SUBMILLIMETER, MILLIMETER, AND MICROWAVE SPECTRAL LINE CATALOG

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Abstract—This paper describes a computer-accessible catalog of submillimeter, millimeter, and microwave spectral lines in the frequency range between 0 and 10,000 GHz (i.e., wavelengths longer than 30 μm). The catalog can be used as a planning guide or as an aid in the identification and analysis of observed spectral lines in the interstellar medium, the Earth’s atmosphere, and the atmospheres of other planets. The information listed for each spectral line includes the frequency and its estimated error, the intensity, the lower state energy, and the quantum number assignment. The catalog is continuously updated and at present has information on 331 atomic and molecular species and includes a total of 1,845,866 lines. The catalog 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 covariance. Future versions of this catalog will add more atoms and molecules and update the present listings as new data appear. The catalog is available on-line via anonymous FTP at spec.jpl.nasa.gov and on the world wide web at http://spec.jpl.nasa.gov. © 1998 Published by Elsevier Science Ltd. All rights reserved.

1. INTRODUCTION

This paper describes a computer-accessible catalog of submillimeter, millimeter, and microwave spectral lines in the frequency range between 0 and 10,000 GHz (i.e., wavelengths longer than 30 μm). The catalog is intended to be used as a guide in the planning of spectral line observations and as a reference that can facilitate identification and analysis of observed spectral lines. The selection of lines for the catalog is based on the project needs of astronomers and atmospheric scientists. A previous version of this catalog has been described.† The present version is changed only by the addition of new and revised species. The catalog is constructed using theoretical least-squares fits and predictions based on spectral lines, mostly obtained from the literature. In subsequent versions of the catalog, more molecules will be added and existing molecular listings will be updated as new data appear.

The catalog is available on-line via anonymous FTP at spec.jpl.nasa.gov and on the world wide web at http://spec.jpl.nasa.gov.

The format of the data is given in Sec. 2. Conversions between different measures of spectral line intensity are given in Sec. 3. General comments on the precision of the spectral line positions and intensities are given in Sec. 4. The format of quantum numbers as they appear in the catalog is given in Sec. 5.

Documentation for each molecular or atomic species is available in printed form as a JPL publication2 and is also available on the catalog web site. Both documentation and the line files use a “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. In many cases, there is a separate tag for each vibration-electronic state of a particular molecule. The catalog contains individual files for each molecular species. Line files are designated as ctttttt.cat, where tttttt is the zero-filled catalog tag number. For example, the H atom line list is in the

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file `c001001.cat`. The documentation files are named `dttttt.cat`. There is also a directory file, named `catdir.cat`, which contains additional information needed to access the line files automatically and to calculate intensities at temperatures other than the standard temperature of 300 K.

Table 1 lists all the species provided in this catalog, by tag and name. There are currently 331 atomic and molecular species and a total of 1,845,866 lines.

### 2. Data Format

#### 2.1. Line files

The catalog line files are composed of 80-character lines, with one line entry per spectral line. The format of each line is:

```
FREQ, ERR, LGINT, DR, ELO, GUP, TAG, QNFMT, QN, QN'
```

- **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 Sect. 3 for conversions to other units.)
- **DR**: Degrees of freedom in the rotational partition function (0 for atoms, 2 for linear molecules, and 3 for nonlinear molecules).
- **ELO**: Lower state energy in cm$^{-1}$ relative to the lowest energy spin-rotation level in ground vibronic state.
- **GUP**: Upper state degeneracy.
- **TAG**: Species tag or molecular identifier. A negative value flags that the line frequency has been measured in the laboratory. The absolute value of TAG is then the species tag and ERR is the reported experimental error. The three most significant digits of the species tag are coded as the mass number of the species, as explained above.
- **QNFMT**: Identifies the format of the quantum numbers given in the field QN. These quantum number formats are given in Sec. 5 and are different from those in the first two editions of the catalog.
- **QN**: Quantum numbers for the upper state coded according to QNFMT.
- **QN’**: Quantum numbers for the lower state.

#### 2.2. Directory file

The catalog contains a special directory file called `catdir.cat`. Each element of this directory is an 80-character record with the following format:

```
TAG, NAME, NLINE, QLOG, VERSION
```

- **TAG**: The species tag or molecular identifier.
- **NAME**: An ASCII name for the species.
- **NLINE**: The number of lines in the catalog.
- **QLOG**: A seven-element vector containing the base 10 logarithm of the partition function for temperatures of 300, 225, 150, 75, 37.5, 18.75, and 9.375 K, respectively.
- **VERSION**: The version of the calculation for this species in the catalog.

#### 2.3. Documentation files

The documentation files are stored natively as ASCII LaTeX files for each species. These documentation files are also included in the printed documentation. This report is freely available from JPL on request. Postscript, LaTeX, and PDF versions of this publication are also available online. The documentation files provide the intensity and frequency cut-offs, partition functions at representative temperatures, assumed dipole moments, literature citations for the experimental lines, and a brief description of the nature of the Hamiltonian model used in the calculation. The
<table>
<thead>
<tr>
<th>Tag</th>
<th>Name</th>
<th>Lines</th>
<th>Tag</th>
<th>Name</th>
<th>Lines</th>
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<td>1</td>
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<td>C2H5OH</td>
<td>709</td>
</tr>
</tbody>
</table>

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Table 1. List of species in the catalog

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documentation file also includes a suggested isotopic correction based on cosmic abundances. This correction includes the appropriate statistics for equivalent nuclei. Note the catalog intensities do not include this isotopic correction.

In this edition of the catalog, several of the species have spectra that are extended to 10,000 GHz, so the documentation includes a maximum frequency cutoff. For almost all species, a strength cutoff was also employed:

$$10^{Q_{\text{LINT}}} > 10^{Q_{\text{LOGSTR0}}} + (\nu/300 \text{ GHz})^2 \cdot 10^{Q_{\text{LOGSTR1}}}$$

A blank entry for LOGSTR1 means that the second term was not included.

We have found that LOGSTR1 is often a useful cut-off parameter to account for the decreased sensitivity of instrumenta-
tion with increasing frequency or as a means to capture lines with comparable transition dipoles. The partition functions listed ($Q$) in the catalog include rotation and spin statistics but usually do not include vibrational or electronic corrections. (Exceptions such as $\text{H}_2\text{O}$ and $\text{O}_3$ are noted.) 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 catalog. The spin statistics included in the partition function are sometimes divided by a common
factor, but the partition functions are always consistent with the statistics used for intensities in the catalog. This common factor is not always documented, but the choice should be clear from the GUP field in the line file.

3. INTENSITY UNITS AND CONVERSIONS

The units of intensity given in the catalog, nm² MHz, are based on the integral of the absorption cross-section over the spectral line shape. The value of the intensity is calculated for 300 K and is directly comparable with the common infrared intensity unit of cm⁻¹/(molecule/cm²). The latter is obtainable by dividing the catalog intensity by 2.99792458 × 10¹⁸.

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

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

(1)

\[
= 4.16231 \times 10^{-5}v_{ba} \times S_{ba} \mu_x^2 \left[ e^{-E'/kT} - e^{-E''/kT} \right]/Q_{rs},
\]

(2)

where \( v_{ba} \) is the line frequency, \( S_{ba} \) 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 \( E'' \)). In Eq. (2), \( I_{ba} \) has units of nm² MHz, \( v_{ba} \) has units of MHz, and \( \mu_x \) has units of Debye. In many molecules, there are several dipole moment projections and there even may be mixing between dipoles. In such cases, \( S_{ba} \mu_x^2 \) is replaced with the sum of the squares of the transition dipoles for each \( M \) component in the line. For magnetic dipole transitions, Eq. (2) can be used with the conversion that a Bohr magneton is equivalent to 0.009274 Debye. 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 is included, except where explicitly stated in the documentation. Care is taken to assure that \( S_{ba} \) and \( Q_{rs} \) are determined with the same state degeneracies. For the catalog, Eq. (2) is evaluated for \( T = T_o = 300 \text{ K} \).

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

\[
I_{ba}(T) = I_{ba}(T_o)[Q_{rs}(T_o)/Q_{rs}(T)]\left[ e^{-E'/kT} - e^{-E''/kT} \right]/\left(e^{-E'/kT_o} - e^{-E''/kT_o}\right),
\]

(3)

\[
\approx I_{ba}(T_o) \cdot (T_o/T)^n e^{-(1/T-1/T_o)E'/k},
\]

(4)

where \( n = 1 \) for a linear molecule and \( \frac{3}{2} \) for a nonlinear molecule. Equation (4) requires that \( E' = E'' \) is small compared with \( kT \) and \( kT_o \).

Absorption coefficients of collision-broadened lines can be obtained from \( I_{ba} \) with the relation

\[
\alpha_{\text{max}} = \frac{I_{ba}(T)}{\Delta \nu} (T_o/T) \times 102.458 \text{ cm}^{-1}
\]

(5)

in which \( \Delta \nu \) is the half-width at half-height in MHz at 1 Torr partial pressure of the absorber at temperature \( T \), \( I_{ba} \) is in units of nm² MHz, and \( \alpha_{\text{max}} \) is in units of cm⁻¹. The power transmission through a uniform medium of length \( L \) at the peak of the line is \( \exp(-\alpha_{\text{max}} L) \). The attenuation is \( \alpha_{\text{max}} L \times 4.3429 \) in dB. The corresponding value of \( \alpha_{\text{max}} \) in the thermal Doppler limit is

\[
\alpha_{\text{max}} = \frac{I_{ba}(T)p}{\Delta \nu_d} (T_o/T) \times 151.194 \text{ cm}^{-1}
\]

(6)

in which \( p \) is the partial pressure of the absorber in Torr, and \( \Delta \nu_d \) is the Doppler half-width at half-height in units of MHz. The Doppler width is given by

\[
\Delta \nu_d = 1.17221 \times 10^{-6} \times v_{ba} \sqrt{(T/T_o)(28/m)}
\]

(7)
in which \( m \) is the mass of the absorber (in atomic mass units). The explicit inverse temperature dependence in Eqs. (5) and (6) is due to the conversion of density to pressure units. There is additional implicit temperature dependence in \( I_{ba}(T) \) and in the widths. In Eqs. (7)–(10), \( v_{ba} \) is the line frequency in MHz.

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

\[
\sigma_{ba} = \frac{I_{ba}}{v_{ba}} \times 2.99792 \times 10^{-9} \text{ cm}^2.
\] (8)

The power transmission through a uniform medium of length \( L \) and number density \( \rho \) is \( \exp(-\sigma_{ba} \rho L) \). 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

\[
A_{ba} = I_{ba}(T) v_{ba}^2 \left[ \frac{Q_{rs}}{g'} \right] \left[ e^{-E'/kT} - e^{-E/kT} \right]^{-1} \times 2.9794 \times 10^{-16} \text{ s}^{-1}
\] (9)

\[
= I_{ba}(T_0) v_{ba} \left[ \frac{Q_{rs}(T_0)}{g'} \right] e^{E/kT_0} \times 1.748 \times 10^{-9} \text{ s}^{-1}
\] (10)

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 catalog. Values of \( Q_{rs} \) are listed in the documentation and on the directory file.

Equation (10) requires that \( h \omega_{ba} \) is small compared with \( kT \) and \( kT_0 \).

It should be noted that the information to make all the intensity conversions given above is available from the directory file and from the line files, with the exception of the collisional broadening coefficients. As a matter of policy, we have not included collisional linewidths in the catalog because of the large variety of different collision partners relevant for the laboratory, the Earth’s atmosphere, and the atmospheres of the other planets.

4. GENERAL COMMENTS ON PRECISION

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

\[
e_n^2 = \sum_{kj} \frac{\partial \nu_n}{\partial \nu_k} \frac{\partial \nu_n}{\partial \nu_j} V_{kj}
\] (11)

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

\[
(V^{-1})_{kj} = \sum_m \frac{\partial \nu_m}{\partial \nu_k} \frac{\partial \nu_m}{\partial \nu_j} \hat{e}_m^{-2}
\] (12)

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

The experimental uncertainties generally given in the literature vary from 1.6-\( \sigma \) estimates to 3-\( \sigma \) estimates and are 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 Eqs. (11) and (12). 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 the input error estimates. Lines with an expected error greater than 1 GHz have been dropped from the catalog.

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 that 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 $x_{Sba}$, and errors in the rotation–spin partition function (the vibration-electronic partition 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 the 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.

The quantum model used to predict frequencies and intensities can also affect accuracy in the catalog. Many molecular models are found in the literature. In principle, a very general model should be able to treat every possible case. In practice, this is hardly ever done. A specific model is most frequently used for every case, mainly because every author starts with a different viewpoint of the problem. In our case, we have tried to develop a program that will treat a wide variety of problems with a minimum of adaptation. This saves a great deal of time in the initial setup, and provides a uniform output format for the final results. Most importantly, the basic treatment is the same for every molecule, regardless of the model used, so that a high degree of consistency can be maintained, facilitating comparisons between different molecules. The particular model needed to analyze a specific problem is treated as a subroutine. For certain problems, this subroutine can be quite simple, but 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.

5. FORMAT OF QUANTUM NUMBERS

For the later editions of this catalog, we have attempted to use a quantum number format convention that allows the quantum numbers to be accessed easily by computer (see Table 2). First, the upper and lower quantum number sets have been separated into distinct fields. Second, the quantum format designations have been defined to have more accessible information encoded in them. The quantum number format designation, QNFMT, is a 4-digit quantity in the catalog. We divide QNFMT into a series of digits so that

$$QNFMT = Q100 + H10 + NQN$$

in which $Q$ determines the type of molecule (see Table 2), $H$ determines the coding of half-integer quantum numbers, and $NQN$ is the number of quantum numbers for each state. $Q$ is defined so that MOD($Q$, 5) is the number of primary quantum numbers. If $NQN$ is greater than the number of primary quantum numbers, the degeneracy is derived from the last quantum number. Otherwise, the degeneracy is derived from the first quantum number. $H$ is a 3-bit binary code for the existence of half-integer quantum numbers for the last three quantum numbers. The least significant bit refers to
Table 2. Quantum number formats

<table>
<thead>
<tr>
<th>Type</th>
<th>( Q )</th>
<th>DR</th>
<th>Quantum order</th>
</tr>
</thead>
<tbody>
<tr>
<td>Atom</td>
<td>0</td>
<td>0</td>
<td>((J), (F), \ldots)</td>
</tr>
<tr>
<td>Linear—( \Xi )</td>
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<td>2</td>
<td>(N, (J), (F_1), (F_2) (F))</td>
</tr>
<tr>
<td>Linear—Case b</td>
<td>2</td>
<td>2</td>
<td>(N, \Lambda, (F_1), (F_2) (F))</td>
</tr>
<tr>
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<td>2</td>
<td>(J, \Omega, \Lambda, (F_1), (F_2) (F))</td>
</tr>
<tr>
<td>Linear—Case a (2S + 1 even)</td>
<td>8</td>
<td>2</td>
<td>(J + \frac{3}{2}, \Omega + \frac{1}{2}, \Lambda, (F_1), (F_2) (F))</td>
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<tr>
<td>Symmetric rotor</td>
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<td>3</td>
<td>(N, K, (J) (F_1), (F_2) (F))</td>
</tr>
<tr>
<td>Symmetric rotor with vibration</td>
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<td>(N, K, \nu, (J), (F_1), (F))</td>
</tr>
<tr>
<td>Asymmetric rotor</td>
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<td>3</td>
<td>(N, K-1, K_\nu, (J), (F_1), (F))</td>
</tr>
<tr>
<td>Asymmetric rotor with vibration</td>
<td>14</td>
<td>3</td>
<td>(N, K-1, K_\nu, \nu, (J), (F))</td>
</tr>
</tbody>
</table>

Conventions: 1. Half-integer quantum numbers are rounded up.
2. The sign of \( \Lambda \) and \( K \) refers to the parity under inversion of spatial coordinates, \textit{not} the sign of the operator.
3. Quantum numbers in parentheses are optional.
4. DR is defined in Sec. 2.1.

The parity given may not always be experimentally determined, but the parity convention is guaranteed to produce parities of the same sign for interacting states and to produce a change in parity across dipole allowed transitions. It should be noted that for symmetric top transitions with no \( K \) splitting, the parity designation is frequently dropped. Unless otherwise stated below, the parity of prolate symmetric tops follows the parity of \( K+1 \) for the corresponding asymmetric top level, while for oblate tops, the parity follows \( K-1 \). For example, the level \( 5_3,2 \) for an asymmetric rotor has \( K = 3 \) for a prolate symmetric top quantum field, and \( K = -2 \) for an oblate top. Hund’s case (b) quanta are similar to symmetric top quanta except that \( K \) is replaced with \( \Lambda \). Hund’s case (a) quanta also have parity encoded in the \( \Lambda \) field. The correlation between parity and \( e,f \) designations should follow the recommendations of Brown et al. For reference, this convention is

For odd-spin multiplicity:

\[
\text{if } p(-1)^{J+1/2} = -1, \text{ then } e, \\
\text{if } p(-1)^{J+1/2} = 1, \text{ then } f.
\]

For even-spin multiplicity:

\[
\text{if } p(-1)^{J} = 1, \text{ then } f, \\
\text{if } p(-1)^{J} = -1, \text{ then } e,
\]

where \( p \) is \( \pm 1 \) according to the parity. Care must be used because this convention is not universally followed in the literature.

6. FUTURE WORK

Future additions of this catalog will add more atoms and molecules and update the present listings as new data appear. We are currently working on an number of molecules of interstellar and atmospheric interest.

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REFERENCES