Submillimeter, Millimeter, and Microwave Spectral Line Catalog

H. M. Pickett E. A. Cohen B. J. Drouin J. C. Pearson

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ABSTRACT

This report 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. 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. This edition of the catalog has information on 298 atomic and molecular species and includes a total of 1,448,153 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 covariances. 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`.

FOREWORD

Revision 2 of the Submillimeter Spectral Line Catalog incorporated a number of changes: (1) a quantum number format, (2) addition of a complete set of partition functions for each species, (3) a computer-accessible directory of species, (4) a table of relative abundances of the isotopes under terrestrial conditions, (5) a new format for the individual species descriptions, (6) eighteen new species, and (7) thirty revised species. The present version is changed only by the addition of new and revised species. The changes are as follows:

NEW SPECIES, REV. 4 (93)

Tag	Name	Tag	Name	Tag	Name
7001	Li-6-H	8001	LiH	8002	Li-6-D
9001	LiD	13003	CH+	19004	H3O+
25002	NaH	27004	C-13-N	28008	HCNH+
28009	CO+	29006	CO-17	29007	HOC+
30010	HOC-13+	30011	NO+	30012	DOC+
31003	HDCO	31004	HO-18-C+	31005	HNO
32006	D2CO	32007	DNO	37002	C3H
37003	c-C3H	38003	C3D	38004	CCC13H
38005	C13CCH	38006	c-C3D	40003	SiC
40004	SiC-v1	40005	KH	41007	SiC-13
41008	CaH	41009	CH3NC	42004	CaD
42005	K-41-H	44010	HCP	44011	AlOH
45009	DCP	45010	HOCO+	45011	AlOD
45012	O-17-CO	46008	CH3OCH3	46009	AlF
46010	NS	46011	DOCO+	46012	HOC-13-O+
46013	O-18-CO	48009	NS-34	49003	C4H
49004	MgCCH	50008	C3N	50009	MgCN
50010	MgNC	51004	HCCNC	51005	HCCNC-v7
51006	HCCNC-v6	51007	HCCNC-v5	51008	HNCCC
52012	DNCCC	53007	C2H3NC	54007	HCCCHO
56007	CCS	56008	C2H3CHO	57001	C-13CS
57002	CC-13S	58001	CCS-34	58002	NaCl
60003	CH3OCHO-A	60004	CH3OCHO-E	60005	NaCl-37
61003	C5H	62005	AlCl	62006	C5D
64003	AlCl-37	66002	OS-34-O	66003	CaNC
69002	C3H7CN	73001	HC6	74001	KCl
74002	C2H5OOCH	75002	H2NCH2COOH-I	75003	H2NCH2COOH-II
76008	KCl-37	76009	C4Si	89001	Sr-88-H
90001	Sr-88-D	92001	C5S	94001	C5-34-S
96001	HOBr-79	98002	HOBr-81	99002	HC7N
112001	Se-80-O2	123001	HC9N	147001	HC11N

REVISED SPECIES, REV. 4 (24)

Tag	Name	Tag	Name	Tag	Name
26001	CN, v = 0, 1	27002	HNC	28001	CO
28007	DNC	29001	C-13-O	30001	CO-18
33001	HO2	34001	O-18-O	34002	H2S
34004	H2O2	38002	c-C3H2	39001	c-HC-13-CCH
39002	c-HCC-13-CH	39005	c-C3HD	41001	CH3CN
46004	C2H5OH	49001	O3-sym-O-17	49002	O3-asym-O-17
52007	SiCC	53001	C2H3CN	55001	C2H5CN
80001	HBr-79	82001	HBr-81	98001	H2SO4

For reference, the changes in Rev. 3 are:

NEW SPECIES, REV. 3 (55)

Tag	Name	Tag	Name	Tag	Name
4001	H2D+	19003	H2O-17	20002	HF
20003	H2O-18	21001	HDO-18	21002	DF
27003	HCN-v2	32005	O2 snglt dlta	33002	O-17-O
37001	DCl	38002	C3H2	39001	C-13-3H2a
39002	C-13-3H2s	39003	C3HD	39004	DCl-37
40002	NaOH	42003	NH2CN	43002	HNCO
43003	AlO	44006	DNCO	44007	HN-15-CO
44008	HNC-13-O	44009	N2O-v2	45005	HCS+
45006	HNCO-18	45007	NN-15-O	45008	N-15-NO
46007	N2O-18	48008	O3-v1,3+v2	50007	CH3Cl-35
51002	ClO-v1	52007	SiCC	52008	CCCO
52009	CH3Cl-37	52010	CH2F2	52011	CH2F2-v4
53003	C-13-CCO	53004	CC-13-CO	53005	CCC-13-O
53006	Cl-37-O-v1	54006	CCCO-18	63002	HNO3-v7
63003	HNO3-v9	63004	HNO3-v6	63005	HNO3-v8
63006	HNO3-v5	66001	COF2	67001	OCl-35-O
68001	CCCS	69001	OCl-37-O	70001	CCCS-34
79001	HOONO2	98001	H2SO4	102001	ClOOCl
104001	Cl-37-OOCl				

REVISED SPECIES, REV. 3 (28)

Tag	Name	Tag	Name	Tag	Name
3001	HD	12001	C-atom	13001	C-13-atom
14002	N-atom-D-state	17001	OH	18003	H2O
19002	HDO	20001	D2O	28001	CO
32001	O2	32002	O2-v1	33001	HO2
34003	PH3	34004	H2O2	36001	HCl
38001	HCl-37	46006	NO2	48004	O3
48005	O3-v2	48006	O3-v1,3	48007	O3-2v2
51002	ClO	52006	HOCl	53002	Cl-37-O
54005	HOCl-37	63001	HNO3	64001	S2
64002	SO2				

For reference, the changes in Rev. 2 are:

NEW SPECIES, REV. 2 (18)

Tag	Name	Tag	Name	Tag	Name
13002	CH	17004	NH3-v2	20001	D2O
25001	CCH	26001	CN	26002	CN-v1
29004	HCO	29005	NNH+	30009	NND+
33001	HO2	46006	NO2	48007	O3-2v2
49001	O3-sym-O-17	49002	O3-asym-O-17	50005	O3-s-O18-v2
50006	O3-a-O18-v2	97002	Cl-35-NO3	99001	Cl-37-NO3

REVISED SPECIES, REV. 2 (30)

Tag	Name	Tag	Name	Tag	Name
16001	O-atom	17001	OH	17002	NH3
18001	OD	18003	H2O	18005	H2O-v2
19001	HO-18	19002	HDO	27001	HCN
29002	HCO+	30002	HC-13-O+	30003	DCO+
31001	HCO-18+	32001	O2	32002	O2-v1
34001	O-18-O	41005	CH3CCD	44001	CS
44002	SiO	45001	C-13-S	46001	CS-34
48004	O3	48005	O3-v2	48006	O3-v1,3
50003	O3-sym-O-18	50004	O3-asym-O-18	52006	HOCl
54005	HOCl-37	63001	HNO3	64002	SO2

For reference, the new and revised species listed in the first revision of this catalog are:

NEW SPECIES, REV. 1 (9)

Tag	Name	Tag	Name	Tag	Name
18004	NH2D	18005	H2O-v2	34004	H2O2
44005	CH3CHO-E	48005	O3-v2	48006	O3-v1,3
52006	HOCl	54005	HOCl-37	63001	HNO3

REVISED SPECIES, REV. 1 (24)

Tag	Name	Tag	Name	Tag	Name
17002	NH3	18002	N-15-H3	18003	H2O
29003	CH2NH	30007	CH2ND	32001	O2
32002	O2-v1	32003	CH3OH	34002	O-18-O
34002	H2S	34003	PH3	45003	NH2CHO
51002	ClO	53002	Cl-37-O	55001	C2H5CN
56001	CH3CH2C-13-N	56002	CH3C-13-H2CN	56003	C-13-H3CH2CN
56005	CH2DCH2CN-s	56006	CH2DCH2CN-a	60001	OCS
61001	OC-13-S	62001	OC-34-S	62002	O-18-CS

Contents

1 INTRODUCTION

This report 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.

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 Section 2. Section 3 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 4, while species-specific comments are reserved for Section 6. Section 5 gives the format of quantum numbers as they appear in the catalog.

Documentation for each molecular or atomic species is listed in Section 6 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.

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

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 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 Section 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
(I6,X,	A13,	I6,	7F7.4,	I2)

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 K, 225 K, 150 K, 75 K, 37.5 K, 18.75 K, 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. Postscript, LaTex, and PDF versions of this publication are also available on line. 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 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:

$$10^{\mathrm{LGINT}} > 10^{\mathrm{LOGSTR0}} + (\nu/300GHz)^2 \cdot 10^{\mathrm{LOGSTR1}}$$

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 instrumentation 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 H_2O and 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, $\mathrm{nm}^2\cdot\mathrm{MHz}$, 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 $\mathrm{cm}^{-1}/(\mathrm{molecule}/\mathrm{cm}^2)$. The latter is obtainable by dividing the catalog intensity by $2.99792458 \times 10^{18}$.

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

$$\begin{aligned} I_{ba}(T) &= (8\pi^3/3\mathrm{hc})\nu_{ba}\, {}^{x}S_{ba}\, \mu_x^2[e^{-E''/kT} - e^{-E'/kT}]/Q_{rs} && (1) \\ &= 4.16231 \times 10^{-5}\nu_{ba}\, {}^{x}S_{ba}\, \mu_x^2[e^{-E''/kT} - e^{-E'/kT}]/Q_{rs} && (2) \end{aligned}$$

where ν_{ba} is the line frequency, ${}^{x}S_{ba}$ is the line strength, μ_x is the dipole moment along the molecular axis x, E″ and E′ are the lower and upper state energies, respectively, and Q_{rs} is the rotation-spin partition function (using the same zero of energy as E' and E″). In Eq.(2), I_{ba} has units of $\mathrm{nm}^2\cdot\mathrm{MHz}$, ν_{ba} has units of MHz, and μ_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, ${}^{x}S_{ba}\, \mu_x^2$ 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 ${}^{x}S_{ba}$ and Q_{rs} are determined with the same state degeneracies. For the catalog, Eq. (2) is evaluated for T = T $_\circ$ = 300 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

$$\begin{aligned} I_{ba}(T) &= I_{ba}(T_\circ)[Q_{rs}(T_\circ)/Q_{rs}(T)]\frac{e^{-E''/kT}-e^{-E'/kT}}{e^{-E''/kT_\circ}-e^{-E'/kT_\circ}} && (3)\\ &\cong I_{ba}(T_\circ)\cdot(T_\circ/T)^{n+1}e^{-(1/T-1/T_\circ)E''/k} && (4)\end{aligned}$$

where n = 1 for a linear molecule and 3/2 for a nonlinear molecule. Eq.(4) requires that $E' - E''$ is small compared with kT and $kT_\circ$.

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

$$\alpha_{\max} = \frac{I_{ba}(T)}{\Delta\nu}(T_\circ/T) \times 102.458\ \mathrm{cm}^{-1} \tag{5}$$

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 $\mathrm{nm}^2\cdot$MHz, and $\alpha_{\max}$ is in units of cm^{-1}. The power transmission through a uniform medium of length L at the peak of the line is $\exp(-\alpha_{\max}L)$. The attenuation is $\alpha_{\max}L \times 4.3429$ in dB. The corresponding value of $\alpha_{\max}$ in the thermal Doppler limit is

$$\alpha_{\max} = \frac{I_{ba}(T)p}{\Delta\nu_d}(T_\circ/T) \times 151.194\ \mathrm{cm}^{-1} \tag{6}$$

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

$$\Delta\nu_d = 1.17221 \times 10^{-6} \times \nu_{ba}\sqrt{(T/T_\circ)(28/m)} \tag{7}$$

in which m is the mass of the absorber (in atomic mass units). The explicit inverse temperature dependence in Eqs.(5) - (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), ν_{ba} is the line frequency in MHz.

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

$$\sigma_{ba} = \frac{I_{ba}}{\nu_{ba}} \times 2.99792 \times 10^{-9}\ \mathrm{cm}^2. \tag{8}$$

The power transmission through a uniform medium of length L and number density ρ is $\exp(-\sigma_{ba}\rho L)$. The inverse of σ_{ba} is the column density per unit optical depth in the same 1 km/s-velocity interval.

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

$$
\begin{aligned}
A_{ba} &= I_{ba}(T)\ \nu_{ba}^2[Q_{rs}/g^{'}][e^{-E^{''}/kT} - e^{-E^{'}/kT}]^{-1} \times 2.7964 \times 10^{-16}\ \mathrm{sec}^{-1} && (9)\\
&\cong I_{ba}(T_\circ)\ \nu_{ba}[Q_{rs}(T_\circ)/g^{'}]e^{E'/kT_\circ} \times 1.748 \times 10^{-9}\ \mathrm{sec}^{-1} && (10)
\end{aligned}
$$

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. Eq.(10) requires that $h\nu_{ba}$ is small compared with kT and $kT_\circ$.

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.

When $\nu \cong \nu_{ba}$, the absorption coefficient is

$$\alpha(\nu) = n \sum_{a,b} I_{ab} f_{ab}(\nu - \nu_{ab}) \tag{11}$$

where n is the number denity of absorbers and $f_{ab}(\delta)$ is an area-normalized line shape. Further away from line center

$$\alpha(\nu) = n\nu \tanh(\nu/2kT) \sum_{a,b} \bar{I}_{ab}\, [f_{ab}(\nu - \nu_{ab}) + f_{ab}(\nu + \nu_{ab})] \tag{12}$$

where $\bar{I}_{ab}$ is defined by

$$I_{ab} = \nu_{ab} \tanh(\nu_{ab}/2kT) \bar{I}_{ab} \tag{13}$$

Note that in Eq. (11) and (12), the sum over a and b is restricted to $\nu_{ab} > 0$.

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:

$$\varepsilon_n^2 = \sum_{kj} \frac{\partial \nu_n}{\partial p_k} \frac{\partial \nu_n}{\partial p_j}\ V_{kj} \tag{14}$$

in which ε_n is the estimated error of frequency ν_n and V_{kj} is an element of the least square variance-covariance matrix for the parameters p_k. This variance-covariance matrix is determined from the observed lines by

$$(V^{-1})_{kj} = \sum_m \frac{\partial \nu_m}{\partial p_k} \frac{\partial \nu_m}{\partial p_j} \ \ \varepsilon_m^{-2} \tag{15}$$

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

The experimental uncertainties generally given in the literature vary from 1.6-σ estimates to 3-σ 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 Eq. (10) and (11). 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 ${}^xS_{ba}$, 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.

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 1). 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

$$\mathrm{QNFMT} = Q \cdot 100 + H \cdot 10 + NQN$$

in which Q determines the type of molecule (see Table 1), H determines the coding of half-integer quantum numbers, and NQN is the number of quantum numbers for each state. Q is defined so that MOD(Q,5) is the number of primary quantum numbers. If NQN is greater than the number of primary quantum numbers, the degeneracy is derived from the last quantum number. Otherwise, the degeneracy is derived from the first quantum number. H is a 3-bit binary code for the existence of half-integer quantum numbers for the *last three* quantum numbers. The least significant bit refers to quantum number NQN and is 1 if the last quantum number is half-integer. In the catalog, all half-integer quantum numbers are rounded **up** to the next integer.

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 Λ. Hunds's case (a) quanta also have parity encoded in the Λ field. The correlation between parity and e,f designations should follow the recommendations of J. M. Brown *et al.*, 1975, J. Mol. Spect. **55**, 500. For reference, this convention is

TABLE 1. QUANTUM NUMBER FORMATS

Type	**Q**	**DR**	**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+$\frac{1}{2}$,$\Omega+\frac{1}{2}$, 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 are rounded up.
2. The sign of Λ and K refers to the parity under inversion of spatial coordinates, *not* the sign of the operator.
3. Quantum numbers in parentheses are optional.

$$\begin{array}{llcrll} & \text{For odd-spin multiplicity:} & & & & \\ \text{if} & p(-1)^{J+1/2} & = & -1, & \text{then} & e \\ \text{if} & p(-1)^{J+1/2} & = & 1, & \text{then} & f \\ & \text{For even-spin multiplicity:} & & & & \\ \text{if} & p(-1)^{J} & = & 1, & \text{then} & f \\ \text{if} & p(-1)^{J} & = & -1, & \text{then} & e \end{array}$$

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

6 DOCUMENTATION BY SPECIES

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

$$10^{\mathrm{LGINT}} > 10^{\mathrm{LOGSTR0}} + (\nu/300GHz)^2 \cdot 10^{\mathrm{LOGSTR1}}$$

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 such as H_2O and 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 are only a partial set but are consistent with the intensities in the catalog.

6.1 Isotope Corrections

For convenience, we have included an isotope correction for the rarer isotopes that includes effects of redundant substitution. The atomic abundances used are listed in Table 2. It should be stressed that the intensities in the catalog do not contain an isotope correction.

TABLE 2. ASSUMED RELATIVE ISOTOPIC ABUNDANCES FOR CATALOG DESCRIPTION

Isotope	Log (abundance)	Isotope	Log (abundance)
^{1}H	0.000	^{2}H	-3.824
^{6}Li	-1.131	^{7}Li	-0.033
^{12}C	0.000	^{13}C	-1.955
^{14}N	0.000	^{15}N	-2.432
^{16}O	0.000	^{17}O	-3.432
^{18}O	-2.690	^{28}Si	-0.035
^{29}Si	-1.327	^{30}Si	-1.506
^{32}S	-0.022	^{33}S	-2.125
^{34}S	-1.376	^{35}Cl	-0.122
^{37}Cl	-0.611	^{79}Br	-0.296
^{81}Br	-0.306		

6.2 List of Species in This Catalog

Table 3 lists all the species provided in this catalog, by tag and name.

TABLE 3. LIST OF SPECIES

Tag	Name	Tag	Name	Tag	Name
1001	H-atom	2001	D-atom	3001	HD
4001	H2D+	7001	Li-6-H	8001	LiH
8002	Li-6-D	9001	LiD	12001	C-atom
13001	C-13-atom	13002	CH	13003	CH+
14001	N-atom	14002	N-atom-D-st	15001	NH
16001	O-atom	17001	OH	17002	NH3
17003	CH3D	17004	NH3-v2	17005	OH-v1,2
18001	OD	18002	N-15-H3	18003	H2O
18004	NH2D	18005	H2O-v2	19001	HO-18
19002	HDO	19003	H2O-17	19004	H3O+
20001	D2O	20002	HF	20003	H2O-18
21001	HDO-18	21002	DF	25001	CCH
25002	NaH	26001	CN, v = 0, 1	27001	HCN
27002	HNC	27003	HCN-v2	27004	C-13-N
28001	CO	28002	HC-13-N	28003	HCN-15
28004	DCN	28005	HNC-13	28006	HN-15-C
28007	DNC	28008	HCNH+	28009	CO+
29001	C-13-O	29002	HCO+ v=0,1,2	29003	CH2NH
29004	HCO	29005	NNH+	29006	CO-17
29007	HOC+	30001	CO-18	30002	HC-13-O+
30003	DCO+	30004	H2CO	30005	C-13-H2NH
30006	CH2N-15-H	30007	CH2ND	30008	NO
30009	NND+	30010	HOC-13+	30011	NO+
30012	DOC+	31001	HCO-18+	31002	H2C-13-O
31003	HDCO	31004	HO-18-C+	31005	HNO
32001	O2	32002	O2-v1	32003	CH3OH
32004	H2CO-18	32005	O2-snglt-dlta	32006	D2CO
32007	DNO	33001	HO2	33002	O-17-O
33003	SH v=0,1	34001	O-18-O	34002	H2S
34003	PH3	34004	H2O2	34005	SD
35001	HDS	36001	HCl	37001	DCl

TABLE 3. (continued)

Tag	Name	Tag	Name	Tag	Name
37002	C3H	37003	c-C3H	38001	HCl-37
38002	c-C3H2	38003	C3D	38004	c-CCC-13-H
38005	c-C-13-CCH	38006	c-C3D	39001	c-HC-13-CCH
39002	c-HCC-13-CH	39003	c-C3HD	39004	DCl-37
40001	CH3CCH	40002	NaOH	40003	SiC
40004	SiC-v1	40005	KH	40006	C2O
40007	MgO	41001	CH3CN v8=0,1	41002	CH3CC-13-H
41003	CH3C-13-CH	41004	C-13-H3CCH	41005	CH3CCD
41006	CH2DCCH	41007	SiC-13	41008	CaH
41009	CH3NC	42001	CH3CN-15	42002	CH2CO
42003	NH2CN	42004	CaD	42005	K-41-H
42006	C-13-H3CN	42007	CH3C-13-N	42008	CH2DCN
42009	H2CSi	42010	SiN	43001	CHDCO
43002	HNCO	43003	AlO	43004	CP
44001	CS	44002	SiO	44003	CH3CHO-a
44004	N2O	44005	CH3CHO-e	44006	DNCO
44007	HN-15-CO	44008	HNC-13-O	44009	N2O-v2
44010	HCP	44011	AlOH	44012	N2O-2v2
45001	C-13-S	45002	Si-29-O	45003	NH2CHO
45005	HCS+	45006	HNCO-18	45007	NN-15-O
45008	N-15-NO	45009	DCP	45010	HOCO+
45011	AlOD	45012	O-17-CO	45013	PN v=0-4
46001	CS-34	46002	Si-30-O	46003	H2CS
46004	C2H5OH	46005	HCOOH	46006	NO2
46007	N2O-18	46008	CH3OCH3	46009	AlF
46010	NS	46011	DOCO+	46012	HOC-13-O+
46013	O-18-CO	47001	H2C-13-S	47002	HC-13-OOH
47003	DCOOH	47004	HCOOD	47005	PO+ v=0-4
47006	PO	48001	SO	48002	SO-v1
48003	H2CS-34	48004	O3	48005	O3-v2
48006	O3-v1,3	48007	O3-2v2	48008	O3-v1,3+v2
48009	NS-34	48010	SO+	49001	O3-sym-O-17
49002	O3-asym-O-17	49003	C4H	49004	MgCCH
50001	S-34-O	50002	SO-18	50003	O3-sym-O-18
50004	O3-asym-O-18	50005	O3-s-O18-v2	50006	O3-a-O18-v2

TABLE 3. (continued)

Tag	Name	Tag	Name	Tag	Name
50007	CH3Cl-35	50008	C3N	50009	MgCN
50010	MgNC	51001	HCCCN	51002	ClO
51003	ClO-v1	51004	HCCNC	51005	HCCNC-v7
51006	HCCNC-v6	51007	HCCNC-v5	51008	HNCCC
52001	HCCC-13-N	52002	HCC-13-CN	52003	HC-13-CCN
52004	HCCCN-15	52005	DCCCN	52006	HOCl
52007	SiCC	52008	CCCO	52009	CH3Cl-37
52010	CH2F2	52011	CH2F2-v4	52012	DNCCC
52013	CNCN	53001	C2H3CN	53002	Cl-37-O
53003	C-13-CCO	53004	CC-13-CO	53005	CCC-13-O
53006	Cl-37-O-v1	53007	C2H3NC	53008	HNCCN+
54001	CH2CHC-13-N	54002	CH2C-13-HCN	54003	C-13-H2CHCN
54004	CH2CDCN	54005	HOCl-37	54006	CCCO-18
54007	HCCCHO	55001	C2H5CN	56001	CH3CH2C-13-N
56002	CH3C-13-H2CN	56003	C-13-H3CH2CN	56004	C2H5CN-15
56005	CH2DCH2CN-s	56006	CH2DCH2CN-a	56007	CCS
56008	C2H3CHO	56009	MgS	57001	C-13CS
57002	CC-13S	58001	CCS-34	58002	NaCl
60001	OCS	60002	SiS	60003	CH3OCHO-A
60004	CH3OCHO-E	60005	NaCl-37	61001	OC-13-S
61002	Si-29-S	61003	C5H	62001	OC-34-S
62002	O-18-CS	62003	Si-30-S	62004	SiS-34
62005	AlCl	62006	C5D	63001	HNO3
63002	HNO3-v7	63003	HNO3-v9	63004	HNO3-v6
63005	HNO3-v8	63006	HNO3-v5	63007	PS
63008	PO2	64001	S2	64002	SO2
64003	AlCl-37	64004	C4O	64005	SO2-v2
65001	S-33-O2	66001	COF2	66002	S-34-O2
66003	CaNC	66004	SOO-18	67001	OCl-35-O
68001	CCCS	69001	OCl-37-O	69002	C3H7CN 1
70001	CCCS-34	71001	MnO	73001	C6H
74001	KCl	74002	C2H5OOCH	75001	HCCCCCN
75002	H2NCH2COOH I	75003	H2NCH2COOH II	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

TABLE 3. (continued)

Tag	Name	Tag	Name	Tag	Name
76008	KCl-37	76009	C4Si	76010	C5O
79001	HOONO2	80001	HBr-79	81001	Cl-35-NO2
82001	HBr-81	88001	C6O	89001	Sr-88-H
90001	Sr-88-D	92001	C5S	94001	C5-34-S
95001	Br-79-O	95002	Br-79-O v=1	96001	HOBr-79
97001	Br-81-O	97002	Cl-35-ONO2	97003	Br-81-O v=1
98001	H2SO4	98002	HOBr-81	99001	Cl-37-ONO2
99002	HC7N	100001	C7O	102001	ClOOCl
104001	Cl-37-OOCl	111001	OBr-79-O	112001	Se-80-O2
112002	C8O	113001	OBr-81-O	123001	HC9N
124001	C9O	147001	HC11N		

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西安分公司：西安高新开发区 20 所(中国电子科技集团导航技术研究所)
西安劳动南路 88 号电子商城二楼 D23 号
TEL：029-81022619 13072977981 FAX:029-88789382