    4001 303 3 1 2 0      2 1 1 0
4548986.3040107.1201  -.2932 3  251.4190  9    4001 303 4 0 4 0      3 0 3 0
5520814.8102366.3745   .1072 3  404.0003 33    4001 303 5 1 5 0      4 1 4 0
5538541.4701349.4946  -.3654 3  403.1568 11    4001 303 5 0 5 0      4 0 4 0
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GX-11D

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Dump of file SCRATCH2:[BROWLAND.WATS]C001001.ED4;1 on 25-FEB-1992 13:23:39.93
File ID (1554,12,0)    End of file block 1 / Allocated 201
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C001001.ED4

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Record number 1 (00000001), 512 (0200) bytes

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GX-11D

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Dump of file SCRATCH2:[BROWLAND.WATS]C002001.ED4;1 on 25-FEB-1992 13:24:54.94
File ID (1574,49958,0)   End of file block 1 / Allocated 201

Record number 1 (00000001), 512 (0200) bytes

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 0A302031 20312032 20202020 20302032 20312033 20333033 20313030 34202020    4001 3
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 00000000 00000000 00000000 00000000 00000000 00000000 00000000 0A302034 4 0.....
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6X - 11 B

**Center for Astrophysics**
60 Garden Street
Cambridge, Massachusetts 02138

Harvard College Observatory
Smithsonian Astrophysical Observatory

July 24, 1984

Dr. Ralph Post
Head of Computing Operations
National Space Science Data Center
NASA/Goddard Space Flight Center
Greenbelt, MD 20771

Dear Dr. Post,

In the past, specifically on 17 September 1982, we have supplied the NSSDC with a tape of our laboratory measurements of the absorption cross section of oxygen.

We should like now to supply a tape containing our measurements of the absorption cross section of sulfur dioxide at 213K in the wavelength region 172-240 nm. Two items are attached to this letter: (a) a preprint of a paper which has been accepted for publication in Planetary and Space Science. In the abstract of that paper reference is made to the deposition of our results at the NSSDC; and (b) a description of the tape format. The tape itself will be mailed under separate cover.

We thank you for providing this valuable service.

Yours sincerely,

Daryl Freeman

D.E. Freeman

Enc.

DEF:ecw

6X-11A

# HIGH RESOLUTION ABSORPTION CROSS SECTION MEASUREMENTS AND BAND OSCILLATOR STRENGTHS OF THE (1,0)-(12,0) SCHUMANN-RUNGE BANDS OF $O_2$

K. Yoshino, D.E. Freeman, J.R. Esmond, and W.H. Parkinson

Harvard-Smithsonian Center for Astrophysics, Cambridge, MA 02138

## Abstract

Cross sections of $O_2$ at 300 K have been obtained from photoabsorption measurements at various pressures throughout the wavelength region 179.3-201.5 nm with a 6.65 m photoelectric scanning spectrometer equipped with a 2400 lines/mm grating and having an instrumental width (FWHM) of 0.0013 nm. The measured absorption cross sections of the Schumann-Runge bands (12,0) through (1,0) in this wavelength region are absolute, i.e., independent of the instrumental width, a result not achieved previously. The measured cross sections are presented graphically and are available at wavenumber intervals of ~ 0.1 $cm^{-1}$ as numerical compilations stored on magnetic tape from the National Space Science Data Center, NASA/ Goddard Space Flight Center, Greenbelt, MD 20771, USA. Band oscillator strengths of the (12,0) through (1,0) bands have been determined by direct numerical integration of the measured cross sections.

Short title for odd-numbered pages

SCHUMANN-RUNGE ABSORPTION CROSS SECTIONS

GX-11A

**Center for Astrophysics**
60 Garden Street
Cambridge, Massachusetts 02138

Harvard College Observatory
Smithsonian Astrophysical Observatory

September 17, 1982

Dr. Ralph Post
Head of Computing Operations
National Space Science Data Center
NASA/Goddard Space Flight Center
Greenbelt, MD 20771

Dear Dr. Post:

Following a phone conversation between you and Jim Esmond, we have sent to you, under separate cover, a tape containing our measured absorption cross sections of the Schumann-Runge bands of oxygen. Two separate pages are attached: One describes the tape format, and the other contains an abstract of our paper which has been submitted for publication in Planetary and Space Science.

If it is your practice to assign an identification number to such a tape of data, please send me that number so that it can be included in the published version of our abstract and paper.

Yours sincerely,

D.E. Freeman

D.E. Freeman

DEF:ng

Enc.

GX-11A

***********************************************************************
O2HCO is the visual label of a nine-track magnetic tape storing data of the cross section of the (1,0) through (12,0) Schumann-Runge bands of molecular oxygen. The tape is magnetically unlabelled and written in fixed recordsize, fixed blocksize format.

The following shows the organization and characteristics of the files stored on magnetic tape O2HCO. There are first 12 files of data, one for each of Schumann-Runge bands (1,0) through (12,0). The division between the files is at arbitrary wavenumbers, but all the files consecutively together create a scan continuous in wavenumber across all those bands. The first file is of the (1,0) band [O2B1X0.PUB], the second is of the (2,0) band [O2B2X0.PUB], etc. The thirteenth file is a comment file containing the title and the abstract of the paper decribing this research, and mention of the journal to which this paper has been submitted for publication. This file has a different recordsize than that of the first twelve files.

Each data file consists of two initial label records-- a title line, and a column label line--, followed by sigma:wavenumber pair records spaced at uneven wavenumber intervals in ascending wavenumber order.

The research producing this data was done at the Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts.
K. Yoshino, D.E. Freeman, J.R. Esmond, and W.H. Parkinson
***********************************************************************

```
15-SEP-1982 23:35:40

Density is 1600 bpi.

Character code is ASCII.

Files are separated by tape-marks, with a double tape-mark at the end.

Record size is  28 bytes.  Block size is  2800 bytes.
(Last block in a file is not padded; it may be as short as  28 bytes.)

Tape file   1:  3641 records copied from VMS file: O2B1X0.PUB
Tape file   2:  7313 records copied from VMS file: O2B2X0.PUB
Tape file   3:  6922 records copied from VMS file: O2B3X0.PUB
Tape file   4:  6806 records copied from VMS file: O2B4X0.PUB
Tape file   5:  3226 records copied from VMS file: O2B5X0.PUB
Tape file   6:  2809 records copied from VMS file: O2B6X0.PUB
Tape file   7:  2347 records copied from VMS file: O2B7X0.PUB
Tape file   8:  3447 records copied from VMS file: O2B8X0.PUB
Tape file   9:  3467 records copied from VMS file: O2B9X0.PUB
Tape file  10:  3405 records copied from VMS file: O2B10X0.PUB
Tape file  11:  2383 records copied from VMS file: O2B11X0.PUB
Tape file  12:  2299 records copied from VMS file: O2B12X0.PUB

Record size is  40 bytes.  Block size is  2800 bytes.
(Last block in a file is not padded; it may be as short as  40 bytes.)

Tape file  13:    46 records copied from VMS file: O2MEMO.PUB

Exit requested after   13 files were copied.
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The following is the description of a 9-track magnetic tape with visual label HCOSO2 containing cross section data of sulfur dioxide at 213 K in the wavelength region 172-240 nm experimentally obtained at the Harvard-Smithsonian Center for Astrophysics.
The tape is magnetically not labelled, and is written in the fixed record-fixed block format described below. The organization of the files on the tape are as follows:

1) File 1: this information file.
2) File 2: the title and abstract of the paper on this work as published in Planetary Space Science.
3) Files 3-20: files of the cross section data within 1000 wavenumber intervals beginning at ~41670 through ~58140 wavenumbers.
4) File 21: repetition of file 1.
5) File 22: repetition of file 2.
6) Files 23-40: repetition of files 3-20.

The cross section data files have two header lines at the beginning, which are followed by wavenumber/sigma pair records for each wavenumber position.

This tape is written with the following characteristics:

Density is 1600 bpi.

Character code is ASCII.

Files are separated by tape-marks, with a double tape-mark at the end.

Record size is 28 bytes.

Block size is 2800 bytes.

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1-JUN-1984 14:17:07

Density is 1600 bpi.

Character code is ASCII.

Files are separated by tape-marks, with a double tape-mark at the end.

Record size is  28 bytes.  Block size is  2800 bytes.
(Last block in a file is not padded; it may be as short as  28 bytes.)

Tape file    1:    62 records copied from VMS file: HCCSC2213.INF
Tape file    2:    57 records copied from VMS file: HCCSC2213.ABS
Tape file    3:  4670 records copied from VMS file: S0241K213.FBB
Tape file    4: 14635 records copied from VMS file: S0242K213.FBB
Tape file    5: 13947 records copied from VMS file: S0243K213.FBB
Tape file    6: 13240 records copied from VMS file: S0244K213.FBB
Tape file    7: 12636 records copied from VMS file: S0245K213.FBB
Tape file    8: 12101 records copied from VMS file: S0246K213.FBB
Tape file    9: 11586 records copied from VMS file: S0247K213.FBB
Tape file   10: 11090 records copied from VMS file: S0248K213.FBB
Tape file   11: 10612 records copied from VMS file: S0249K213.FBB
Tape file   12: 10198 records copied from VMS file: S0250K213.FBB
Tape file   13:  9797 records copied from VMS file: S0251K213.FBB
Tape file   14:  9434 records copied from VMS file: S0252K213.FBB
Tape file   15:  6502 records copied from VMS file: S0253K213.FBB
Tape file   16:  2892 records copied from VMS file: S0254K213.FBB
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Tape file   18:  2693 records copied from VMS file: S0256K213.FBB
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Tape file   20:  1143 records copied from VMS file: S0258K213.FBB
Tape file   21:    62 records copied from VMS file: HCCSC2213.INF
Tape file   22:    57 records copied from VMS file: HCCSC2213.ABS
Tape file   23:  4670 records copied from VMS file: S0241K213.FBB
Tape file   24: 14635 records copied from VMS file: S0242K213.FBB
Tape file   25: 13947 records copied from VMS file: S0243K213.FBB
Tape file   26: 13240 records copied from VMS file: S0244K213.FBB
Tape file   27: 12636 records copied from VMS file: S0245K213.FBB
Tape file   28: 12101 records copied from VMS file: S0246K213.FBB
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Tape file   30: 11090 records copied from VMS file: S0248K213.FBB
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Tape file   32: 10198 records copied from VMS file: S0250K213.FBB
Tape file   33:  9797 records copied from VMS file: S0251K213.FBB
Tape file   34:  9434 records copied from VMS file: S0252K213.FBB
Tape file   35:  6502 records copied from VMS file: S0253K213.FBB
Tape file   36:  2892 records copied from VMS file: S0254K213.FBB
Tape file   37:  2777 records copied from VMS file: S0255K213.FBB
Tape file   38:  2693 records copied from VMS file: S0256K213.FBB
Tape file   39:  2595 records copied from VMS file: S0257K213.FBB
Tape file   40:  1143 records copied from VMS file: S0258K213.FBB

Exit requested after   40 files were copied.
```

# High Resolution Absorption Cross Section Measurements of Sulfur Dioxide at 213 K in the Wavelength Region 172-240 nm

D.E.Freeman, K.Yoshino,
J.Esmond, and W.H.Parkinson

Harvard-Smithsonian
Center for Astrophysics

Cambridge, MA 02138, U.S.A.

Published in
Planetary Space Science

ABSTRACT-Laboratory measurements at high resolution of the absorption cross section of sulfur dioxide at the temperature 213 K have been performed in the wavelength region [illegible]72-240 nm with a 6.65 m scanning spectrometer/spectrograph operated at an instrumental width of 0.002 nm. The measured cross sections are presented graphically in representative wavelength regions and are available throughout the region 172-240 nm at wavenumber intervals of 0.4-0.1 wavenumbers as a numerical tabulation stored on magnetic tape from the National Space Science Data Center, Greenbelt, MD 20771, U.S.A. The measured cross sections, which are relevant to the photochemistry of planetary atmospheres, possess significantly more spectroscopic structure, and are more accurate, than previous measurements made [illegible] lower resolution.

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1-JUN-1984 14:17:07

Density is 1600 bpi.

Character code is ASCII.

Files are separated by tape-marks, with a double tape-mark at the end.

Record size is  28 bytes.  Block size is  2800 bytes.
(Last block in a file is not padded; it may be as short as  28 bytes.)

Tape file    1:    62 records copied from VMS file: HCCSO2213.INF
Tape file    2:    57 records copied from VMS file: HCCSO2213.ABS
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Tape file    5: 13947 records copied from VMS file: SO243K213.FBB
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Tape file   19:  2595 records copied from VMS file: SO257K213.FBB
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Tape file   25: 13947 records copied from VMS file: SO243K213.FBB
Tape file   26: 13240 records copied from VMS file: SO244K213.FBB
Tape file   27: 12636 records copied from VMS file: SO245K213.FBB
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Tape file   29: 11586 records copied from VMS file: SO247K213.FBB
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Tape file   32: 10198 records copied from VMS file: SO250K213.FBB
Tape file   33:  9797 records copied from VMS file: SO251K213.FBB
Tape file   34:  9434 records copied from VMS file: SO252K213.FBB
Tape file   35:  6502 records copied from VMS file: SO253K213.FBB
Tape file   36:  2892 records copied from VMS file: SO254K213.FBB
Tape file   37:  2777 records copied from VMS file: SO255K213.FBB
Tape file   38:  2693 records copied from VMS file: SO256K213.FBB
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Tape file   40:  1143 records copied from VMS file: SO258K213.FBB

Exit requested after   40 files were copied.
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The following is the description of a 9-track magnetic tape with visual label HCOSO2 containing cross section data of sulfur dioxide at 213 K in the wavelength region 172-240 nm experimentally obtained at the Harvard-Smithsonian Center for Astrophysics.
The tape is magnetically not labelled, and is written in the fixed record-fixed block format described below. The organization of the files on the tape are as follows:

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The cross section data files have two header lines at the beginning, which are followed by wavenumber/sigma pair records for each wavenumber position.

This tape is written with the following characteristics:

Density is 1600 bpi.

Character code is ASCII.

Files are separated by tape-marks, with a double tape-mark at the end.

Record size is 28 bytes.

Block size is 2800 bytes.

section there. Thus, the changes in column density and consequent adjustments to the provisional cross section of the previous scan are made by interpolation. This procedure is repeated until the entire 172-240 nm region has been covered by overlapping scans. Each 1 nm scan is performed with 3 to 5 different column densities of $SO_2$.

The photoelectric scanning is continuous, not stepwise, and counts are recorded on magnetic tape at intervals of 0.375 sec. In regions of highly structured absorption, $\lambda > 186$ nm, datum points are taken at intervals of 6.7 μm or 0.0004 nm in wavelength ($\simeq 0.1$ cm$^{-1}$) in the focal surface of the spectrometer; in regions of less highly structured absorption, $\lambda < 186$ nm, the corresponding intervals are 20 μm or 0.0012 nm. The background continuum is obtained by scanning the empty cell before and after each photoabsorption measurement. The small decrease in background continuum found to occur during a scan is taken into account by interpolation, and is attributed to the decrease with time of the transmittance of the silica windows of the cell. The effect of decreases in the window transmittance and column density during a scan requires a net adjustment of the provisional cross section by an amount which is typically only a few percent.

Before performing the photoelectric cross section measurements described above, we have used the 6.65 m spectrometer/spectrograph to photograph the absorption spectrum of $SO_2$ at 213 K and 300 K throughout the region 172-240 nm at a resolution of 0.0007 nm, together with standard hollow cathode and CO emission lines needed for wavelength calibration.

## 3. RESULTS AND DISCUSSION

In the wavelength region 172-240 nm the intense $SO_2$ absorption system $\tilde{C}\ ^1B_2 - \tilde{X}\ ^1A_1$ (Brand and Srikameswaran, 1972; Brand <u>et</u> <u>al</u>., 1976) dominates the other near-ultraviolet transitions of $SO_2$. In Figure 1 we present the results of our absorption cross section measurements of $SO_2$ at 213 K throughout the wavelength region 172-240 nm (58140-41670 cm$^{-1}$). The compressed wavenumber scale does scant justice to the small instrumental width (FWHM = 0.7-0.4 cm$^{-1}$), but does permit the overall pattern of the absorption to be seen; the bands are strongly degraded towards low energies and large changes in the cross section occur over small wavenumber intervals, especially in the region 42500-51000 cm$^{-1}$ (235-196 nm). Brand <u>et</u> <u>al</u>. (1976) have established that the origin of the system is at 42573.5 cm$^{-1}$, and they have made vibrational assignments and rotational analyses of bands near the origin; at higher energies the vibrational intervals in the $\tilde{C}$ state become quite irregular, principally as a result of a double minimum in the upper state potential of the antisymmetric stretching mode.

The two-photon excitation spectrum of $SO_2$ in the region of the $\tilde{C}$-$\tilde{X}$ transition has been studied by Vasudev and McClain (1981) who conclude that the photopredissociation threshold lies in the interval 219.56 ± 0.71 nm and that vibronic coupling of the $\tilde{C}$ state with $A_1$ states is very weak. However, the coupling of the $\tilde{C}$ state with the $\tilde{X}\ ^1A_1$ state is sufficient to permit Sharfin <u>et</u> <u>al</u>. (1982) and Ivanco <u>et</u> <u>al</u>. (1983) to observe quantum interference phenomena in the radiative decay of low lying levels of the $\tilde{C}$ state; these quantum beats disappear abruptly for bands of wavelength less than 218.06 nm, and lifetimes, which are characteristically 27-36 ns for the low lying vibronic levels, become progressively shorter beginning with the 218.06 nm band which marks the onset of the photopredissociation corresponding to a ground state dissociation limit of 217.9 ± 0.4 nm.

In absorption, the broadening associated with the photopredissociation is observed at somewhat shorter wavelengths because it must be detected in the presence of the combined Doppler and instrumental widths. Below ~196 nm (i.e., above ~51000 cm$^{-1}$) the absorption bands are quite diffuse (Figure 1), but near 210 nm the absorption spectrum is still rich in structure (Figures 1 and 2), so that previous cross section measurements made at low resolution (Table 1) in such highly structured regions are seriously in error. Thus, in Figure 2 our photographic spectrum obtained at a resolution of 0.0007 nm reveals a wealth of fine structure, almost all of which is absent from the recent cross section measurements obtained at a resolution of 0.06 nm by Wu and Judge (1981); and Table 1 shows, as an example, that the cross sections previously measured for the absorption peak near 210.2 nm are lower by about a factor of 3, than the present high resolution photoelectric measurements. Although we have yet to investigate the temperature dependence of the cross section at high resolution, it is known generally that, at a given temperature, the effects of loss of structure and diminution in the peaks of the cross section occur if the instrumental width is comparable with or larger than the width of the spectral feature of which the cross section is being measured (Hudson, 1971).

In Figure 3, we show a spectrogram and, in Figure 4, cross section determinations for SO$_2$ at 213 K in the region 43510-43545 cm$^{-1}$ (229.83-229.65 nm) of the band head of the (100)-(000) band, where no predissociation broadening of the line structure occurs. Comparison of the spectrogram, Figure 3, with the cross section plot, Figure 4a, reveals that essentially all of the structure present in the former is also present in the latter. The photoabsorption data for Figure 4a have been collected at wavelength intervals of 0.0001 nm and subjected to a smoothing procedure in which weighted averages are taken over adjacent wavenumber channels. Since the collection of data at intervals of 0.0001 nm requires impracticably long scanning times to cover an extended wavelength region, we show in Figure 4b the effects produced in the cross section by collecting data at intervals of 0.0004 nm (see Section 2) and subjecting them to a similar smoothing procedure. The four-fold increase in experimental speed results principally in reduction of the peaks and troughs in the cross section by ~10%, together with some loss of spectroscopic detail.

At energies above ~51000 cm$^{-1}$ the broadening effects of predissociation ensure that our cross section measurements are absolute in the sense of their being independent of the instrumental function. At energies below ~51000 cm$^{-1}$ the measured cross sections are probably close to absolute because the spectral features being measured are often not individual rotational lines, of Doppler width (FWHM) ~0.06 cm$^{-1}$, but clusters of overlapping lines; the view that these cross sections are close to absolute is supported by our observation that the optical depths on which the cross sections in Figure 4a are based vary linearly with the SO$_2$ pressure for optical depths up to 1.7.

The uncertainty in the measured cross sections resulting from uncertainties in the path length, pressure and temperature is less than 2%. Statistical errors in the measured optical depths contribute an additional 2% to the uncertainty in the measured cross sections. Systematic errors that are difficult to estimate in regions of sharp spectral structure may arise from a possible lack of spectroscopic resolution and from the use of scanning speeds chosen, as discussed above in relation to Figure 4, to permit practicable scanning times. The wavelength acuracy for the cross section measurements is estimated to vary from 0.01 nm (~3 $cm^{-1}$) in the most diffuse spectral regions to 0.0007 nm (~0.1 $cm^{-1}$) for the sharpest bands.

The absorption cross sections we have measured for $SO_2$ at 213 K with an instrumental width (FWHM) of 0.002 nm (0.7-0.4 $cm^{-1}$) throughout the region 172-240 nm (58140-41667 $cm^{-1}$) shown in Figure 1 are available, at wavenumber intervals of 0.4-0.1 $cm^{-1}$, as a numerical tabulation stored on magnetic tape from the National Space Science Data Center, NASA/Goddard Space Flight Center, Greenbelt, MD 20771, U.S.A. From these results we present in Figures 5-8 plots of the measured cross section in four representative energy regions, each spanning 1000 $cm^{-1}$. Figure 5 shows the cross section in the region 43000-44000 $cm^{-1}$ (232.5-227.3 nm) where predissociaton does not occur; this region includes the smaller region shown on an expanded scale in Figures 3 and 4. Figure 6 shows the cross section in the region 47000-48000 $cm^{-1}$ (212.7-208.4 nm) where considerable rovibronic structure persists in spite of the onset of predissociation at 217.9 nm; this region includes the smaller region shown in Figure 2. Figure 7 shows the cross section in the region 52000-53000 $cm^{-1}$ (192.3-188.7 nm) where the increasing loss of detailed structure with increasing energy reflects the rate of predissociation. Figure 8 shows the cross section in the region 54000-55000 $cm^{-1}$ (185.1-181.9 nm) where the diffuseness resulting from predissociation is very pronounced; within this region, Warneck et al. (1964) have found, using the mercury line at 185 nm (54069 $cm^{-1}$) as a source, that the apparent cross section of $SO_2$ at room temperature varies from $4x10^{-18}$ to $1x10^{-18}$ $cm^2$ as the $SO_2$ pressure is increased from 1 to 16 torr, whereas the cross section we have measured at 213 K at pressures in the range 0.1-0.5 torr is $3.64x10^{-18}$ $cm^2$, compared with the value ~$2.8x10^{-18}$ $cm^2$ measured at room temperature with relatively low resolution by Golomb et al. (1962). Most of the apparent cross sections measured at 185 nm by Warneck et al. (1964), viz., those obtained with pressures 4-16 torr and optical depths 5-7, are probably subject to considerable errors resulting from saturation effects present at these large optical depths.

## 4. CONCLUDING REMARK

In our present high resolution absorption cross section measurements of $SO_2$ at 213 K, hot bands originating from vibrationally excited ground state levels are largely suppressed. Future measurements are planned at 300 K to study the temperature dependence of the cross section in selected wavelength intervals of the spectrum of the $\tilde{C} - \tilde{X}$ transition of $SO_2$.

## ACKNOWLEDGEMENT

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# HIGH RESOLUTION ABSORPTION CROSS SECTION MEASUREMENTS OF $SO_2$ AT 213 K IN THE WAVELENGTH REGION 172-240 nm

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# HIGH RESOLUTION ABSORPTION CROSS SECTION MEASUREMENTS OF $SO_2$ AT 213 K IN THE WAVELENGTH REGION 172-240 nm

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## ABSTRACT

Laboratory measurements at high resolution of the absorption cross section of $SO_2$ at the temperature 213 K have been performed in the wavelength region 172-240 nm with a 6.65 m scanning spectrometer/spectrograph operated at an instrumental width of 0.002 nm. The measured cross sections are presented graphically in representative wavelength regions and are available throughout the region 172-240 nm at wavenumber intervals of 0.4-0.1 $cm^{-1}$ as a numerical tabulation stored on magnetic tape from the National Space Science Data Center, NASA/Goddard Space Flight Center, Greenbelt, MD 20771, U.S.A. The measured cross sections, which are relevant to the photochemistry of planetary atmospheres, possess significantly more spectroscopic structure, and are more accurate, than previous measurements made at lower resolution.

## 1. INTRODUCTION

Not only does $SO_2$ occur in the Earth's stratosphere as a trace species (Jaeschke et al., 1976; Sagawa and Itoh, 1977; Krueger, 1983) but it is also an important constituent of the atmosphere of Venus where $SO_2$ has been identified from Earth-based observations in the wavelength region 300–330 nm (Barker, 1979), from Pioneer orbiter observations in the region 206–280 nm (Stewart et al., 1979), and from International Ultraviolet Explorer observations in the region 208–218 nm (Conway et al., 1979). In addition, calculations on the heating of Io's atmosphere (Kumar, 1980, 1982) are based on the assumption that the dominant mechanism is the absorption by $SO_2$ of solar radiation with wavelengths below 221 nm. The need for improved laboratory measurements of the absorption cross section of $SO_2$ in the region 200–340 nm has recently been emphasized in some detail (Belton, 1982) in connection with the elucidation of the atmospheric compositions of Venus and Io.

In this paper we present an account of high resolution absorption cross section measurements on $SO_2$ at 213 K in the wavelength region 172–240 nm. These laboratory measurements have been performed with a 6.65 m photoelectric scanning spectrometer/spectrograph equipped with a 2400 lines $mm^{-1}$ grating and operated at an instrumental width, full width at half maximum (FWHM), of 0.002 nm.

## 2. EXPERIMENTAL PROCEDURE

The 6.65 m scanning spectrometer/spectrograph, used here with entrance and exit slit widths of 15 and 10 μm, respectively, has been described previously (Yoshino et al., 1980), as have the general methods for the reduction of such data (Yoshino et al., 1983; Freeman et al., 1983). The $SO_2$ in the 27 cm optical path of a Pyrex cell fitted with Suprasil-1 (silica) windows is cooled to 213 K by immersing the cell in stirred methanol cooled by a cold finger connected to an external refrigeration unit. The cell is located between the $H_2$ continuum source and the entrance slit of the 6.65 m instrument. The $SO_2$, of initial purity 99.98%, is purified further by fractional distillation. The $SO_2$ pressure, which varies over the range 0.03–40 torr, is monitored by an MKS Baratron gauge.

Photoabsorption measurements throughout the 172–240 nm region have been made, by the following technique, in a series of overlapping scans, with each scan covering a range of ~1 nm. A typical scan, say for the region 230–229 nm, begins at 230 nm where the measured values of the optical depth $\ln(I_0/I)$ and the column density N of the pure $SO_2$ are used to calculate the cross section $\sigma = (1/N)\ln(I_0/I)$. This value of N is adopted provisionally for the column density of $SO_2$ throughout the 1 nm scan, and provisional values of the cross section are thereby obtained from the measured values of $\ln(I_0/I)$ in this 1 nm region. We recognize that some photolysis of $SO_2$ occurs during the time (15–20 min) taken for the 1 nm scan, although no detectable change in pressure is observed. Since the direction of each scan is from long to short wavelength, the column density of $SO_2$ at the short wavelength end of a scan will really be somewhat less than it was at the start of the scan. Hence, the cross section at the short wavelength end of a scan, obtained provisionally by temporary neglect of the photolysis, will be smaller than the true cross section. The start of the next 1 nm scan, at which point the column density is accurately known because a fresh sample of pure $SO_2$ is used, overlaps the end of the previous scan, so that the true cross section in the overlap region is obtained from the current scan, and the result is applied to the end of the previous scan to obtain the corrected column density and corrected cross

## FIGURE CAPTIONS

Figure 1. The absorption cross section, plotted logarithmically, of $SO_2$ at 213 K in the region 41670–58140 $cm^{-1}$ (240–172 nm), obtained with an instrumental width (FWHM) of 0.4–0.7 $cm^{-1}$ (0.002 nm).

Figure 2. The spectrogram of $SO_2$ at 300 K has been photographed at a pressure of 0.098 torr in a path length of 17.5 cm by a 6.65 m spectrometer/spectrograph with an instrumental width (FWHM) of 0.0007 nm. The cross section plot is that of Wu and Judge (1981) obtained with an instrumental width of 0.06 nm; the solid dots in the cross section plot are data of Thompson _et al_. (1963). See Table 1. Both wavelength scales in Figure 2 are in air nanometers.

Figure 3. Spectrogram of $SO_2$ at 213 K in the region 43510–43545 $cm^{-1}$ photographed by a 6.65 m spectrometer/spectrograph with an instrumental width (FWHM) of 0.0007 nm. See Section 3 of the text and Figure 4. The wavelength scale in Figure 3 is in vacuum nanometers.

Figure 4. Cross sections of $SO_2$ at 213 K in the region 43510–43545 $cm^{-1}$ obtained with a 6.65 m scanning spectrometer/spectrograph with an instrumental width (FWHM) of 0.002 nm. The photoabsorption data for Figures 4a and 4b have been collected at intervals of 0.0001 and 0.0004 nm, respectively. See Section 3 of the text and Figure 3.

Figure 5. High resolution absorption cross section of $SO_2$ at 213 K in the region 43000–44000 $cm^{-1}$ (see Section 3). The upper state vibrational assignments ($v_1v_2v_3$) are those of Brand _et al_. (1976) for the transitions ($v_1v_2v_3$)-(000).

Figure 6. High resolution absorption cross section of $SO_2$ at 213 K in the region 47000–48000 $cm^{-1}$ (see Section 3).

Figure 7. High resolution absorption cross section of $SO_2$ at 213 K in the region 52000–53000 $cm^{-1}$ (see Section 3).

Figure 8. High resolution absorption cross section of $SO_2$ a 213 K in the region 54000–55000 $cm^{-1}$ (see Section 3).

Table 1. Absorption Cross Section Measurements of $SO_2$ at Wavelengths Overlapping the Range 172-240 nm of the $\tilde{C}$-$\tilde{X}$ Transition

| Range nm | Resolution nm | Source | Pressure torr | Cell length cm | Temperature K | $\sigma$(210.2 nm)[a] | Reference |
|---|---|---|---|---|---|---|---|
| 172-240 | 0.002 | $H_2$ discharge | 0.03-40 | 27 | 213 | 24.0 | Present work |
| 208-228 | 0.06 | synchrotron | 0.01-40 | 11, 51 | 294 | ~7.5 | Wu and Judge (1981) |
| 200-240 | 0.033 | ?[b] | 5 | ?[b] | ~300 | ?[b] | Conway _et_ _al_. (1979) |
| 185-315 | 0.1 | $H_2$ discharge; Hg lines | 2-10 | 12.4 | ~300 | ~9 | Warneck _et_ _al_. (1964) |
| 185-325[c] | ?[b] | ?[b] | 0.26-5 | 10 | ~300 | ~7.5 | Thompson _et_ _al_. (1963) |
| 105-217 | 0.1 | $H_2$ discharge | 0.03-1 | 4.7 | ~300 | ~9 | Golomb _et_ _al_. (1962) |

a. Cross section, in units of $10^{-18}$ $cm^2$, at the absorption peak near 210.2 nm (see Fig. 2).

b. Not published.

c. Wavelengths of absorption features too small by ~0.5 nm (Hudson, 1974).

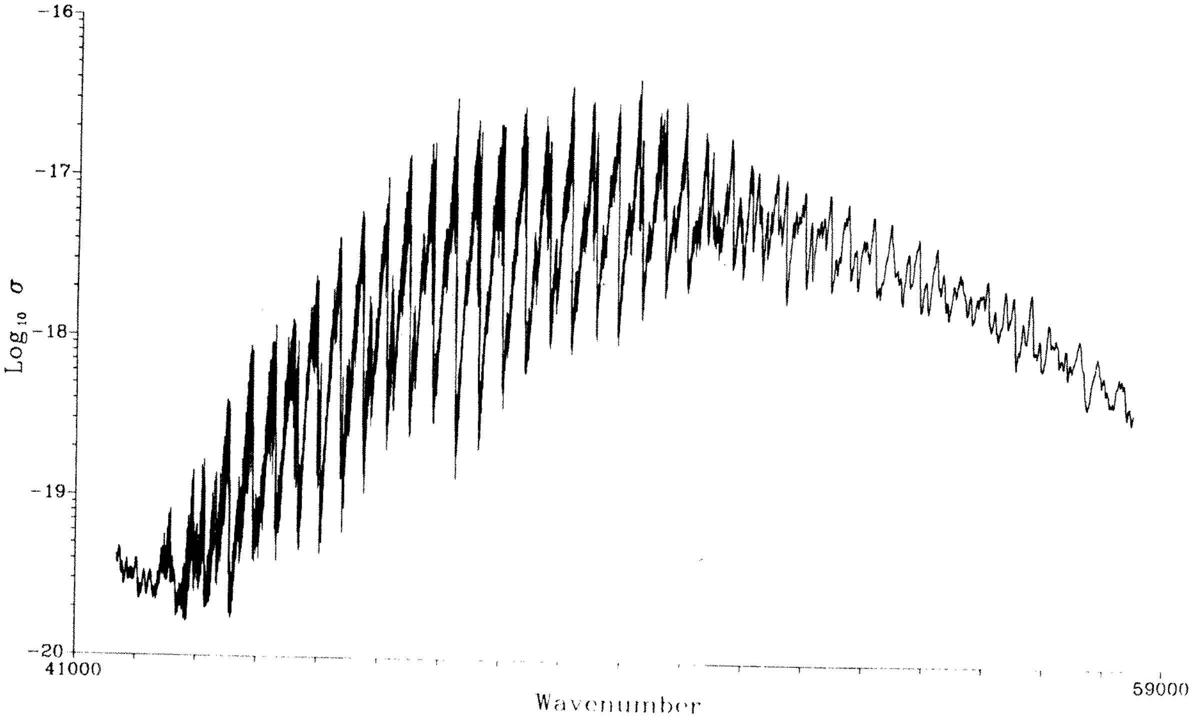


Figure 1

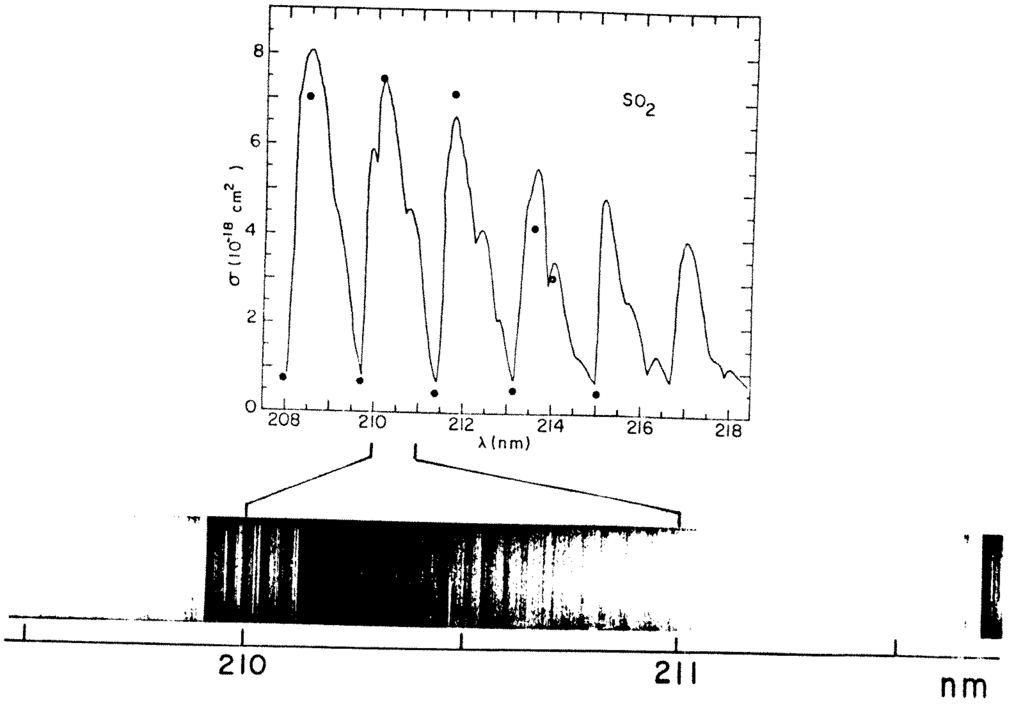


Figure 2

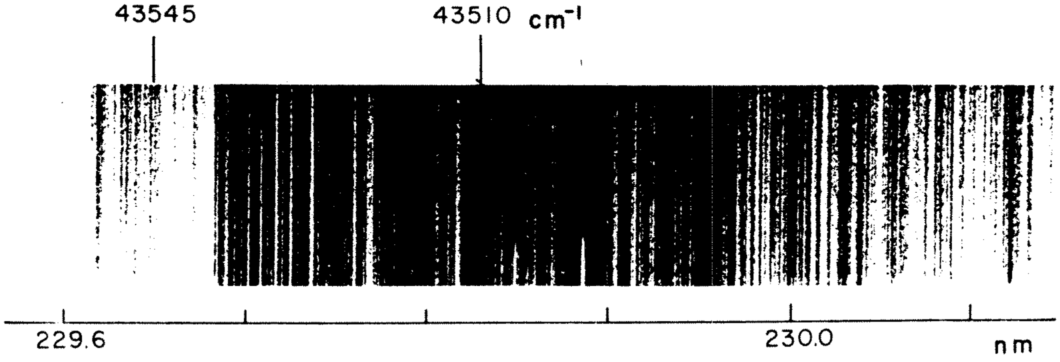
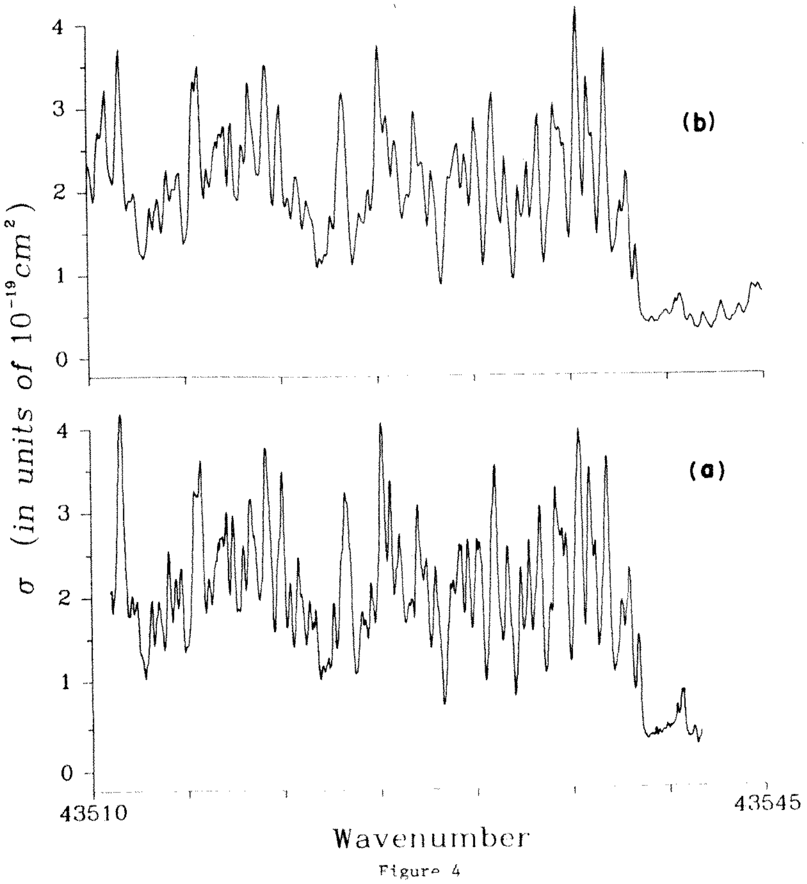


Figure 3



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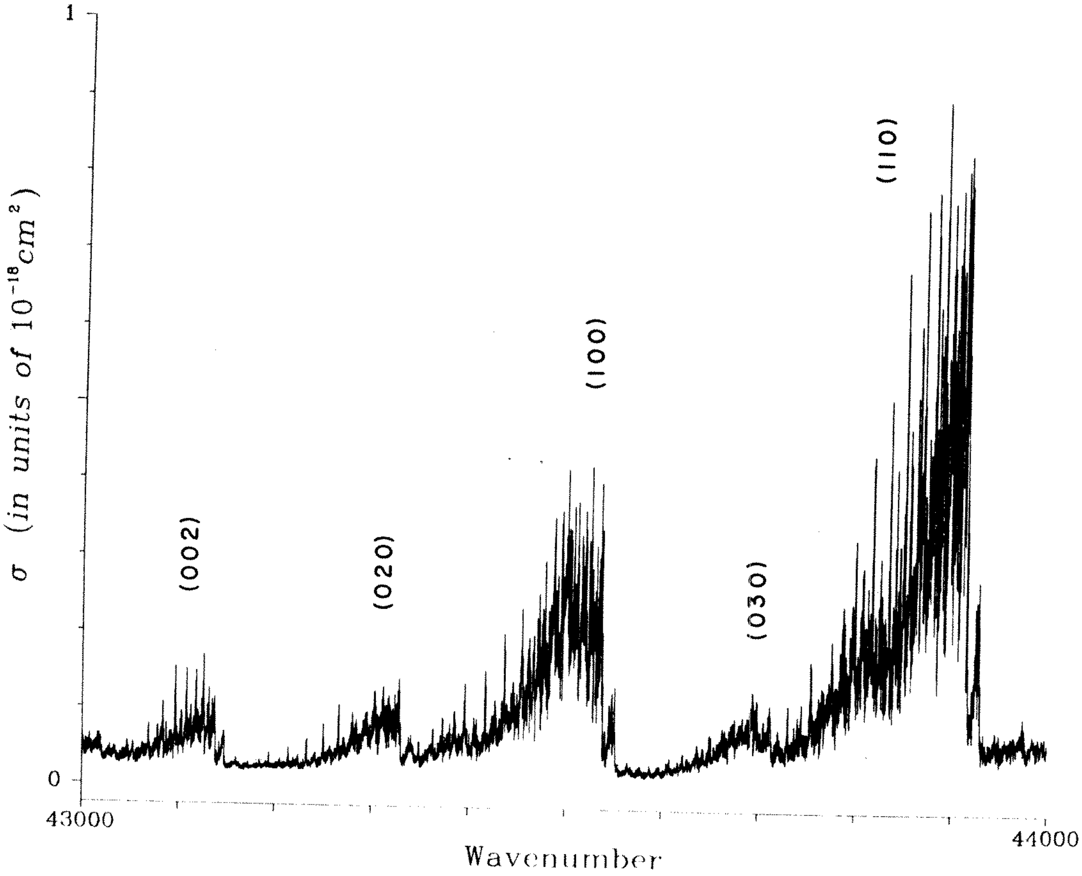

Figure 5

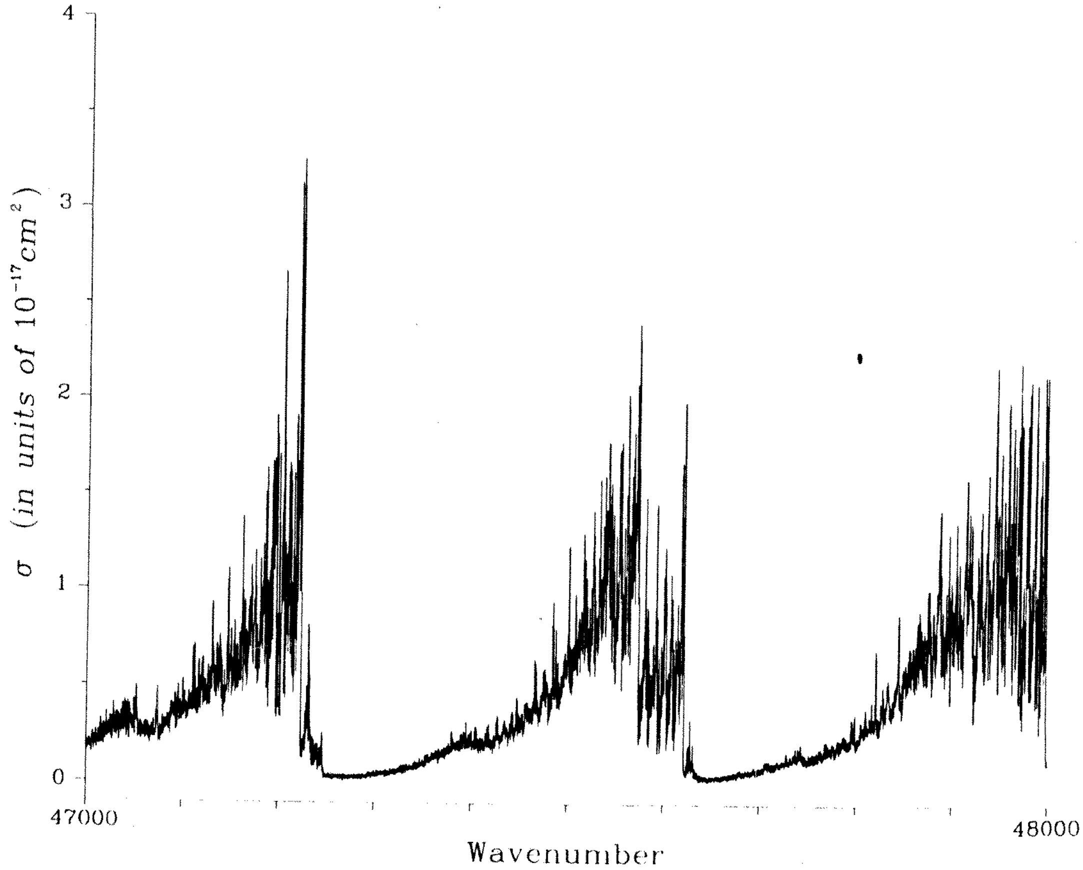

Figure 6

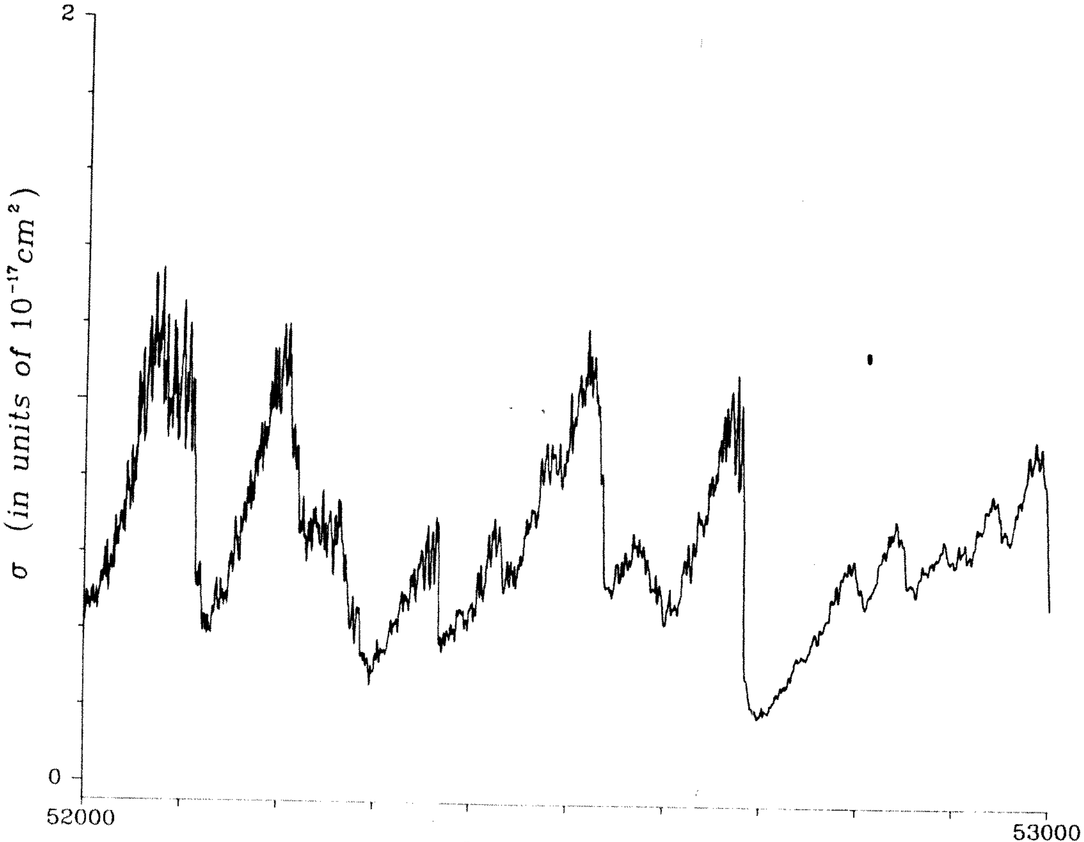

Figure 7

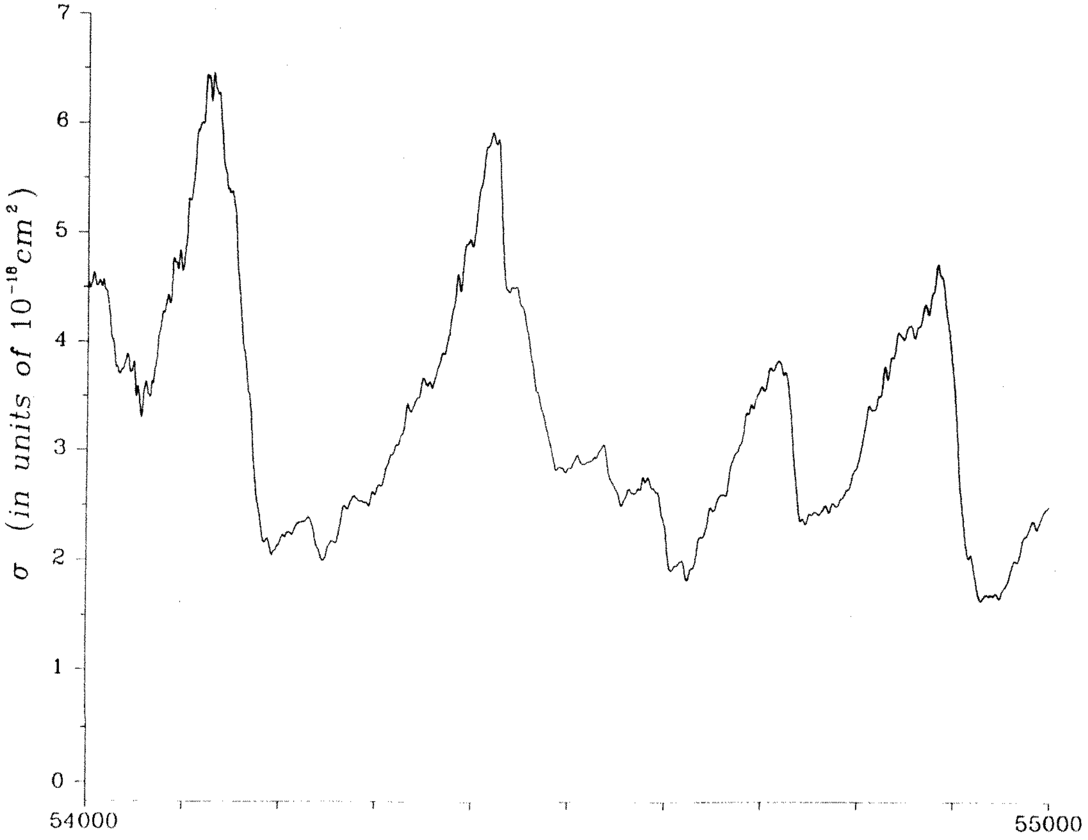

Figure 8

Joe King

GX - 11 C

**Center for Astrophysics**
60 Garden Street
Cambridge, Massachusetts 02138

Harvard College Observatory
Smithsonian Astrophysical Observatory

August 6, 1987

Dr. James Green
National Space Science Data Center
NASA/Goddard Space Flight Center
Greenbelt, MD 20771

Dear Dr. Green,

In the past we have supplied the NSSDC with tapes of our laboratory measurements of the absorption cross sections of oxygen at 295K and sulfur dioxide at 213K.

Enclosed under a separate cover is a 9-track magnetic tape on which are written files containing our high resolution laboratory measurements of absorption cross sections of oxygen at 79 K. The first file on the tape is a copy of the abstract from the paper in which the data is published and discussed (Planetary and Space Science). Next follows the 11 files of the cross sections of $^{16}O_2$ versus wavenumber of the (2,0)-(12,0) bands of oxygen, and then a duplicate copy in the same sequence.

The naming of the files follows the convention that O6LB is the general stem of the filename, and the digits following identify the upper level of the band included: i.e., for file O6LB11.SNG, this contains the cross sections of the B(11)-X(0) band.

The tape is an unlabelled ASCII tape written at 1600 bpi in fixed-blocksize, fixed-recordsize format where the recordsize is 24 bytes (characters), and the blocksize is 2400 bytes.

Two separate papers are enclosed here: one describes the tape format, and the other contains the abstract of our paper which has been submitted for publication in Planetary and Space Science.

Thank you again for the valuable service you provide.

Sincerely,

Kouichi Yoshino
Jim Esmond

617-495-7240

# HIGH RESOLUTION ABSORPTION CROSS-SECTIONS AND BAND OSCILLATOR STRENGTHS OF THE SCHUMANN–RUNGE BANDS OF OXYGEN AT 79 K

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(*Received* 11 *March* 1987)

**Abstract**—Cross-sections of $O_2$ at 79 K have been obtained from photoabsorption measurements at various pressures throughout the wavelength region 179.3–198.0 nm with a 6.65 m photoelectric scanning spectrometer equipped with a 2400 lines $mm^{-1}$ grating and having an instrumental width (FWHM) of 0.0013 nm. The measured absorption cross-sections of the Schumann–Runge bands (12, 0) through (2, 0) are independent of the instrumental width. The measured cross-sections are presented graphically here and are available at wavenumber intervals of $\sim 0.1$ $cm^{-1}$ as numerical compilations stored on magnetic tape from the National Space Science Data Center, NASA/Goddard Space Flight Center, Greenbelt, MD 20771, U.S.A. Band oscillator strengths of these bands have been determined by direct numerical integration of the measured cross-sections.

NSDF FREE TEXT ENTRY SHEET (Working Copy)

NSDF ID: GX-11C

Originator: ______ Date: ______

Short Name: SCHUMANN-RUNGE BAND OF O2 AT 79K

Agent Assigned: SJK Date: 9/13/87

File Coord.: ______ Date: ______

☒ Brief Description
☐ Full Name
☐ Data Set Documentation

☒ New
☐ Addition (explain below)
☐ Replacement (explain below)

---

This data set contains high resolution absorption cross-sections of the Schumann-Runge bands of oxygen at 79 K. The cross-sections were obtained in the wavelength region 179.3 - 198.0 nm with an instrumental width (FWHM) of 0.0013 nm. The measured cross-sections of the Schumann-Runge bands (12,0) through (2,0) are independent of the instrument width. The cross-sections are available at wavenumber intervals of about 0.1 cm-1 on a 9 track, 1600 bpi, ASCII tape. The first file on the tape is a copy of the abstract from the paper in which the data are published and discussed (submitted to Planetary and Space Science, March 1987). Next follows the 11 files of the cross-sections of oxygen versus wavenumber of the (2,0)-(12,0) bands, and then a duplicate copy in the same sequence. The naming of the files follows the convention that 06LB is the general stem of the filename, and the digits following identify the upper level of the band included: i.e., for file 06LB11.SNG, this contains the cross-sections of the B(11)-X(0) band. The absorption cross-sections of oxygen at 295 K for the same band are available at NSSDC under a data set ID GX-11A.

TAPE Visual ID: 016K79

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Density is 1600 bpi.

Character code is ASCII.

Files are separated by tape-marks, with a double tape-mark at the end.

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(Last block in a file is not padded; it may be as short as  24 bytes.)

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51375.015     0.7577E-22
51375.091     0.8654E-22
51375.167     0.9677E-22
51375.243     0.1076E-21
51375.319     0.1194E-21
51375.395     0.1312E-21
51375.471     0.1412E-21
51375.547     0.1490E-21
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fourth file on tape OZHC
which contains cross-sectio
data versus wavenumber
For the (4,0) Schumann-Rung
band of molecular oxygen.

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51375.851     0.1853E-21
51375.927     0.1964E-21
51376.003     0.2055E-21
51376.079     0.2122E-21
51376.155     0.2171E-21
51376.231     0.2207E-21
51376.307     0.2238E-21
51376.383     0.2265E-21
51376.459     0.2282E-21
51376.535     0.2286E-21
51376.611     0.2277E-21
51376.687     0.2261E-21
51376.763     0.2245E-21
51376.839     0.2218E-21
51376.915     0.2163E-21
51376.991     0.2076E-21
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GX-11A
D-51695
C-22901

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$NOP
$NOP
$NOP ********* GOUT-1 *********
$EXEC TPLIST BS

INPUT PARAMETERS ARE:  AS SR=1=2 2

 TAPE NO.   1                FILE NO.   1
 RECORD   1                  LENGTH   2800
 BAND 1,0; 0231XCC                  WNO          SIGMA         49623.232     0.7449E-23      49623.302
   0.8721E-23     49623.582     0.9887E-23     49623.652     0.1135E-22     49623.722     0.1319E-22
    49623.792     0.1482E-22     49623.862     0.1517E-22     49624.002     0.1369E-22     49624.071
  0.1119E-22     49624.211     0.9068E-23     49624.281     0.7952E-23     49624.351     0.7686E-23
  49624.421     0.8053E-23     49624.561     0.8782E-23     49624.701     0.9315E-23     49624.771     0
.9171E-23     49625.190     0.8591E-23     49625.260     0.8284E-23     49625.330     0.8560E-23     4
9625.540     0.8963E-23     49625.610     0.8641E-23     49625.820     0.7281E-23     49625.890     0.5
818E-23     49625.960     0.5942E-23     49626.030     0.8619E-23     49626.100     0.1294E-22     496
26.310     0.1659E-22     49626.519     0.1780E-22     49626.589     0.1671E-22     49626.799     0.147
6E-22     49627.009     0.1318E-22     49627.079     0.1206E-22     49627.149     0.1093E-22     49627
.219     0.1303E-22     49627.289     0.1002E-22     49627.569     0.1105E-22     49627.849     0.1265E
-22     49627.989     0.1424E-22     49628.059     0.1541E-22     49628.269     0.1595E-22     49628.5
49     0.1600E-22     49628.689     0.1594E-22     49629.039     0.1565E-22     49629.109     0.1464E-2
2     49629.249     0.1296E-22     49629.319     0.1117E-22     49629.389     0.9664E-23     49629.949
   0.8539E-23     49630.229     0.8134E-23     49630.299     0.8829E-23     49630.369     0.1026E-22
    49630.439     0.1103E-22     49630.579     0.9947E-23     49630.789     0.7470E-23     49630.929
  0.5266E-23     49631.139     0.4392E-23     49631.279     0.4624E-23     49631.349     0.5166E-23
   49631.489     0.5555E-23     49631.559     0.6009E-23     49631.629     0.7125E-23.    49631.769
0.9110E-23     49631.909     0.1119E-22     49631.979     0.1193E-22     49632.049     0.1057E-22
49632.119     0.8287E-23     49632.189     0.7271E-23     49632.259     0.8540E-23     49632.399     0.
1092E-22     49632.680     0.1245E-22     49632.750     0.1231E-22     49632.890     0.1103E-22     49
633.030     0.9451E-23     49633.170     0.8178E-23     49633.310     0.7575E-23     49633.520     0.75
19E-23     49633.590     0.7711E-23     49633.730     0.8231E-23     49634.081     0.9236E-23     4963
4.151     0.1044E-22     49634.711     0.1147E-22     49634.922     0.1208E-22     49634.992     0.1181
E-22     49635.062     0.1033E-22     49635.132     0.8363E-23     49635.202     0.7333E-23     49635.
272     0.8072E-23     49635.342     0.1020E-22     49635.412     0.1244E-22     49635.482     0.1355E-
22     49635.903     0.1322E-22     49635.973     0.1204E-22     49636.253     0.1064E-22     49636.81
4     0.9446E-23     49636.884     0.8805E-23     49636.954     0.8685E-23     49637.024     0.8740E-23
     49637.094     0.8756E-23

 TAPE NO.   1                FILE NO.   1
 RECORD   2                  LENGTH   2800
     49637.375     0.8692E-23     49637.445     0.8599E-23     49637.585     0.8620E-23     49637.655
   0.8869E-23     49637.796     0.9563E-23     49637.866     0.1092E-22     49637.936     0.1235E-22
    49638.006     0.1280E-22     49638.076     0.1239E-22     49638.146     0.1214E-22     49638.497
  0.1214E-22     49638.707     0.1158E-22     49638.777     0.1024E-22     49638.848     0.8885E-23
  49638.988     0.8385E-23     49639.268     0.8845E-23     49639.619     0.9577E-23     49639.759     0
.9989E-23     49639.829     0.1020E-22     49640.110     0.1066E-22     49640.461     0.1126E-22     4
9640.601     0.1119E-22     49640.812     0.1020E-22     49640.952     0.9293E-23     49641.092     0.9
434E-23     49641.162     0.1050E-22     49641.233     0.1199E-22     49641.584     0.1374E-22     496
41.724     0.1549E-22     49641.794     0.1706E-22     49641.864     0.1894E-22     49642.285     0.212
5E-22     49642.355     0.2294E-22     49642.426     0.2291E-22     49642.566     0.2093E-22     49642
.706     0.1724E-22     49642.847     0.1272E-22     49642.917     0.9278E-23     49643.057     0.8246E
-23     49643.128     0.8846E-23     49643.408     0.9337E-23     49643.479     0.8967E-23     49643.5
49     0.8047E-23     49643.619     0.6958E-23     49643.689     0.5926E-23     49643.900     0.5242E-2
3     49643.970     0.5153E-23     49644.040     0.5696E-23     49644.110     0.6740E-23     49644.321
   0.8097E-23     49644.391     0.9393E-23     49644.461     0.9972E-23     49644.532     0.9486E-23
    49644.602     0.8608E-23     49644.883     0.8463E-23     49644.953     0.9369E-23     49645.164
  0.1038E-22     49645.374     0.1023E-22     49645.445     0.8824E-23     49645.585     0.7331E-23
   49645.796     0.6964E-23     49645.866     0.8273E-23     49646.006     0.1101E-22     49646.077
 0.1381E-22     49646.428     0.1493E-22     49646.849     0.1491E-22     49646.920     0.1249E-22
49647.060     0.1157E-22     49647.130     0.1210E-22     49647.411     0.1334E-22     49647.482     0.
1382E-22     49647.622     0.1306E-22     49647.692     0.1236E-22     49647.763     0.1307E-22     49
647.833     0.1503E-22     49647.903     0.1707E-22     49647.973     0.1803E-22     49648.114     0.17
77E-22     49648.325     0.1716E-22     49648.536     0.1677E-22     49648.606     0.1619E-22     4964
8.746     0.1512E-22     49649.028     0.1425E-22     49649.168     0.1426E-22     49649.309     0.1478
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 22     49650.433     0.1182E-22     49650.765     0.1067E-22     49650.925     0.8751E-23     49651.06
 6    0.7281E-23     49651.136     0.6722E-23     49651.207     0.6736E-23     49651.488     0.7164E-23
        49651.699     0.8233E-23

  TAPE NO.   1              FILE NO.   2
  RECORD   1                LENGTH   2800
  BAND 2,0; 02B2X0C                    WNO         SIGMA          50050.057     0.1785E-22     50050.130
    0.2093E-22     50050.203     0.2242E-22     50050.275     0.2086E-22     50050.421     0.1739E-22
     50050.494     0.1452E-22     50050.713     0.1373E-22     50050.786     0.1446E-22     50050.859
    0.1529E-22     50050.932     0.1470E-22     50051.077     0.1272E-22     50051.150     0.1139E-22
   50051.223     0.1269E-22     50051.369     0.1624E-22     50051.442     0.1971E-22     50051.588     0
 .2149E-22     50051.661     0.2174E-22     50051.880     0.2081E-22     50051.952     0.1844E-22     5
 0052.025     0.1517E-22     50052.098     0.1270E-22     50052.171     0.1208E-22     50052.244     0.1
 251E-22     50052.317     0.1282E-22     50052.390     0.1304E-22     50052.463     0.1367E-22     500
 52.682     0.1442E-22     50052.755     0.1478E-22     50052.828     0.1500E-22     50052.901     0.155
 8E-22     50052.974     0.1627E-22     50053.046     0.1672E-22     50053.119     0.1771E-22     50053
 .338     0.2015E-22     50053.411     0.2318E-22     50053.630     0.2430E-22     50053.703     0.2194E
 -22     50053.776     0.1741E-22     50053.849     0.1370E-22     50053.922     0.1241E-22     50053.9
 95     0.1282E-22     50054.068     0.1344E-22     50054.141     0.1328E-22     50054.287     0.1209E-2
 2     50054.505     0.1038E-22     50054.724     0.9103E-23     50054.797     0.8897E-23     50054.870
     0.9717E-23     50054.943     0.1101E-22     50055.016     0.1215E-22     50055.089     0.1282E-22
      50055.162     0.1292E-22     50055.381     0.1249E-22     50055.454     0.1188E-22     50055.527
   0.1148E-22     50055.673     0.1127E-22     50055.819     0.1104E-22     50055.965     0.1055E-22
    50056.184     0.9809E-23     50056.257     0.9337E-23     50056.330     0.9599E-23     50056.549
 0.1028E-22     50056.622     0.1059E-22     50056.695     0.1031E-22     50056.768     0.9878E-23
 50056.841     0.9595E-23     50056.914     0.9584E-23     50056.987     0.1025E-22     50057.060     0.
 1161E-22     50057.133     0.1265E-22     50057.352     0.1254E-22     50057.498     0.1201E-22     50
 057.717     0.1244E-22     50057.790     0.1424E-22     50057.863     0.1677E-22     50058.009     0.19
 05E-22     50058.082     0.1993E-22     50058.374     0.1875E-22     50058.520     0.1652E-22     5005
 8.666     0.1517E-22     50058.739     0.1528E-22     50058.885     0.1560E-22     50059.031     0.1499
 E-22     50059.104     0.1381E-22     50059.250     0.1339E-22     50059.542     0.1417E-22     50059.
 615     0.1512E-22     50059.761     0.1488E-22     50059.834     0.1337E-22     50059.907     0.1183E-
 22     50060.127     0.1160E-22     50060.200     0.1282E-22     50060.273     0.1436E-22     50060.34
 6     0.1462E-22     50060.419     0.1291E-22     50060.492     0.1017E-22     50060.565     0.8177E-23
        50060.711     0.7877E-23

  TAPE NO.   1              FILE NO.   2
  RECORD   2                LENGTH   2800
        50060.784     0.8644E-23     50061.003     0.9406E-23     50061.222     0.9813E-23     50061.295
     0.9994E-23     50061.441     0.9823E-23     50061.514     0.9068E-23     50061.588     0.8068E-23
      50061.734     0.7843E-23     50061.807     0.9323E-23     50061.880     0.1226E-22     50062.026
   0.1527E-22     50062.099     0.1728E-22     50062.172     0.1808E-22     50062.245     0.1756E-22
    50062.318     0.1569E-22     50062.464     0.1301E-22     50062.537     0.1031E-22     50062.611     0
 .8360E-23     50062.684     0.7790E-23     50062.757     0.8592E-23     50062.830     0.1008E-22     5
 0063.122     0.1152E-22     50063.195     0.1253E-22     50063.268     0.1310E-22     50063.414     0.1
 354E-22     50063.487     0.1431E-22     50063.561     0.1520E-22     50063.707     0.1489E-22     500
 63.780     0.1239E-22     50063.853     0.8757E-23     50063.999     0.6233E-23     50064.072     0.631
 8E-23     50064.145     0.8820E-23     50064.218     0.1216E-22     50064.438     0.1465E-22     50064
 .511     0.1607E-22     50064.584     0.1745E-22     50064.876     0.1914E-22     50064.949     0.1993E
 -22     50065.096     0.1864E-22     50065.169     0.1562E-22     50065.315     0.1273E-22     50065.4
 61     0.1186E-22     50065.534     0.1324E-22     50065.754     0.1506E-22     50066.119     0.1543E-2
 2     50066.192     0.1436E-22     50066.266     0.1310E-22     50066.339     0.1222E-22     50066.412
     0.1136E-22     50066.485     0.1055E-22     50066.631     0.1011E-22     50066.851     0.9671E-23
      50066.997     0.8788E-23     50067.070     0.7961E-23     50067.143     0.8025E-23     50067.289
   0.8843E-23     50067.363     0.9492E-23     50067.509     0.9402E-23     50067.582     0.8882E-23
    50067.801     0.8630E-23     50067.948     0.8879E-23     50068.021     0.9330E-23     50068.094
 0.9716E-23     50068.313     0.9841E-23     50068.387     0.9456E-23     50068.460     0.8738E-23
 50068.533     0.8402E-23     50068.752     0.8855E-23     50068.899     0.9688E-23     50068.972     0.
 1016E-22     50069.045     0.9962E-23     50069.118     0.9538E-23     50069.265     0.9433E-23     50
 069.338     0.9405E-23     50069.411     0.8783E-23     50069.484     0.7667E-23     50069.557     0.69
 90E-23     50069.630     0.7637E-23     50069.704     0.9808E-23     50069.777     0.1264E-22     5006
 9.923     0.1458E-22     50069.996     0.1473E-22     50070.070     0.1377E-22     50070.216     0.1317
 E-22     50070.289     0.1368E-22     50070.362     0.1496E-22     50070.435     0.1608E-22     50070.
 509     0.1630E-22     50070.582     0.1545E-22     50070.728     0.1404E-22     50070.801     0.1289E-
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      50071.826    0.1605E-22

   ***** JOB DONE.
   $AVF IN 11
   $EXEC TPLIST BS

   INPUT PARAMETERS ARE:  AS SR=1=2 2

    TAPE NO.   1              FILE NO.   1
    RECORD   1                LENGTH   2800
    BAND 12,0; L02B12X0C                 WNO            SIGMA          55450.372    0.4072E-20     55451.272
      0.3873E-20     55452.173     0.2364E-20     55453.073     0.2657E-20     55453.974     0.3155E-20
      55454.875    0.3012E-20     55455.775    0.2278E-20     55456.676    0.2518E-20     55457.577
    0.4802E-20     55457.755     0.5099E-20     55457.844     0.6137E-20     55457.934     0.6981E-20
    55458.023    0.7373E-20     55458.112    0.7605E-20     55458.202    0.8155E-20     55458.291     0
   .9217E-20     55458.381     0.1093E-19     55458.470     0.1421E-19     55458.559     0.1948E-19     5
   5458.682    0.2548E-19     55458.772    0.3007E-19     55458.861    0.3172E-19     55458.951     0.3
   095E-19     55459.006     0.2859E-19     55459.096     0.2499E-19     55459.185     0.2040E-19     554
   59.274    0.1559E-19     55459.364    0.1174E-19     55459.453    0.9168E-20     55459.543     0.781
   8E-20     55459.632     0.7519E-20     55459.721     0.7179E-20     55459.811     0.6647E-20     55459
   .900     0.6368E-20     55459.990     0.5930E-20     55460.079     0.5083E-20     55460.168     0.4575E
   -20     55460.258     0.4965E-20     55460.347     0.5708E-20     55460.436     0.5919E-20     55460.5
   26     0.5812E-20     55460.615     0.5888E-20     55460.705     0.6113E-20     55460.794     0.6317E-2
   0     55460.883     0.6748E-20     55460.973     0.7575E-20     55461.062     0.9028E-20     55461.152
      0.1181E-19     55461.241     0.1609E-19     55461.364     0.2069E-19     55461.453     0.2384E-19
     55461.543     0.2551E-19     55461.632     0.2678E-19     55461.722     0.2756E-19     55461.777
    0.2712E-19     55461.900     0.2515E-19     55461.956     0.2198E-19     55462.045     0.1851E-19
     55462.135     0.1536E-19     55462.224     0.1267E-19     55462.314     0.1122E-19     55462.403
   0.1121E-19     55462.492     0.1145E-19     55462.582     0.1127E-19     55462.671     0.1120E-19
   55462.761     0.1203E-19     55462.850     0.1357E-19     55462.939     0.1532E-19     55463.029     0.
   1712E-19     55463.118     0.1931E-19     55463.208     0.2194E-19     55463.331     0.2387E-19     55
   463.420     0.2429E-19     55463.476     0.2356E-19     55463.565     0.2218E-19     55463.655     0.20
   25E-19     55463.744     0.1767E-19     55463.833     0.1459E-19     55463.923     0.1190E-19     5546
   4.012     0.1027E-19     55464.102     0.9203E-20     55464.191     0.8376E-20     55464.280     0.7953
   E-20     55464.370     0.7258E-20     55464.459     0.6174E-20     55464.549     0.5498E-20     55464.
   638     0.5130E-20     55464.783     0.4444E-20     55465.684     0.4155E-20     55466.585     0.5604E-
   20     55466.694     0.6829E-20     55466.784     0.8432E-20     55466.873     0.1037E-19     55466.96
   3     0.1196E-19     55467.052     0.1201E-19     55467.141     0.1345E-19     55467.231     0.8691E-20
      55467.320     0.7335E-20

    TAPE NO.   1              FILE NO.   1
    RECORD   2                LENGTH   2800
      55467.410     0.6103E-20     55467.499     0.5440E-20     55467.588     0.5617E-20     55467.678
     0.5696E-20     55467.767     0.5435E-20     55467.857     0.5472E-20     55467.946     0.5829E-20
     55468.035     0.6018E-20     55468.125     0.6009E-20     55468.337     0.5514E-20     55469.195
    0.7328E-20     55470.006     0.1871E-19     55470.181     0.1936E-19     55470.271     0.2253E-19
    55470.394     0.2686E-19     55470.483     0.3159E-19     55470.573     0.3686E-19     55470.662     0
   .4341E-19     55470.752     0.5161E-19     55470.830     0.6141E-19     55470.919     0.7308E-19     5
   5471.023     0.8525E-19     55471.105     0.9538E-19     55471.194     0.1017E-18     55471.284     0.1
   025E-18     55471.377     0.9760E-19     55471.467     0.9102E-19     55471.552     0.8519E-19     554
   71.634     0.7870E-19     55471.724     0.7124E-19     55471.813     0.6359E-19     55471.903     0.579
   1E-19     55471.992     0.5638E-19     55472.081     0.5811E-19     55472.171     0.6080E-19     55472
   .260     0.6360E-19     55472.350     0.6662E-19     55472.439     0.7061E-19     55472.529     0.7631E
   -19     55472.613     0.8327E-19     55472.719     0.9042E-19     55472.804     0.9772E-19     55472.8
   93     0.1033E-18     55472.983     0.1051E-18     55473.072     0.1029E-18     55473.166     0.9715E-1
   9     55473.255     0.9175E-19     55473.345     0.8975E-19     55473.430     0.8928E-19     55473.523
      0.8923E-19     55473.609     0.9075E-19     55473.698     0.9204E-19     55473.788     0.9058E-19
      55473.881     0.8613E-19     55473.971     0.8086E-19     55474.049     0.7588E-19     55474.138
     0.7041E-19     55474.228     0.6410E-19     55474.317     0.5720E-19     55474.407     0.5027E-19
     55474.496     0.4405E-19     55474.597     0.3932E-19     55474.686     0.3664E-19     55474.764
   0.3500E-19     55474.865     0.3251E-19     55474.921     0.2943E-19     55475.044     0.2644E-19
   55475.100     0.2372E-19     55475.189     0.2135E-19     55475.279     0.1943E-19     55475.368     0.
   1797E-19     55475.457     0.1684E-19     55475.547     0.1549E-19     55475.597     0.1331E-19     55
   476.499     0.6760E-20     55477.400     0.4776E-20     55478.301     0.3527E-20     55479.203     0.26
```

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E-20     55486.416     0.2494E-20      55487.318     0.2829E-20      55488.219     0.2284E-20      55489.
121     0.2644E-20      55490.023     0.3242E-20      55490.925     0.3873E-20      55491.827     0.4947E-
20     55492.729     0.5342E-20      55493.537     0.8787E-20      55493.617     0.9166E-20      55493.70
7     0.9446E-20      55493.796     0.1034E-19      55493.886     0.1187E-19      55493.975     0.1289E-19
      55494.065     0.1360E-19

  TAPE NO.   1               FILE NO.   2
  RECORD   1                 LENGTH   1840
 ****************************************HIGH RESOLUTION ABSORPTION CROSS         SECTION MEASUREMENT
S AND BAND          OSCILLATOR STRENGTHS OF THE (1,0)-(12,0)SCHUMANN-RUNGE BANDS OF MOLECULAR
  OXYGEN                                                                           K. Yoshino, D.E.
Freeman, J.R. Esmond,  and W.H. Parkinson
    Harvard-Smithsonian Center for           Astrophysics, Cambridge, MA 02138
                               Abstract:
          Cross sections of molecular oxygen    at 300 K have been obtained from         photoabsorpti
on measurements at various pressures throughout the wavelength     region 179.3-201.5 nm with a 6.6
5 m     photoelectric scanning spectrometer     equipped with a 2400 lines/mm grating   and having
an instrumental width (FWHM) of 0.0013 nm.  The measured absorption  cross sections of the Schumann
-Runge    bands (12,0) through (1,0) in this      wavelength region are absolute, i.e.,   independe
nt of the instrumental width,  a result not achieved previously.  The  measured cross sections are
presented   graphically and are available           at wavenumber intervals of              approxi
mately 0.1 wavenumbers             as numerical compilations stored on    magnetic tape from the Nat
ional Space   Science Data Center, Greenbelt,           MD 20771, USA.  Band ocsillator          stren
gths of the (12,0) through (1,0)   bands have been determined by direct    numerical integration of
 the measured   cross sections.                                                                  The
 paper describing this research has  been submitted for publication in       PLANETARY AND SPACE SC
IENCE.          ****************************************

***** JOB DONE.
$WEO LFS

$$
```

and last 3 records

```
$NOP
$NOP **** LIST OF THE FIRST 3 RECORDS OF FILE 1 ****
$EXEC TPLIST BS

INPUT PARAMETERS ARE:  AS FL=3=3 1 1 1

 TAPE NO.   1             FILE NO.   1
 RECORD   1               LENGTH   1736
                                                                                   The following i
s the       description of a 9-track    magnetic tape with visual   label HCOSO2 containing     cr
oss section data of sulfurdioxide at 213 K in the     wavelength region 172-240 nmexperimentally ob
tained at  the Harvard-Smithsonian     Center for Astrophysics.   The tape is magnetically notlabe
lled, and is written in the fixed record-fixed blockformat described below. The organization of the
 files onthe tape are as follows:    1) File 1: this information file.                      2) Fil
e 2: the title and    abstract of the paper on    this work as published in   Planetary Space Scien
ce.   3) Files 3-20: files of the cross section data within  1000 wavenumber intervals   beginnin
g at ~41670      through ~58140 wavenumbers. 4) File 21: repetition of   file 1.
    5) File 22: repetition of   file 2.                        6) Files 23-40: repetition  of files 3
-20.          The cross section data fileshave two header lines at thebeginning, which are
   followed by wavenumber/sigmapair records for each       wavenumber position.
                                                                        This tape is written with
 the following             characteristics:                                            Density is 160
0 bpi.                                      Character code is ASCII.                               F
iles are separated by      tape-marks, with a double   tape-mark at the end.
                 Record size is 28 bytes.                                 Block size is 2800 bytes.


***** JOB DONE.
$WEO LPS


$$
$WEO LO
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GX-11B
Sulfur Dioxide
Cross Sections
D-65017
C-252466

```
$EXEC TPLIST BS

INPUT PARAMETERS ARE:  AS FL=3=3 1 1 2

 TAPE NO.   1            FILE NO.   2
 RECORD   1              LENGTH   1596
                                                                                High Resolution
 Absorption  Cross Section Measurements  of Sulfur Dioxide at 213 K  in the Wavelength Region   17
2-240 nm                                                  D.E.Freeman, K.Yoshino,     J.Esmond, and W.H
.Parkinson                                     Harvard-Smithsonian        Center for Astrophysics
                           Cambridge, MA 02138, U.S.A.                                     Published in
          Planetary Space Science                                  ABSTRACT-Laboratory         measur
ements at high        resolution of the absorptioncross section of sulfur    dioxide at the temper
ature  213 K have been performed inthe wavelength region       172-240 nm with a 6.65 m    scanning
                   spectrometer/spectrograph   operated at an instrumental width of 0.002 nm. The
     measured cross sections are presented graphically in    representative wavelength   regions an
d are available   throughout the region       172-240 nm at wavenumber    intervals of 0.4-0.1
   wavenumbers as a numerical  tabulation stored on        magnetic tape from the      National Spa
ce Science Data Center, Greenbelt, MD 20771,U.S.A. The measured cross   sections, which are
 relevant to the            photochemistry of planetary atmospheres, possess       significantly
more          spectroscopic structure, andare more accurate, than     previous measurements made  a
t lower resolution.

***** JOB DONE.
$WEO LPS




















$$
$NOP
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$NOP
$NOP
$NOP ***** LIST OF FIRST 3 AND LAST 3 RECORDS OF FILE 40 *****
$EXEC TPLIST BS

INPUT PARAMETERS ARE:  AS FL=3=3 1 1 40

 TAPE NO.    1              FILE NO.   40
 RECORD   1                 LENGTH   2800
-1  SO2;58000-58453;213K          WN            SIGMA          58000.104    0.5225E-18      58000.498
0.5222E-18      58000.892    0.5221E-18      58001.285    0.5224E-18      58001.679    0.5228E-18
58002.073    0.5236E-18      58002.467    0.5244E-18      58002.860    0.5256E-18      58003.254    0.
5271E-18      58003.648    0.5287E-18      58004.042    0.5305E-18      58004.436    0.5324E-18      58
004.830    0.5345E-18      58005.223    0.5366E-18      58005.617    0.5385E-18      58006.011    0.54
04E-18      58006.405    0.5424E-18      58006.799    0.5441E-18      58007.193    0.5459E-18      5800
7.586    0.5477E-18      58007.980    0.5496E-18      58008.374    0.5519E-18      58008.768    0.5542
E-18      58009.162    0.5567E-18      58009.556    0.5593E-18      58009.950    0.5618E-18      58010.
344    0.5637E-18      58010.737    0.5653E-18      58011.131    0.5661E-18      58011.525    0.5661E-
18      58011.919    0.5653E-18      58012.313    0.5637E-18      58012.707    0.5618E-18      58013.10
1    0.5593E-18      58013.495    0.5564E-18      58013.889    0.5535E-18      58014.283    0.5507E-18
     58014.677    0.5480E-18      58015.071    0.5456E-18      58015.465    0.5436E-18      58015.859
    0.5416E-18      58016.253    0.5400E-18      58016.647    0.5388E-18      58017.041    0.5379E-18
    58017.435    0.5373E-18      58017.829    0.5372E-18      58018.223    0.5378E-18      58018.617
  0.5390E-18      58019.011    0.5409E-18      58019.405    0.5434E-18      58019.799    0.5462E-18
 58 020 .193    0.5493E-18      58020.587    0.5523E-18      58020.981    0.5545E-18      58021.375    0
.5559E-18      58021.769    0.5561E-18      58022.163    0.5554E-18      58022.557    0.5536E-18      5
8022.951    0.5511E-18      58023.345    0.5481E-18      58023.739    0.5452E-18      58024.133    0.5
425E-18      58024.527    0.5404E-18      58024.922    0.5387E-18      58025.316    0.5375E-18      580
25.710    0.5366E-18      58026.104    0.5359E-18      58026.498    0.5351E-18      58026.892    0.533
9E-18      58027.286    0.5327E-18      58027.680    0.5313E-18      58028.075    0.5298E-18      58028
.469    0.5283E-18      58028.863    0.5267E-18      58029.257    0.5252E-18      58029.651    0.5240E
-18      58030.045    0.5227E-18      58030.439    0.5212E-18      58030.834    0.5196E-18      58031.2
28    0.5176E-18      58031.622    0.5156E-18      58032.016    0.5132E-18      58032.410    0.5107E-1
8      58032.805    0.5081E-18      58033.199    0.5056E-18      58033.593    0.5034E-18      58033.987
    0.5013E-18      58034.381    0.4994E-18      58034.776    0.4973E-18      58035.170    0.4954E-18
    58 035 .564    0.4932E-18      58035.958    0.4905E-18      58036.353    0.4874E-18      58036.747
  0.4840E-18      58037.141    0.4801E-18      58037.535    0.4763E-18      58037.930    0.4724E-18
  58038.324    0.4689E-18

 TAPE NO.    1              FILE NO.   40
 RECORD   2                 LENGTH   2800
  58038.718    0.4659E-18      58039.113    0.4637E-18      58039.507    0.4621E-18      58039.901
0.4612E-18      58040.295    0.4607E-18      58040.690    0.4607E-18      58041.084    0.4609E-18
58041.478    0.4610E-18      58041.873    0.4609E-18      58042.267    0.4604E-18      58042.661    0.
4596E-18      58043.056    0.4582E-18      58043.450    0.4566E-18      58043.844    0.4547E-18      58
044.239    0.4526E-18      58044.633    0.4505E-18      58045.028    0.4487E-18      58045.422    0.44
74E-18      58045.816    0.4467E-18      58046.211    0.4465E-18      58046.605    0.4467E-18      5804
6.999    0.4476E-18      58047.394    0.4486E-18      58047.788    0.4498E-18      58048.183    0.4508
E-18      58048.577    0.4516E-18      58048.971    0.4517E-18      58049.366    0.4514E-18      58049.
760    0.4507E-18      58050.155    0.4493E-18      58050.549    0.4479E-18      58050.944    0.4465E-
18      58051.338    0.4453E-18      58051.733    0.4446E-18      58052.127    0.4441E-18      58052.52
2    0.4441E-18      58052.916    0.4446E-18      58053.310    0.4452E-18      58053.705    0.4458E-18
     58054.099    0.4461E-18      58054.494    0.4462E-18      58054.888    0.4462E-18      58055.283
    0.4459E-18      58055.677    0.4455E-18      58056.072    0.4447E-18      58056.467    0.4440E-18
    58056.861    0.4433E-18      58057.256    0.4430E-18      58057.650    0.4430E-18      58058.045
  0.4433E-18      58058.439    0.4443E-18      58058.834    0.4459E-18      58059.228    0.4483E-18
  58059.623    0.4510E-18      58060.017    0.4539E-18      58060.412    0.4569E-18      58060.807    0
.4597E-18      58061.201    0.4621E-18      58061.596    0.4640E-18      58061.990    0.4652E-18      5
8062.385    0.4659E-18      58062.780    0.4664E-18      58063.174    0.4668E-18      58063.569    0.4
674E-18      58063.964    0.4681E-18      58064.358    0.4690E-18      58064.753    0.4701E-18      580
65.147    0.4710E-18      58065.542    0.4714E-18      58065.937    0.4711E-18      58066.331    0.470
2E-18      58066.726    0.4686E-18      58067.121    0.4665E-18      58067.515    0.4640E-18      58067
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 73     0.4581E-18      58071.068      0.4584E-18      58071.462      0.4584E-18      58071.857      0.4578E-1
 8        58072.252      0.4567E-18      58072.647      0.4553E-18      58073.041      0.4535E-18      58073.436
      0.4514E-18      58073.831      0.4496E-18      58074.226      0.4479E-18      58074.620      0.4465E-18
       58075.015      0.4458E-18      58075.410      0.4455E-18      58075.805      0.4459E-18      58076.200
   0.4470E-18      58076.594      0.4483E-18      58076.989      0.4502E-18      58077.384      0.4521E-18
    58077.779      0.4539E-18

  TAPE NO.    1                FILE NO.    40
  RECORD    3                  LENGTH    2800
    58078.174      0.4554E-18      58078.568      0.4566E-18      58078.963      0.4572E-18      58079.358
 0.4572E-18      58079.753      0.4566E-18      58080.148      0.4553E-18      58080.543      0.4538E-18
 58080.937      0.4520E-18      58081.332      0.4499E-18      58081.727      0.4479E-18      58082.122      0.
 4461E-18      58082.517      0.4447E-18      58082.912      0.4439E-18      58083.307      0.4436E-18      58
 083.702      0.4437E-18      58084.097      0.4446E-18      58084.491      0.4461E-18      58084.886      0.44
 77E-18      58085.281      0.4493E-18      58085.676      0.4508E-18      58086.071      0.4523E-18      5808
 6.466      0.4533E-18      58086.861      0.4541E-18      58087.256      0.4542E-18      58087.651      0.4541
 E-18      58088.046      0.4538E-18      58088.441      0.4532E-18      58088.836      0.4523E-18      58089.
 231      0.4513E-18      58089.626      0.4502E-18      58090.021      0.4492E-18      58090.416      0.4481E-
 18      58090.811      0.4474E-18      58091.206      0.4470E-18      58091.601      0.4470E-18      58091.99
 6      0.4473E-18      58092.391      0.4479E-18      58092.786      0.4487E-18      58093.181      0.4498E-18
       58093.576      0.4508E-18      58093.971      0.4516E-18      58094.366      0.4523E-18      58094.761
      0.4527E-18      58095.156      0.4530E-18      58095.551      0.4532E-18      58095.946      0.4532E-18
      58096.341      0.4533E-18      58096.736      0.4535E-18      58097.131      0.4538E-18      58097.526
   0.4544E-18      58097.921      0.4550E-18      58098.317      0.4560E-18      58098.712      0.4575E-18
   58099.107      0.4593E-18      58099.502      0.4612E-18      58099.897      0.4634E-18      58100.292      0
 .4659E-18      58100.687      0.4684E-18      58101.082      0.4707E-18      58101.477      0.4726E-18      5
 8101.873      0.4741E-18      58102.268      0.4748E-18      58102.663      0.4750E-18      58103.058      0.4
 744E-18      58103.453      0.4730E-18      58103.848      0.4711E-18      58104.244      0.4690E-18      581
 04.639      0.4668E-18      58105.034      0.4647E-18      58105.429      0.4628E-18      58105.824      0.461
 5E-18      58106.219      0.4609E-18      58106.615      0.4609E-18      58107.010      0.4613E-18      58107
 .405      0.4622E-18      58107.800      0.4633E-18      58108.196      0.4646E-18      58108.591      0.4655E
 -18      58108.986      0.4659E-18      58109.381      0.4658E-18      58109.777      0.4653E-18      58110.1
 72      0.4644E-18      58110.567      0.4631E-18      58110.962      0.4616E-18      58111.358      0.4601E-1
 8      58111.753      0.4587E-18      58112.148      0.4573E-18      58112.543      0.4560E-18      58112.939
      0.4547E-18      58113.334      0.4532E-18      58113.729      0.4516E-18      58114.125      0.4498E-18
       58114.520      0.4479E-18      58114.915      0.4459E-18      58115.311      0.4443E-18      58115.706
   0.4428E-18      58116.101      0.4418E-18      58116.497      0.4412E-18      58116.892      0.4410E-18
    58117.287      0.4413E-18

  TAPE NO.    1                FILE NO.    40
  RECORD   10                  LENGTH    2800
    58355.870      0.4039E-18      58356.269      0.4071E-18      58356.668      0.4105E-18      58357.066
 0.4138E-18      58357.465      0.4167E-18      58357.863      0.4193E-18      58358.262      0.4213E-18
 58358.661      0.4228E-18      58359.059      0.4240E-18      58359.458      0.4247E-18      58359.857      0.
 4253E-18      58360.255      0.4259E-18      58360.654      0.4265E-18      58361.053      0.4271E-18      58
 361.451      0.4276E-18      58361.850      0.4277E-18      58362.249      0.4276E-18      58362.647      0.42
 71E-18      58363.046      0.4262E-18      58363.445      0.4247E-18      58363.844      0.4227E-18      5836
 4.242      0.4206E-18      58364.641      0.4185E-18      58365.040      0.4166E-18      58365.438      0.4150
 E-18      58365.837      0.4138E-18      58366.236      0.4133E-18      58366.635      0.4133E-18      58367.
 033      0.4141E-18      58367.432      0.4154E-18      58367.831      0.4170E-18      58368.230      0.4193E-
 18      58368.628      0.4216E-18      58369.027      0.4243E-18      58369.426      0.4270E-18      58369.82
 5      0.4292E-18      58370.224      0.4311E-18      58370.622      0.4326E-18      58371.021      0.4333E-18
       58371.420      0.4335E-18      58371.819      0.4330E-18      58372.218      0.4323E-18      58372.617
      0.4313E-18      58373.015      0.4302E-18      58373.414      0.4293E-18      58373.813      0.4286E-18
      58374.212      0.4280E-18      58374.611      0.4277E-18      58375.010      0.4274E-18      58375.409
   0.4273E-18      58375.807      0.4273E-18      58376.206      0.4273E-18      58376.605      0.4273E-18
   58377.004      0.4273E-18      58377.403      0.4274E-18      58377.802      0.4276E-18      58378.201      0
 .4276E-18      58378.600      0.4276E-18      58378.999      0.4274E-18      58379.398      0.4271E-18      5
 8379.796      0.4268E-18      58380.195      0.4268E-18      58380.594      0.4268E-18      58380.993      0.4
 274E-18      58381.392      0.4284E-18      58381.791      0.4299E-18      58382.190      0.4320E-18      583
 82.589      0.4341E-18      58382.988      0.4360E-18      58383.387      0.4376E-18      58383.786      0.438
 5E-18      58384.185      0.4387E-18      58384.584      0.4379E-18      58384.983      0.4363E-18      58385
 .382      0.4344E-18      58385.781      0.4323E-18      58386.180      0.4302E-18      58386.579      0.4284E
 -18      58386.978      0.4270E-18      58387.377      0.4261E-18      58387.776      0.4253E-18      58388.1
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      0.4181E-18     58391.368     0.4169E-18     58391.767     0.4161E-18     58392.166     0.4157E-18
       58392.565     0.4154E-18     58392.964     0.4151E-18     58393.363     0.4150E-18     58393.762
    0.4147E-18     58394.162     0.4142E-18     58394.561     0.4133E-18     58394.960     0.4121E-18
     58395.359     0.4105E-18

   TAPE NO.   1               FILE NO.   40
   RECORD   11                LENGTH   2800
    58395.758     0.4089E-18     58396.157     0.4071E-18     58396.556     0.4052E-18     58395.956
  0.4033E-18     58397.355     0.4015E-18     58397.754     0.3999E-18     58398.153     0.3982E-18
  58398.552     0.3969E-18     58398.952     0.3957E-18     58399.351     0.3947E-18     58399.750     0.
  3939E-18     58400.149     0.3935E-18     58400.548     0.3935E-18     58400.948     0.3938E-18      58
  401.347     0.3942E-18     58401.746     0.3948E-18     58402.145     0.3956E-18     58402.545     0.39
  59E-18     58402.944     0.3959E-18     58403.343     0.3954E-18     58403.742     0.3945E-18     5840
  4.142     0.3930E-18     58404.541     0.3910E-18     58404.940     0.3884E-18     58405.339     0.3856
  E-18     58405.739     0.3827E-18     58406.138     0.3796E-18     58406.537     0.3764E-18     58406.
  937     0.3733E-18     58407.336     0.3704E-18     58407.735     0.3680E-18     58408.134     0.3659E-
  18     58408.534     0.3646E-18     58408.933     0.3637E-18     58409.332     0.3636E-18     58409.73
  2     0.3640E-18     58410.131     0.3646E-18     58410.531     0.3653E-18     58410.930     0.3658E-18
        58411.329     0.3656E-18     58411.729     0.3647E-18     58412.128     0.3633E-18     58412.527
       0.3612E-18     58412.927     0.3587E-18     58413.326     0.3559E-18     58413.726     0.3532E-18
      58414.125     0.3510E-18     58414.524     0.3490E-18     58414.924     0.3477E-18     58415.323
   0.3467E-18     58415.723     0.3459E-18     58416.122     0.3455E-18     58416.521     0.3449E-18
   58416.921     0.3443E-18     58417.320     0.3436E-18     58417.720     0.3427E-18     58418.119     0
  .3421E-18     58418.519     0.3418E-18     58418.918     0.3418E-18     58419.318     0.3427E-18     5
  8419.717     0.3441E-18     58420.117     0.3465E-18     58420.516     0.3496E-18     58420.916     0.3
  530E-18     58421.315     0.3567E-18     58421.715     0.3601E-18     58422.114     0.3630E-18     584
  22.514     0.3649E-18     58422.913     0.3658E-18     58423.313     0.3655E-18     58423.712     0.364
  1E-18     58424.112     0.3621E-18     58424.511     0.3596E-18     58424.911     0.3569E-18     58425
  .310     0.3544E-18     58425.710     0.3523E-18     58426.109     0.3508E-18     58426.509     0.3501E
  -18     58426.909     0.3499E-18     58427.308     0.3501E-18     58427.708     0.3507E-18     58428.1
  07     0.3514E-18     58428.507     0.3521E-18     58428.907     0.3529E-18     58429.306     0.3535E-1
  8     58429.706     0.3541E-18     58430.105     0.3550E-18     58430.505     0.3559E-18     58430.905
      0.3570E-18     58431.304     0.3585E-18     58431.704     0.3604E-18     58432.104     0.3627E-18
       58432.503     0.3652E-18     58432.903     0.3679E-18     58433.303     0.3707E-18     58433.702
    0.3735E-18     58434.102     0.3760E-18     58434.502     0.3782E-18     58434.901     0.3800E-18
     58435.301     0.3813E-18

   TAPE NO.   1               FILE NO.   40
   RECORD   12                LENGTH   1204
    58435.701     0.3824E-18     58436.100     0.3828E-18     58436.500     0.3831E-18     58436.900
  0.3830E-18     58437.299     0.3827E-18     58437.699     0.3822E-18     58438.099     0.3818E-18
  58438.499     0.3812E-18     58438.898     0.3804E-18     58439.298     0.3797E-18     58439.698     0.
  3788E-18     58440.098     0.3779E-18     58440.497     0.3772E-18     58440.897     0.3766E-18      58
  441.297     0.3761E-18     58441.697     0.3761E-18     58442.096     0.3764E-18     58442.496     0.37
  70E-18     58442.896     0.3781E-18     58443.296     0.3793E-18     58443.696     0.3806E-18     5844
  4.095     0.3819E-18     58444.495     0.3833E-18     58444.895     0.3844E-18     58445.295     0.3855
  E-18     58445.695     0.3865E-18     58446.095     0.3876E-18     58446.494     0.3889E-18     58446.
  894     0.3904E-18     58447.294     0.3920E-18     58447.694     0.3936E-18     58448.094     0.3953E-
  18     58448.494     0.3967E-18     58448.894     0.3979E-18     58449.294     0.3988E-18     58449.69
  3     0.3991E-18     58450.093     0.3991E-18     58450.493     0.3988E-18     58450.893     0.3984E-18
        58451.293     0.3978E-18     58451.693     0.3972E-18     58452.093     0.3967E-18     58452.493
      0.3964E-18

  ***** JOB DONE.
  $EXEC TPDUMP BS
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 $NOP
 $NOP ************** SOUT40 ************
 $EXE TPLIST BS

 INPUT PARAMETERS ARE:  AS FL=2=2 23 1 1

  TAPE NO.   1                FILE NO.   1
  RECCRC   1                  LENGTH   1200
 HIGH RESOLUTION ABSORP- TICN CROSS-SECTIONS AND BAND OSCILLATOR STRENGTHOF THE SCHUMANN-RUNGE   BAN
 DS OF OXYGEN AT 79 K K. Yoshino, D.E.Freeman,J.R.Esmond and W.H.       Parkinson -- Harvard-   Smiths
 onian Center for  Astrophysics, Cambridge,MA 02138, U.S.A.         (Received 11 March 1987)Abstract-
 Cross-sectiors cf C2 at 79K have been  cbtainec from photo-    absorption measurements at various p
 ressures    throughout the wave-    length region 179.3-    198.0 nm with a 6.65 m  photoelectric s
 canning  spectrometer equipped   with a 2400 lines/nm    grating and having an   instrumental width
 (FWHM)of 0.0013 nm.  The meas-ured absorption cross-  sections of the Schumann-Rurge bancs (12,0)-
    (2,0) are incepercent ofthe instrurertal wicth. The measured cross-     secticrs are preserted
 graphically here and areavailable at wavenumber intervals of ~0.1 wave- numbers as numerical    com
 pilations stored on  magnetic tape from the  National Space Science  Data Center, NASA/     Goddar
 d Space Flight    Center, Greenbelt, MD   20771, U.S.A.  Band      oscillator strengths of these ban
 ds have been   ceterrined by direct    rumerical integration ofthe measured cross-     sections.


  TAPE NO.   1                FILE NO.   2
  RECCRD   1                  LENGTH   2400
 -1        1602;B2-X0;79K         WNO            SIGMA  50530.077    1.0410E-23 50530.136    1.2570E-23 50
 530.194    1.5470E-23 50530.253    1.4730E-23 50530.312    1.1100E-23 50530.371    1.1810E-23 50530
 .430    8.9100E-24 50530.489    3.1420E-24 50530.548    4.5690E-24 50530.607    1.3220E-23 50530.66
 5    1.6840E-23 50530.724    1.3930E-23 50530.783    1.6100E-23 50530.842    1.7540E-23 50530.901
   1.6080E-23 50530.960    1.6790E-23 50531.019    1.7510E-23 50531.078    2.2610E-23 50531.136    2
 .8470E-23 50531.195    3.1400E-23 50531.254    2.8450E-23 50531.313    2.1110E-23 50531.372    1.23
 70E-23 50531.431    2.9870E-24 50531.490    1.5420E-24 50531.549    3.6850E-24 50531.607    2.9570E
 -24 50531.666    5.1030E-24 50531.725    9.4150E-24 50531.784    1.8840E-23 50531.843    2.3950E-23
  50531.902    2.1010E-23 50531.961    1.6630E-23 50532.020    7.9270E-24 50532.079    1.4450E-24 50
 532.137    7.5070E-24 50532.196    1.2960E-23 50532.255    1.2220E-23 50532.314    7.1570E-24 50532
 .373    3.5490E-24 50532.432    2.8220E-24 50532.491    6.6070E-25 50532.550    1.3680E-24 50532.60
 8    1.3580E-24 50532.667    2.6316E-23 50532.726    2.5592E-23 50532.785    2.5582E-23 50532.844
   2.2006E-23 50532.903    2.2709E-23 50532.962    2.3412E-23 50533.021    2.7688E-23 50533.079    4
 .8710E-24 50533.138    4.8610E-24 50533.197    6.2910E-24 50533.256    6.2810E-24 50533.315    2.67
 60E-24 50533.374    2.7630E-23 50533.433    1.9390E-24 50533.492    8.4060E-24 50533.551    8.3960E
 -24 50533.609    6.2230E-24 50533.668    1.1270E-23 50533.727    1.4880E-23 50533.786    1.6330E-23
  50533.845    1.4860E-23 50533.904    9.0600E-24 50533.963    3.2880E-24 50534.022    2.6808E-23 50
 534.081    2.4654E-23 50534.139    2.6788E-23 50534.198    3.9670E-24 50534.257    7.5580E-24 50534
 .316    1.6240E-23 50534.375    1.4780E-23 50534.434    8.2500E-24 50534.493    6.0780E-24 50534.55
 2    2.6721E-23 50534.610    1.8872E-23 50534.669    1.5321E-23 50534.728    1.6021E-23 50534.787
   1.6711E-23 50534.846    1.6701E-23 50534.905    2.0955E-23 50534.964    2.3082E-23 50535.023    2
 .5213E-23 50535. 82    5.9810E-24 50535.140    1.1030E-23 50535.199    7.4030E-24 50535.258    9.55
 90E-24 50535.317    1.3900E-23 50535.376    1.2440E-23 50535.435    7.3640E-24 50535.494    2.3170E
 -24 50535.553    2.5126E-23 50535.612    2.1550E-23 50535.670    1.5861E-23 50535.729    1.0201E-23
  50535.788    7.3810E-24

  TAPE NO.   1                FILE NO.   2
  RECORD   2                  LENGTH   2400
  50535.847    1.0181E-23 50535.906    1.2591E-23 50535.965    1.6521E-23 50536.024    2.2507E-23 50
 536.083    2.2200E-24 50536.142    6.5260E-24 50536.200    9.4040E-24 50536.259    2.9090E-24 50536
 .318    1.7171E-23 50536.377    9.3910E-24 50536.436    1.2201E-23 50536.495    2.1405E-23 50536.55
 4    5.7380E-24 50536.613    1.3680E-23 50536.672    1.4400E-23 50536.731    1.0760E-23 50536.789
   3.5400E-24 50536.848    1.9924E-23 50536.907    1.5661E-23 50536.966    1.7061E-23 50537.025    2
 .3456E-23 50537. 84    2.4874E-23 50537.143    2.7009E-23 50537.202    2.5569E-23 50537.261    2.12
 79E-23 50537.319    2.3407E-23 50537.378    2.4111E-23 50537.437    2.0538E-23 50537.496    2.4092E
 -23 50537.555    2.6226E-23 50537.614    2.7648E-23 50537.673    1.9788E-23 50537.732    1.7651E-23
  50537.791    1.8348E-23 50537.850    2.7609E-23 50537.908    1.2020E-23 50537.967    2.1470E-23 50
 538.026    2.6600E-23 50538.085    1.9260E-23 50538.144    7.6390E-24 50538.203    2.4689E-23 50538
 .262    1.8980E-23 50538.321    2.0392E-23 50538.380    2.4660E-23 50538.438    3.9880E-24 50538.49
 7    1.0470E-23 50538.556    8.2930E-24 50538.615    7.5610E-24 50538.674    1.7930E-[illegible] 50538.733
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GX-11C
Schumann-Range
Band & O2 at 79K
D 76163
23F

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71E-23 50539.263    6.7330E-24 50539.322    1.4690E-23 50539.381    1.6130E-23 50539.440    1.7580E
-23 50539.499    1.1030E-23 50539.558    3.0840E-24 50539.616    2.5171E-23 50539.675    2.3732E-23
 50539.734    2.4437E-23 50539.793    2.7289E-23 50539.852    8.0800E-24 50539.911    2.1150E-23 50
539.970    2.7010E-23 50540.029    2.6270E-23 50540.088    1.4560E-23 50540.147    1.1580E-25 50540
.205    2.4359E-23 50540.264    2.5779E-23 50540.323    2.7201E-23 50540.382    2.2189E-23 50540.44
1    2.0043E-23 50540.500    2.4311E-23 50540.559    2.6446E-23 50540.618    2.5721E-23 50540.677
  2.4281E-23 50540.736    2.2844E-23 50540.795    2.0696E-23 50540.853    2.1399E-23 50540.912    1
.9965E-23 50540.971    2.0667E-23 50541.030    2.7801E-23 50541.089    7.8760E-24 50541.148    1.00
40E-23 50541.207    8.5790E-24 50541.266    7.8470E-24 50541.325    5.6720E-24 50541.384    4.2220E
-24 50541.443    6.1930E-25 50541.501    2.1292E-23 50541.560    1.9858E-23 50541.619    2.1985E-23
 50541.678    2.2689E-23

 TAPE NO.   1               FILE NO.   2
 RECORD   38                LENGTH   2400
 50748.966    2.5100E-24 50749.026    2.5143E-23 50749.085    1.9970E-23 50749.145    1.9960E-23 50
749.204    2.3630E-23 50749.264    2.7323E-23 50749.323    3.1930E-24 50749.383    4.6710E-24 50749
.442    2.7293E-23 50749.502    2.0636E-23 50749.561    1.8420E-23 50749.621    1.9880E-23 50749.68
0    1.9870E-23 50749.740    1.9125E-23 50749.799    1.6181E-23 50749.859    2.2787E-23 50749.918
  6.8160E-24 50749.978    1.2040E-23 50750.037    1.4290E-23 50750.097    1.0520E-23 50750.156    5
.2850E-24 50750.216    9.7550E-24 50750.275    1.6500E-23 50750.335    1.9510E-23 50750.394    2.25
30E-23 50750.454    2.7070E-23 50750.514    3.4700E-23 50750.573    3.6220E-23 50750.633    2.7040E
-23 50750.692    9.6750E-24 50750.752    2.9520E-24 50750.811    2.4102E-23 50750.871    2.0405E-23
 50750.930    2.4082E-23 50750.990    2.3334E-23 50751.049    2.6281E-23 50751.109    8.8570E-24 50
751.168    1.5600E-23 50751.228    1.9360E-23 50751.287    2.1620E-23 50751.347    2.3120E-23 50751
.406    1.8570E-23 50751.466    1.4040E-23 50751.525    1.1030E-23 50751.585    8.0290E-24 50751.64
4    2.0580E-24 50751.704    2.1738E-23 50751.763    1.9518E-23 50751.823    1.7301E-23 50751.882
  2.0234E-23 50751.942    1.7281E-23 50752.001    7.0510E-24 50752.061    1.2141E-23 50752.120    2
.0194E-23 50752.180    2.0184E-23 50752.240    1.5031E-23 50752.299    1.6491E-23 50752.359    2.38
41E-23 50752.418    4.4210E-25 50752.478    5.6390E-24 50752.537    5.6290E-24 50752.597    5.6190E
-24 50752.656    5.6080E-24 50752.716    6.3440E-24 50752.775    1.0820E-23 50752.835    1.3060E-23
 50752.894    1.6060E-23 50752.954    1.9070E-23 50753.013    1.8300E-23 50753.073    1.3020E-23 50
753.132    4.7830E-24 50753.192    2.1487E-23 50753.251    1.7061E-23 50753.311    2.1466E-23 50753
.370    2.2194E-23 50753.430    1.8502E-23 50753.489    1.2631E-23 50753.549    1.1161E-23 50753.60
9    1.6271E-23 50753.668    2.2882E-23 50753.728    2.5829E-23 50753.787    2.1100E-25 50753.847
  3.1730E-24 50753.906    1.9090E-25 50753.966    2.3570E-23 50754.025    1.7080E-25 50754.085    4
.6220E-24 50754.144    1.6360E-24 50754.204    8.8290E-25 50754.263    8.7280E-25 50754.323    2.42
49E-23 50754.382    1.3941E-23 50754.442    7.3610E-24 50754.501    7.3510E-24 50754.561    8.0710E
-24 50754.620    9.5210E-24 50754.680    1.3161E-23 50754.740    1.9016E-23 50754.799    1.8271E-23
 50754.859    1.0201E-23

 TAPE NO.   1               FILE NO.   2
 RECORD   39                LENGTH   72
 50754.918    4.3810E-24 50754.978    7.5100E-25 50755.039    1.1000E-26

 TAPE NO.   1               FILE NO.   3
 RECORD   1                 LENGTH   2400
-1  16C2;B3-X0;79K          WNO          SIGMA  51150.080    3.0080E-23 51150.140    2.5754E-23 51
150.201    2.1451E-23 51150.261    2.3591E-23 51150.322    1.7861E-23 51150.383    1.2881E-23 51150
.443    2.1421E-23 51150.504    3.2208E-23 51150.564    1.2630E-24 51150.625    3.4360E-24 51150.68
5    5.6140E-24 51150.746    5.6090E-24 51150.806    5.1610E-25 51150.867    3.0009E-23 51150.928
  2.9282E-23 51150.988    2.8556E-23 51151.049    2.5673E-23 51151.109    2.4949E-23 51151.170    3
.1426E-23 51151.230    3.4314E-23 51151.291    3.4309E-23 51151.351    4.6710E-25 51151.412    2.85
18E-23 51151.472    2.9233E-23 51151.533    3.3563E-23 51151.594    4.0770E-24 51151.654    6.2560E
-24 51151.715    5.5220E-24 51151.775    1.8800E-24 51151.836    3.2812E-23 51151.896    3.2806E-23
 51151.957    3.2078E-23 51152.017    2.7024E-23 51152.078    2.3431E-23 51152.139    1.8411E-23 51
152.199    1.9841E-23 51152.260    1.7691E-23 51152.320    2.4121E-23 51152.381    3.3487E-23 51152
.441    3.3481E-23 51152.502    3.6360E-25 51152.562    4.7170E-24 51152.623    7.6280E-24 51152.68
4    6.1630E-24 51152.744    8.3470E-24 51152.805    5.4240E-24 51152.865    1.0560E-24 51152.926
  2.6942E-23 51152.986    1.9051E-23 51153.047    1.9761E-23 51153.107    2.5488E-23 51153.168    2
.9802E-23 51153.229    3.1963E-23 51153.289    3.0513E-23 51153.350    3.1230E-23 51153.410    2.61
79E-23 51153.471    2.8333E-23 51153.531    3.1213E-23 51153.592    2.6560E-25 51153.652    8.2660E
-24 51153.713    1.7060E-23 51153.774    1.4850E-23 51153.834    1.1910E-23 51153.895    8.2440E-24
 51153.955    9.5810E-25 51154.016    3.0448E-23 51154.076    2.9720E-23 51154.137    6.7620E-24 51
154.197    2.1450E-23 51154.258    3.1850E-23 51154.319    3.4090E-23 51154.379    3.3340E-23 51154
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  3.3258E-23 51154.985     1.4030E-25 51155.045     2.6751E-23 51155.106     2.7466E-23 51155.166     1
 .2390E-25 51155.227     7.3940E-24 51155.288     5.9290E-24 51155.348     3.3944E-23 51155.409     8.27
 40E-25 51155.469     4.4560E-24 51155.53      6.6370E-24 51155.590     3.7170E-24 51155.651     1.5310E
 -24 51155.711     5.1620E-24 51155.772     1.2470E-23 51155.833     1.0260E-23 51155.893     7.3340E-24
  51155.954     5.8690E-24

  TAPE NO.    1                 FILE NO.    3
  RECORD    2                   LENGTH    2400
  51156.014     1.4650E-23 51156.075     1.6110E-23 51156.135     1.0240E-23 51156.196     3.6630E-24 51
 156.257     2.2030E-24 51156.317     3.3857E-23 51156.378     3.0235E-23 51156.438     3.0230E-23 51156
 .499     2.1810E-24 51156.559     9.4660E-24 51156.620     1.1660E-23 51156.680     1.5320E-23 51156.74
 1     2.3440E-23 51156.802     2.5660E-23 51156.862     2.7150E-23 51156.923     2.2690E-23 51156.983
   1.3090E-23 51157.044     4.3140E-24 51157.104     2.1270E-24 51157.165     1.3950E-24 51157.226     3
 .3775E-23 51157.286     2.8710E-23 51157.347     2.7984E-23 51157.407     3.0865E-23 51157.468     1.36
 80E-24 51157.528     8.6480E-24 51157.589     9.3730E-24 51157.650     9.3680E-24 51157.710     7.9000E
 -24 51157.771     3.5210E-24 51157.831     3.1549E-23 51157.892     2.9377E-23 51157.952     2.9372E-23
  51158.013     2.6484E-23 51158.073     3.2974E-23 51158.134     7.1320E-24 51158.195     1.1520E-23 51
 158.255     1.0780E-23 51158.316     1.0040E-23 51158.376     1.2230E-23 51158.437     1.0030E-23 51158
 .497     4.9110E-24 51158.558     5.4400E-25 51158.619     3.4450E-24 51158.679     5.6240E-24 51158.74
 0     1.0730E-23 51158.800     1.5130E-23 51158.861     8.5280E-24 51158.921     3.4170E-24 51158.982
   1.9580E-24 51159.043     3.4336E-23 51159.103     3.0712E-23 51159.164     2.9263E-23 51159.224     3
 .2871E-23 51159.285     3.4314E-23 51159.345     2.9246E-23 51159.406     2.9963E-23 51159.467     3.21
 25E-23 51159.527     3.2844E-23 51159.588     5.5420E-24 51159.648     5.1880E-24 51159.709     9.9150E
 -24 51159.769     9.1770E-24 51159.830     5.5200E-24 51159.891     3.0641E-23 51159.951     2.0571E-23
  51160.012     1.8421E-23 51160.072     1.6271E-23 51160.133     1.2711E-23 51160.193     1.2701E-23 51
 160.254     1.4831E-23 51160.315     1.7681E-23 51160.375     2.5552E-23 51160.436     2.7706E-23 51160
 .496     2.5542E-23 51160.557     2.6255E-23 51160.617     2.6250E-23 51160.678     2.6964E-23 51160.73
 9     2.9121E-23 51160.799     3.0559E-23 51160.860     3.1277E-23 51160.920     2.7663E-23 51160.981
   2.6217E-23 51161.041     1.9761E-23 51161.102     1.5471E-23 51161.163     1.4751E-23 51161.223     1
 .1901E-23 51161.284     1.0481E-23 51161.344     1.0471E-23 51161.405     1.1181E-23 51161.465     1.75
 71E-23 51161.526     2.5449E-23 51161.587     2.6163E-23 51161.647     2.6157E-23 51161.708     2.2561E
 -23 51161.768     2.1121E-23 51161.829     2.3981E-23 51161.889     2.7575E-23 51161.950     3.0456E-23
  51162.011     2.8285E-23

  TAPE NO.    1                 FILE NO.    3
  RECORD    44                  LENGTH    2400
  51411.410     1.9830E-23 51411.471     2.4360E-23 51411.532     3.2740E-23 51411.593     3.1970E-23 51
 411.654     1.8300E-23 51411.715     1.0840E-24 51411.776     3.4157E-23 51411.837     1.8150E-24 51411
 .898     4.7840E-24 51411.959     4.0340E-24 51412.021     7.7550E-24 51412.082     4.0230E-24 51412.14
 3     3.2730E-24 51412.204     3.2680E-24 51412.265     3.2620E-24 51412.326     1.0280E-24 51412.387
   2.5080E-24 51412.448     5.4780E-24 51412.509     5.4730E-24 51412.570     3.9780E-24 51412.631     5
 .4620E-24 51412.692     3.3333E-23 51412.753     9.8950E-25 51412.814     1.7260E-24 51412.875     2.81
 46E-23 51412.936     2.4461E-23 51412.997     1.8601E-23 51413.059     2.3721E-23 51413.120     2.2981E
 -23 51413.181     2.4441E-23 51413.242     2.5170E-23 51413.303     2.5164E-23 51413.364     2.5159E-23
  51413.425     2.2221E-23 51413.486     2.2211E-23 51413.547     2.3671E-23 51413.608     2.7343E-23 51
 413.669     1.6480E-24 51413.730     1.1340E-23 51413.791     2.2640E-23 51413.852     2.7950E-23 51413
 .913     2.8700E-23 51413.974     2.3380E-23 51414.035     8.3180E-24 51414.097     2.8035E-23 51414.15
 8     2.5086E-23 51414.219     2.7287E-23 51414.280     3.0780E-24 51414.341     9.7860E-24 51414.402
   1.4280E-23 51414.463     1.2020E-23 51414.524     6.7800E-24 51414.585     6.7750E-24 51414.646     1
 .0510E-23 51414.707     9.7530E-24 51414.768     9.7470E-24 51414.829     1.1240E-23 51414.890     1.34
 80E-23 51414.951     1.2730E-23 51415.012     1.5730E-23 51415.074     1.1970E-23 51415.135     4.4880E
 -24 51415.196     3.1624E-23 51415.257     2.6456E-23 51415.318     2.6451E-23 51415.379     2.4975E-23
  51415.440     2.7176E-23 51415.501     2.9381E-23 51415.562     2.9375E-23 51415.623     3.0846E-23 51
 415.684     3.1580E-23 51415.745     3.4576E-23 51415.806     3.6830E-24 51415.867     3.6770E-24 51415
 .928     1.4420E-24 51415.990     3.1552E-23 51416.051     2.1981E-23 51416.112     1.6861E-23 51416.17
 3     1.3941E-23 51416.234     1.8301E-23 51416.295     2.6362E-23 51416.356     3.1519E-23 51416.417
   2.9297E-23 51416.478     2.4141E-23 51416.539     2.1931E-23 51416.600     2.1201E-23 51416.661     2
 .2661E-23 51416.722     2.8532E-23 51416.783     3.1480E-23 51416.844     3.3694E-23 51416.905     3.07
 29E-23 51416.967     2.5565E-23 51417.028     2.2621E-23 51417.089     2.6289E-23 51417.150     1.3300E
 -24 51417.211     9.5240E-24 51417.272     1.1770E-23 51417.333     8.7650E-24 51417.394     6.5180E-24
  51417.455     6.5130E-24

  TAPE NO.    1                 FILE NO.    3
  RECORD    45                  LENGTH    816
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-22 55493.227    8.9880E-22 55493.298    9.1550E-22 55493.370    9.2380E-22 55493.442    9.0270E-22
 55493.513    9.0260E-22 55493.585    9.3620E-22 55493.656    9.5730E-22 55493.728    9.7000E-22 55
493.800    9.6560E-22 55493.871    8.9800E-22 55493.943    8.6870E-22 55494.014    8.6030E-22 55494
.086    8.8930E-22 55494.157    9.5240E-22 55494.229    9.8220E-22 55494.301    9.9920E-22 55494.37
2    1.0290E-21 55494.444    1.0470E-21 55494.515    1.0380E-21 55494.587    1.0420E-21 55494.659
  1.0770E-21 55494.730    1.0990E-21 55494.802    1.1120E-21 55494.873    1.1070E-21 55494.945    1
.1380E-21 55495.017    1.2140E-21 55495.088    1.2870E-21 55495.160    1.3850E-21 55495.231    1.48
10E-21 55495.303    1.5880E-21 55495.374    1.7040E-21 55495.446    1.8550E-21 55495.518    2.0160E
-21 55495.589    2.1450E-21 55495.661    2.2080E-21 55495.732    2.2540E-21 55495.804    2.2780E-21
 55495.876    2.2250E-21 55495.947    2.1500E-21 55496.019    2.0490E-21 55496.090    1.9290E-21 55
496.162    1.8550E-21 55496.234    1.7960E-21 55496.305    1.7750E-21 55496.377    1.7900E-21 55496
.448    1.8060E-21 55496.520    1.8110E-21 55496.592    1.8210E-21 55496.663    1.8580E-21 55496.73
5    1.9060E-21 55496.806    1.9660E-21 55496.878    2.0480E-21 55496.950    2.1210E-21 55497.021
  2.2060E-21 55497.093    2.2880E-21 55497.164    2.3410E-21 55497.236    2.3590E-21 55497.308    2
.3890E-21 55497.379    2.4250E-21 55497.451    2.4310E-21 55497.522    2.3710E-21 55497.594    2.29
90E-21 55497.666    2.2340E-21 55497.737    2.1820E-21 55497.809    2.1650E-21 55497.880    2.1200E
-21 55497.952    2.0580E-21 55498.023    1.9750E-21 55498.095    1.8560E-21 55498.167    1.7520E-21
 55498.238    1.6700E-21

 TAPE NO.   1               FILE NO.   22
 RECORD   50                LENGTH   576
 55498.310    1.5600E-21 55498.381    1.4330E-21 55498.453    1.2920E-21 55498.525    1.1870E-21 55
498.596    1.1470E-21 55498.668    1.1330E-21 55498.739    1.1160E-21 55498.811    1.0670E-21 55498
.883    1.0060E-21 55498.954    9.8470E-22 55499.026    9.6320E-22 55499.098    9.2070E-22 55499.16
9    8.9540E-22 55499.241    8.7020E-22 55499.312    8.7840E-22 55499.384    8.9090E-22 55499.456
  8.8660E-22 55499.527    8.5730E-22 55499.599    8.3650E-22 55499.670    8.0760E-22 55499.742    7
.9110E-22 55499.814    7.9510E-22 55499.885    7.9090E-22 55499.957    8.0310E-22

 TAPE NO.   1               FILE NO.   23
 RECORD   1                 LENGTH   2400
-1  1602;B12-X0;79K         WNO          SIGMA  55537.118    1.0990E-21 55537.190    1.0370E-21 55
537.262    9.5210E-22 55537.333    8.7380E-22 55537.405    8.1400E-22 55537.477    8.1390E-22 55537
.549    8.1970E-22 55537.620    8.3740E-22 55537.692    8.3730E-22 55537.764    7.8970E-22 55537.83
6    7.2480E-22 55537.907    6.0840E-22 55537.979    5.0530E-22 55538.051    4.3740E-22 55538.123
  3.9800E-22 55538.194    4.0340E-22 55538.266    4.1450E-22 55538.338    3.6410E-22 55538.410    3
.0290E-22 55538.482    2.8630E-22 55538.553    2.8610E-22 55538.625    2.5300E-22 55538.697    2.42
00E-22 55538.769    2.4180E-22 55538.840    2.2530E-22 55538.912    2.0340E-22 55538.984    2.3050E
-22 55539.056    2.7420E-22 55539.127    2.6310E-22 55539.199    2.5200E-22 55539.271    2.3000E-22
 55539.343    2.0800E-22 55539.415    2.6810E-22 55539.486    3.3970E-22 55539.558    3.6740E-22 55
539.630    3.4500E-22 55539.702    3.0610E-22 55539.773    3.0600E-22 55539.845    3.3910E-22 55539
.917    3.2780E-22 55539.989    3.1660E-22 55540.060    2.6690E-22 55540.132    2.2840E-22 55540.20
4    2.5010E-22 55540.276    2.6100E-22 55540.348    2.8280E-22 55540.419    2.8820E-22 55540.491
  2.6610E-22 55540.563    2.3850E-22 55540.635    2.3290E-22 55540.706    2.0550E-22 55540.778    2
.0540E-22 55540.850    2.2160E-22 55540.922    2.0510E-22 55540.994    2.1590E-22 55541.065    2.21
20E-22 55541.137    2.2110E-22 55541.209    1.7740E-22 55541.281    1.3940E-22 55541.352    1.2840E
-22 55541.424    1.5530E-22 55541.496    1.9310E-22 55541.568    2.6410E-22 55541.639    3.1360E-22
 55541.711    3.1900E-22 55541.783    2.8570E-22 55541.855    2.5810E-22 55541.927    2.6340E-22 55
541.998    2.8530E-22 55542.070    3.1830E-22 55542.142    2.9060E-22 55542.214    2.6840E-22 55542
.285    2.6280E-22 55542.357    2.2430E-22 55542.429    1.6970E-22 55542.501    1.2630E-22 55542.57
3    7.2500E-23 55542.644    2.9710E-23 55542.716    3.0450E-24 55542.788    8.2110E-24 55542.860
  3.9950E-23 55542.931    9.8630E-23 55543.003    1.6860E-22 55543.075    2.2290E-22 55543.147    2
.4470E-22 55543.219    2.3360E-22 55543.290    2.1710E-22 55543.362    1.9510E-22 55543.434    1.84
10E-22 55543.506    1.7310E-22 55543.578    1.2430E-22 55543.649    9.7310E-23 55543.721    1.1870E
-22 55543.793    1.3470E-22 55543.865    1.6710E-22 55543.936    1.9410E-22 55544.008    1.7220E-22
 55544.080    1.3420E-22

 TAPE NO.   1               FILE NO.   23
 RECORD   2                 LENGTH   2400
 55544.152    1.5030E-22 55544.224    1.6100E-22 55544.295    1.6080E-22 55544.367    1.8790E-22 55
544.439    2.2590E-22 55544.511    2.4770E-22 55544.582    1.9830E-22 55544.654    1.7100E-22 55544
.726    1.8720E-22 55544.798    2.0340E-22 55544.870    2.6900E-22 55544.941    3.2410E-22 55545.01
3    2.7420E-22 55545.085    2.1920E-22 55545.157    2.3000E-22 55545.229    2.2440E-22 55545.300
  2.0250E-22 55545.372    1.4800E-22 55545.444    7.7910E-23 55545.516    1.3790E-23 55545.587    4
.2191E-23 55545.659    3.6771E-23 55545.731    1.3390E-23 55545.803    6.6540E-23 55545.875    9.85
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 55546.521    9.7380E-23 55546.592    8.1150E-23 55546.664    8.1020E-23 55546.736    9.6990E-23 55
546.808    1.1300E-22 55546.880    1.3440E-22 55546.951    1.1810E-22 55547.023    1.0720E-22 55547
.095    1.0170E-22 55547.167    1.3390E-22 55547.239    1.6630E-22 55547.310    1.6610E-22 55547.38
2    1.8770E-22 55547.454    2.0940E-22 55547.526    2.4760E-22 55547.598    2.4750E-22 55547.669
  2.4180E-22 55547.741    2.2530E-22 55547.813    1.6520E-22 55547.885    1.3800E-22 55547.957    1
.5950E-22 55548.028    1.8650E-22 55548.100    2.0820E-22 55548.172    2.2450E-22 55548.244    2.73
80E-22 55548.316    3.2900E-22 55548.387    3.6780E-22 55548.459    3.6210E-22 55548.531    3.7880E
-22 55548.603    4.0670E-22 55548.674    4.1210E-22 55548.746    3.9520E-22 55548.818    4.0630E-22
 55548.890    3.7250E-22 55548.962    3.2220E-22 55549.033    2.9440E-22 55549.105    2.5020E-22 55
549.177    2.0620E-22 55549.249    2.1160E-22 55549.321    2.3880E-22 55549.392    2.8270E-22 55549
.464    3.2690E-22 55549.536    3.3780E-22 55549.608    3.6000E-22 55549.680    3.8780E-22 55549.75
1    3.8210E-22 55549.823    3.4850E-22 55549.895    3.5390E-22 55549.967    3.9290E-22 55550.039
  3.5360E-22 55550.110    3.1460E-22 55550.182    3.3110E-22 55550.254    3.3650E-22 55550.326    2
.5200E-22 55550.398    2.3680E-22 55550.469    2.0380E-22 55550.541    1.7650E-22 55550.613    1.65
50E-22 55550.685    1.8160E-22 55550.757    2.3070E-22 55550.828    2.9660E-22 55550.900    3.0760E
-22 55550.972    3.0740E-22 55551.044    2.8520E-22 55551.116    2.8500E-22 55551.187    2.5180E-22
 55551.259    2.2430E-22

 TAPE NO.    1                FILE NO.    23
 RECORD    44                 LENGTH    24
 55847.491    1.1190E-21 55847.564    1.2490E-21 55847.636    1.5140E-21 55847.709    1.8270E-21 55
847.782    2.2970E-21 55847.854    2.9560E-21 55847.927    3.6730E-21 55848.000    4.4170E-21 55848
.072    5.7190E-21 55848.145    6.5880E-21 55848.218    7.1500E-21 55848.290    7.3950E-21 55848.36
3    7.1340E-21 55848.436    6.4690E-21 55848.508    5.6530E-21 55848.581    4.8360E-21 55848.654
  3.3130E-21 55848.726    2.8500E-21 55848.799    2.5050E-21 55848.872    2.2080E-21 55848.944    1
.9300E-21 55849.017    1.6700E-21 55849.090    1.5330E-21 55849.162    1.5330E-21 55849.235    1.59
00E-21 55849.308    1.7500E-21 55849.380    2.0130E-21 55849.453    2.3260E-21 55849.526    2.7460E
-21 55849.598    3.2560E-21 55849.671    3.8160E-21 55849.744    5.0620E-21 55849.816    6.1980E-21
 55849.889    7.4080E-21 55849.962    8.4600E-21 55850.034    9.1130E-21 55850.107    9.3590E-21 55
850.180    9.3770E-21 55850.252    9.2230E-21 55850.325    8.9510E-21 55850.398    8.8340E-21 55850
.471    8.9680E-21 55850.543    9.2100E-21 55850.616    9.4610E-21 55850.688    9.5500E-21 55850.76
1    9.3410E-21 55850.834    8.9330E-21 55850.906    8.3070E-21 55850.979    7.4460E-21 55851.052
  6.4880E-21 55851.124    5.5510E-21 55851.197    4.1680E-21 55851.270    3.4850E-21 55851.343    2
.9840E-21 55851.415    2.5740E-21 55851.488    2.2820E-21 55851.561    2.0240E-21 55851.633    1.81
20E-21 55851.706    1.5780E-21 55851.779    1.4070E-21 55851.851    1.3230E-21 55851.924    1.2470E
-21 55851.997    1.1850E-21 55852.069    1.1040E-21 55852.142    1.0770E-21 55852.215    1.0370E-21
 55852.287    9.8330E-22 55852.360    9.5670E-22 55852.433    9.1710E-22 55852.505    8.4520E-22 55
852.578    7.3560E-22 55852.651    6.0250E-22 55852.723    5.7730E-22 55852.796    6.1480E-22 55852
.869    6.7770E-22 55852.941    7.0300E-22 55853.014    7.3470E-22 55853.087    7.4100E-22 55853.16
0    7.4180E-22 55853.232    7.3430E-22 55853.305    7.5330E-22 55853.378    7.6600E-22 55853.450
  7.5950E-22 55853.523    7.2090E-22 55853.596    6.7000E-22 55853.668    6.6980E-22 55853.741    6
.8230E-22 55853.814    7.0130E-22 55853.886    7.9070E-22 55853.959    8.2940E-22 55854.032    7.90
50E-22 55854.104    7.3900E-22 55854.177    6.8150E-22 55854.250    6.1190E-22 55854.322    5.4920E
-22 55854.395    5.2420E-22 55854.468    4.9930E-22 55854.541    5.0530E-22 55854.613    5.4240E-22
 55854.686    6.0470E-22

 TAPE NO.    1                FILE NO.    23
 RECORD    45                 LENGTH    672
 55854.759    6.2350E-22 55854.831    6.1700E-22 55854.904    6.0430E-22 55854.977    5.7290E-22 55
855.049    4.9810E-22 55855.122    4.7330E-22 55855.195    4.9780E-22 55855.267    5.0390E-22 55855
.340    4.9140E-22 55855.413    5.4080E-22 55855.486    5.9690E-22 55855.558    6.0930E-22 55855.63
1    6.0290E-22 55855.704    5.7770E-22 55855.776    5.4010E-22 55855.849    5.2750E-22 55855.922
  4.9640E-22 55855.994    5.0240E-22 55856.067    5.5820E-22 55856.140    5.7680E-22 55856.212    5
.6420E-22 55856.285    5.5780E-22 55856.358    5.5140E-22 55856.430    5.5130E-22 55856.503    5.32
40E-22 55856.576    5.3850E-22 55856.649    6.2600E-22 55856.724    6.5740E-22

***** JOB DONE.
$WEO LPS



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$ASS IN HT. CUT TB
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