



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.¹ 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 *tttttt.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 *dtttttt.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, (F13.4,	ERR, F8.4,	LGINT, F8.4,	DR, I2,	ELO, F10.4,	GUP, I3,	TAG, I7,	QNFMT, I4,	QN', QN'' 6I2, 6I2)
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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, (I6,X,	NAME, A13,	NLINE, I6,	QLOG, 7F7.4,	VERSION I2)
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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.² This report is freely available from JPL on request. 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

Table 1. List of species in the catalog

Tag	Name	Lines	Tag	Name	Lines	Tag	Name	Lines
1001	H-atom	1	30011	NO+	154	44001	CS	51
2001	D-atom	1	30012	DOC+	40	44002	SiO	31
3001	HD	1	31001	HCO-18+	34	44003	CH3CHO-a	1347
4001	H2D+	19	31002	H2C-13-O	601	44004	N2O	61
7001	Li-6-H	33	31003	HDCO	4204	44005	CH3CHO-e	691
8001	LiH	40	31004	HO-18-C+	40	44006	DNCO	5504
8002	Li-6-D	40	31005	HNO	10 293	44007	HN-15-CO	888
9001	LiD	40	32001	O2	237	44008	HNC-13-O	4332
12001	C-atom	2	32002	O2-v1	237	44009	N2O-v2	146
13001	C-13-atom	7	32003	CH3OH	709	44010	HCP	34
13002	CH	324	32004	H2CO-18	449	44011	AlOH	766
13003	CH+	9	32005	O2-snglt-dlta	67	44012	N2O-2v2	194
14001	N-atom	2	32006	D2CO	3682	45001	C-13-S	29
14002	N-atom-D-state	6	32007	DNO	14 739	45002	Si-29-O	66
15001	NH	926	33001	HO2	21 954	45003	NH2CHO	3476
16001	O-atom	2	33002	O-17-O	10 787	45005	HCS+	64
17001	OH	788	33003	SH v = 0, 1	646	45006	HNCO-18	4929
17002	NH3	446	34001	O-18-O	400	45007	NN-15-O	85
17003	CH3D	80	34002	H2S	1525	45008	N-15-NO	87
17004	NH3-v2	442	34003	PH3	728	45009	DCP	34
18001	OD	912	34004	H2O2	38 357	45010	HOCO+	1745
18002	N-15-H3	235	34005	SD	1125	45011	AlOD	70
18003	H2O	783	35001	HDS	1138	45012	O-17-CO	285
18004	NH2D	5036	36001	HCl	137	45013	PN v = 0-4	1637
18005	H2O-v2	292	37001	DCI	228	46001	CS-34	34
19001	HO-18	295	37002	C3H	4990	46002	Si-30-O	67
19002	HDO	1401	37003	c-C3H	2973	46003	H2CS	517
19003	H2O-17	404	38001	HCl-37	137	46004	C2H5OH	12 557
19004	H3O+	420	38002	c-C3H2	30 436	46005	HCOOH	1888
20001	D2O	1137	38003	C3D	1560	46006	NO2	16 444
20002	HF	8	38004	c-CCC-13-H	6541	46007	N2O-18	88
20003	H2O-18	726	38005	c-C-13-CCH	9753	46008	CH3OCH3	21 735
21001	HDO-18	952	38006	c-C3D	6001	46009	AlF	1188
21002	DF	20	39001	c-HC-13-CCH	17 768	46010	NS	2402
25001	CCH	114	39002	c-HCC-13-CH	6892	46011	DOC0+	677
25002	NaH	52	39003	c-C3HD	21 610	46012	HOC-13-O+	1735
26001	CN, v = 0, 1	874	39004	DCI-37	228	46013	O-18-CO	91
27001	HCN	40	40001	CH3CCH	813	47001	H2C-13-S	110
27002	HNC	49	40002	NaOH	91	47002	HC-13-OOH	1194
27003	HCN-v2	132	40003	SiC	982	47003	DCOOH	628
27004	C-13-N	1218	40004	SiC-v1	703	47004	HCOOD	612
28001	CO	91	40005	KH	40	47005	PO+ v = 0-4	239
28002	HC-13-N	45	40006	C2O	354	47006	PO	743
28003	HCN-15	35	40007	MgO v = 0, 1	88	48001	SO	330
28004	DCN	54	41001	CH3CN v8 = 0, 1	29 304	48002	SO-v1	261
28005	HNC-13	34	41002	CH3CC-13-H	822	48003	H2CS-34	111
28006	HN-15-C	33	41003	CH3C-13-CH	813	48004	O3	7089
28007	DNC	53	41004	C-13-H3CCH	821	48005	O3-v2	4947
28008	HCNH+	74	41005	CH3CCD	822	48006	O3-v1, 3	9685
28009	CO+	88	41006	CH2DCCH	223	48007	O3-2v2	3031
29001	C-13-O	60	41007	SiC-13	2417	48008	O3-v1, 3+v2	10 912
29002	HCO+ v = 0, 4	246	41008	CaH	387	48009	NS-34	2364
29003	CH2NH	2957	41009	CH3NC	1798	48010	SO+	194
29004	HCO	2454	42001	CH3CN-15	2755	49001	O3-sym-O-17	26 092
29005	NNH+	34	42002	CH2CO	835	49002	O3-asym-O-17	52 613
29006	CO-17	50	42003	NH2CN	13 898	49003	C4H	742
29007	HOC+	40	42004	CaD	501	49004	MgCCH	274
30001	CO-18	60	42005	K-41-H	40	50001	S-34-O	280
30002	HC-13-O+	34	42006	C-13-H3CN	9015	50002	SO-18	179
30003	DCO+	41	42007	CH3C-13-N	8951	50003	O3-sym-O-18	3184
30004	H2CO	611	42008	CH2DCN	19 256	50004	O3-asym-O-18	7304
30005	C-13-H2NH	439	42009	H2CSi	670	50005	O3-s-O18-v2	2387
30006	CH2N-15-H	440	42010	SiN	614	50006	O3-a-O18-v2	4213
30007	CH2ND	1834	43001	CHDCO	886	50007	CH3Cl-35	6372
30008	NO	1909	43002	HNCO	6078	50008	C3N	1351
30009	NND+	41	43003	AlO	1023	50009	MgCN	273
30010	HOC-13+	40	43004	CP	397	50010	MgNC	269

continued

Table 1—*continued*

Tag	Name	Lines	Tag	Name	Lines	Tag	Name	Lines
51001	<i>HCCCN</i>	139	56008	C2H3CHO	24 051	73001	C6H	3031
51002	<i>CIO</i>	2585	56009	MgS	99	74001	KCl	99
51003	<i>CIO-v1</i>	2112	57001	C-13CS	1013	74002	C2H5OOC	60 671
51004	<i>HCCNC</i>	563	57002	CC-13S	1015	75001	HCCCCCN	99
51005	<i>HCCNC-v7</i>	291	58001	CCS-34	565	75002	H2NCH2COOH I	27 217
51006	<i>HCCNC-v6</i>	291	58002	NaCl	99	75003	H2NCH2COOH II	26 544
51007	<i>HCCNC-v5</i>	278	60001	OCS	99	76001	HCCCC-13-N	99
51008	<i>HNCCC</i>	574	60002	SiS	97	76002	HCCCC-13-CN	99
52001	<i>HCCC-13-N</i>	152	60003	HCO(O) CH3-A	16 153	76003	HCCC-13-CCN	99
52002	<i>HCC-13-CN</i>	146	60004	HCO(O) CH3-E	17 260	76004	HCC-13-CCCN	99
52003	<i>HC-13-CCN</i>	144	60005	NaCl-37	99	76005	HC-13-CCCN	99
52004	<i>HCCCN-15</i>	99	61001	OC-13-S	99	76006	HCCCCCN-15	99
52005	<i>DCCCN</i>	156	61002	Si-29-S	98	76007	DCCCCCN	99
52006	<i>HOCl</i>	6929	61003	C5H	2594	76008	KCl-37	99
52007	<i>SiCC</i>	304	62001	OC-34-S	99	76009	C4Si	229
52008	<i>CCCO</i>	99	62002	O-18-CS	99	76010	C5O	99
52009	<i>CH3Cl-37</i>	6403	62003	Si-30-S	99	79001	HOONO2	50 775
52010	<i>CH2F2</i>	11 942	62004	SiS-34	99	80001	HBr-79	143
52011	<i>CH2F2-v4</i>	7808	62005	AlCl	11 525	81001	Cl-35-NO2	3520
52012	<i>DNCCC</i>	3098	62006	C5D	4436	82001	HBr-81	143
52013	<i>CNCN</i>	206	63001	HNO3	36 551	88001	C6O	567
53001	<i>C2H3CN gs, v's</i>	75 697	63002	HNO3-v7	16 478	89001	Sr-88-H	391
53002	<i>Cl-37-O</i>	2624	63003	HNO3-v9	32 404	90001	Sr-88-D	922
53003	<i>C-13-CCO</i>	99	63004	HNO3-v6	15704	92001	C5S	99
53004	<i>CC-13-CO</i>	99	63005	HNO3-v8	14 537	94001	C5-34-S	99
53005	<i>CCC-13-O</i>	99	63006	HNO3-v5	13 269	95001	Br-79-O	1892
53006	<i>Cl-37-O-v1</i>	2132	63007	PS	2340	96001	HOBr-79	9898
53007	<i>C2H3NC</i>	9362	63008	PO2	7323	97001	Br-81-O	1892
53008	<i>HNCCN+</i>	99	64001	S2	174	97002	Cl-35-ONO2	78 323
54001	<i>CH2CHC-13-N</i>	118	64002	SO2	13 573	98001	H2SO4	5690
54002	<i>CH2C-13-HCN</i>	117	64003	AlCl-37	11 326	98002	HOBr-81	9920
54003	<i>C-13-H2CHCN</i>	116	64004	C4O	535	99001	Cl-37-ONO2	49 505
54004	<i>CH2CDN</i>	6381	64005	SO2-v2	9225	99002	HC7N	518
54005	<i>HOCl-37</i>	6925	65001	S-33-O2	19 048	100001	C7O	99
54006	<i>CCCO-18</i>	99	66001	COF2	23 090	102001	ClOCl	17 266
54007	<i>HCCCHO</i>	8407	66002	S-34-O2	11 894	104001	Cl-37-OOCl	17 482
55001	<i>C2H5CN</i>	52 883	66003	CaNC	259	111001	OBr-79-O	52 631
56001	<i>CH3CH2C-13-N</i>	1183	66004	SOO-18	9758	112001	Se-80-O2	7484
56002	<i>CH3C-13-HCN</i>	1252	67001	OCl-35-O	57 232	112002	C8O	644
56003	<i>C-13-H3CH2CN</i>	1183	68001	CCCS	99	113001	OBr-81-O	52 840
56004	<i>C2H5CN-15</i>	1621	69001	OCl-37-O	49 388	123001	HC9N	99
56005	<i>CH2DCH2CN-s</i>	1166	69002	C3H7CN	131 349	124001	C9O	100
56006	<i>CH2DCH2CN-a</i>	1286	70001	CCCS-34	99	147001	HC11N	99
56007	<i>CCS</i>	563						

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:

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

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 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 H₂O and O₃ 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, $\text{nm}^2 \text{ MHz}$, 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 $\text{cm}^{-1}/(\text{molecule}/\text{cm}^2)$. 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

$$I_{ba}(T) = (8\pi^3/3hc)v_{ba} {}^xS_{ba} \mu_x^2 [e^{-E''/kT} - e^{-E'/kT}]/Q_{rs} \quad (1)$$

$$= 4.16231 \times 10^{-5} v_{ba} {}^xS_{ba} \mu_x^2 [e^{-E''/kT} - e^{-E'/kT}]/Q_{rs}, \quad (2)$$

where v_{ba} is the line frequency, ${}^xS_{ba}$ 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 $\text{nm}^2 \text{ MHz}$, v_{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, ${}^xS_{ba} \mu_x^2$ 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 ${}^xS_{ba}$ and Q_{rs} are determined with the same state degeneracies. For the catalog, Eq. (2) is evaluated for $T = T_0 = 300 \text{ K}$.

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

$$I_{ba}(T) = I_{ba}(T_0) [Q_{rs}(T_0)/Q_{rs}(T)] \frac{e^{-E''/kT} - e^{-E'/kT}}{e^{-E''/kT_0} - e^{-E'/kT_0}} \quad (3)$$

$$\cong I_{ba}(T_0) \cdot (T_0/T)^{n+1} e^{-(1/T-1/T_0)E'/k}, \quad (4)$$

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_0 .

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

$$\alpha_{\max} = \frac{I_{ba}(T)}{\Delta\nu} (T_0/T) \times 102.458 \text{ cm}^{-1} \quad (5)$$

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 $\text{nm}^2 \text{ MHz}$, and α_{\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 α_{\max} in the thermal Doppler limit is

$$\alpha_{\max} = \frac{I_{ba}(T)p}{\Delta\nu_d} (T_0/T) \times 151.194 \text{ cm}^{-1} \quad (6)$$

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

$$\Delta\nu_d = 1.17221 \times 10^{-6} \times v_{ba} \sqrt{(T/T_0)(28/m)} \quad (7)$$

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), 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

$$\sigma_{ba} = \frac{I_{ba}}{\nu_{ba}} \times 2.99792 \times 10^{-9} \text{ cm}^2. \quad (8)$$

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

$$A_{ba} = I_{ba}(T) \nu_{ba}^2 [Q_{rs}/g'] [e^{-E''/kT} - e^{-E'/kT}]^{-1} \times 2.7964 \times 10^{-16} \text{ s}^{-1} \quad (9)$$

$$\cong I_{ba}(T_0) \nu_{ba} [Q_{rs}(T_0)/g'] e^{E'/kT_0} \times 1.748 \times 10^{-9} \text{ s}^{-1} \quad (10)$$

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 $h\nu_{ba}$ 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:

$$\varepsilon_n^2 = \sum_{kj} \frac{\partial \nu_n}{\partial p_k} \frac{\partial \nu_n}{\partial p_j} V_{kj} \quad (11)$$

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

$$(V^{-1})_{kj} = \sum_m \frac{\partial \nu_m}{\partial p_k} \frac{\partial \nu_m}{\partial p_j} \varepsilon_m^{-2} \quad (12)$$

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

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 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 $^xS_{ba}$, 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.

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

$$\text{QNFMT} = Q100 + H10 + NQN$$

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 $\text{MOD}(Q, 5)$ 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

Type	Q	DR	Quantum order
Atom	0	0	$(J), (F), \dots$
Linear— Σ	1	2	$N, (J), (F_1), (F_2), (F)$
Linear—Case b	2	2	$N, \Lambda, (F_1), (F_2), (F)$
Linear—Case a ($2S + 1$ odd)	3	2	$J, \Omega, \Lambda, (F_1), (F_2), (F)$
Linear—Case a ($2S + 1$ even)	8	2	$J + \frac{1}{2}, \Omega + \frac{1}{2}, \Lambda, (F_1), (F_2), (F)$
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.
 4. DR is defined in Sec. 2.1.

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 . Hund'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 Brown et al.³ 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 ± 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

1. Poynter, R. L. and Pickett, H. M., Submillimeter, Millimeter, and Microwave Spectral Line Catalog. *Appl. Opt.*, 1985, **24**, 2235.
2. Pickett, H. M., Poynter, R. L., Cohen, E. A., Delitsky, M. L., Pearson, J. C. and Müller, H. S. P., *Submillimeter, Millimeter, and Microwave Spectral Line Catalog*. JPL Publication 80-23, Rev. 4, 1996, p. 4.
3. Brown, J. M. et al, *J. Mol. Spectrosc.*, 1975, **55**, 500.