

Submillimeter, Millimeter, and Microwave Spectral Line Catalog

H. M. Pickett, R. L. Poynter, E. A. Cohen,
M. L. Delitsky, J. C. Pearson, and H. S. P. Müller
Jet Propulsion Laboratory, California Institute of Technology,
Pasadena, CA 91109

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](ftp://spec.jpl.nasa.gov) and on the world wide web at <http://spec.jpl.nasa.gov>.

1 INTRODUCTION

This paper describes a publicly accessible catalog of submillimeter, millimeter, and microwave spectral lines in the frequency range between 0 and 10,000 GHz (i.e., wavelengths longer than $30\ \mu\text{m}$). 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 Section 2. Conversions between different measures of spectral line intensity are given in Section 3. General comments on the precision of the spectral line positions and intensities are given in Section 4. The format of quantum numbers as they appear in the catalog is given in Section 5.

Documentation for each molecular or atomic species is available in printed form as a JPL publication 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 *cttttt.cat*, where *ttttt* is the zero-filled catalog tag number. For example, the H atom line list is in the 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, LG INT, DR, ELO, GUP, **T A G**, QNF MT, QN', QN''
(F13.4, F8.4, F8.4, 12, 1"10.1, 13, 17, I4, 612, 612)

- FREQ: Frequency of the line in MHz.
 ERR: Estimated or experimental error of FREQ in MHz.
 LGINT: Base 10 logarithm of the integrated intensity in units of $\text{nm}^2 \cdot \text{MHz}$ 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).
 EL(): Lower state energy in eV relative to the lowest energy spire 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
(16,X,         A13,           I6,           7F7.4,      12)
```

- 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. 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 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:

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

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, 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 2.9'3792458 X 10*⁸.

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

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

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

where ν_{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 nm²·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, ${}^xS_{ba} \mu_x^2$ 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 vibrational-electronic state of the species. No vibrational partition function is included, except where explicitly stated in the documentation. Care is taken to assure that I_{ba} and Q_{rs} are determined with the same state degeneracies. For the catalog, Eq. (2) is evaluated for $T = T_0 = 300$ 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

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

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

where $n = 1$ for a linear molecule and $3/2$ for a nonlinear molecule. Eq. (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 $\text{nm}^2 \cdot \text{MHz}$, 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 $\alpha_{\max}L$, 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

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

in which m is the mass of the absorber (in atomic mass units). The explicit inverse temperature dependence in Eqs. (5) - (6) is due to the conversion of density to pressure units. There is also 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 p is $\exp(-\sigma_{ba}pL)$. 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

$$\begin{aligned}
 A_{ba} &= I_{ba}(T) \nu_{ba}^2 [Q_{rs}/g'] [e^{-E''/kT} - e^{-E'/kT}]^{-1} \times 2.7964 \times 10^{-16} \text{ sec}^{-1} & (9) \\
 &\cong I_{ba}(T_0) \nu_{ba} [Q_{rs}(T_0)/g] e^{E'/kT_0} \times 1.748 \times 10^9 \text{ sec}^{-1} & (10)
 \end{aligned}$$

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_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 anti 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.(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 $^x S_{ba}$, 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

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

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 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 A. Hund's case (a) quanta also have parity encoded in the A field. The correlation between parity and e,f designations should follow the recommendations of J. M. Brown *et al.*³ For reference, this convention is

TABLE 2. QUANTUM NUMBER FORMATS

Type	Q	D R	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 A 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 section 2.1.

For odd-spin multiplicity:
 if $p(-1)^{J+1/2} = -1$, then e
 if $p(-1)^{J+1/2} = 1$, then f

For even-spin multiplicity:
 if $p(-1)^J = 1$, then f
 if $p(-1)^J = -1$, 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.

ACKNOWLEDGEMENT

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

REFERENCES

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

Table 1: List of Species in the Catalog

Tag	Name	lines	Tag	Name	lines	Tag	Name	lines
1001	H-atom	1	41001	CH3CN v8= 0,1	29304	52013	CNCN	206
2001	D-atom	1	41002	CH3CC-13-H	822	53001	C2H3CN gs,v's	75697
3001	HD	1	41003	CH3C-13-CH	813	53002	Cl-37-O	2624
4001	H2D+	19	4100.1	C-13-H3CCH	821	53003	C-13-CCO	99
7001	Li-6-H	33	41005	CH3CCD	822	53004	CC-13-CO	99
8001	LiH	40	41006	CH2DCCH	223	53005	CC-C13-O	99
8002	Li-6-D	40	41007	SiC-13	2417	53006	Cl-37-O-v1	2132
9001	LiD	40	41008	CaH	387	53007	C2H3NC	9362
12001	C-atom	2	41009	CH3NC	1798	53008	HNCCN+	99
13001	C-13-atom	7	42001	CH3CN-15	2755	54001	CH2CHC-13-N	118
13002	CH	324	42002	CH2CO	835	54002	CH2C-13-HCN	117
13003	CH+	9	42003	NH2CN	13898	54003	C-13-H2CHCN	116
14001	N-atom	2	42004	CaD	501	54004	CH2CDCN	6381
14002	N-atom-1)-state	6	42005	K-41-H	40	54005	HOCl-37	6925
15001	NH	926	42006	C-13-H3CN	9015	54006	COCO-18	99
16001	C)-atom	2	42007	CH3C-13-N	8951	51007	HCCCHO	8407
17001	OH	788	42008	CH2DCN	19256	55001	C2H5CN	52883
17002	NH3	446	42009	H2CSi	670	56001	CH3CH2C-13-N	1183
17003	CH3D	80	42010	SiN	614	56002	CH3C-13-H2CN	1252
17004	NH3-v2	442	43001	CHDCO	886	56003	C-13-H3CH2CN	1183
18001	OD	912	43002	HNCO	6078	56004	C2H5CN-15	1621
18002	N-15-113	235	43003	AlO	1023	56005	CH2DCH2CN-s	1166
18003	H2O	783	43004	CP	397	56006	CH2DCH2CN-a	1286
18004	NH2D	5036	44001	Cs	51	56007	Ccs	563
18005	H2O-v2	292	44002	SiO	31	56008	C2H3CHO	24051
19001	HO-18	295	44003	CH3CHO-a	1347	56009	Mgs	99
19002	HDO	1401	44004	N2O	61	57001	C-13CS	1013
19003	1120-17	404	44005	CH3CHO-e	691	57002	CC-13S	1015
19004	H3O+	420	44006	DNCO	5504	58001	CCS-34	565
20001	1)20	1137	44007	HN-15-CO	888	58002	NaCl	99
20002	HF	8	44008	HNC-13-O	4332	60001	OCS	99
20003	H2O-18	726	44009	N2O-v2	146	60002	SiS	97
21001	1100-18	952	44010	HCP	34	60003	HCO(O)CH3-A	16153
21002	DF	20	44011	AlOH	766	60004	11 CO(O) CH3-E	17260
25001	CCH	114	44012	N2O-2v2	194	60005	NaCl-37	99
25002	NaH	52	45001	C-13-S	29	61001	OC-13-S	99
26001	CN, v = 0, 1	874	45002	Si-29-0	66	61002	Si-29-S	98
27001	HCN	40	45003	NH2CHO	3476	61003	C5H	2594
27002	HNC	49	45005	HCS+	64	62001	OC-34-S	99
27003	HCN-v2	132	45006	HNCO-18	4929	62002	O-18-CS	99
27004	C-13-N	1218	45007	NN-15-O	85	62003	Si-30-S	99
28001	c o	91	45008	N-15-NO	87	62004	SiS-34	99
28002	HC-13-N	45	45009	DCP	34	62005	AlCl	11525
28003	HCN-15	35	45010	HO CO+	1745	62006	C5D	4436
28004	DCN	54	45011	AlOD	70	63001	HNO3	36551
28005	HNC-13	34	45012	O-17-CO	285	63002	HNO3-v7	16478
28006	HN-15-C	33	45013	PN v= O-4	1637	63003	HNO3-v9	32404
28007	DNC	53	46001	CS-34	34	63001	HNO3-v6	15704
28008	HCNH+	74	46002	Si-30-O	67	63005	HNO3-v8	14537
28009	c o +	88	46003	H2CS	517	63006	HNO3-v5	13269
23001	C-13-O	60	46004	C2H5OH	12557	63007	PS	2340
29002	HCO+ v=0,4	246	46005	HCOOH	1888	G3008	PO2	7323
29003	CH2NH	2957	46006	NO2	16444	G1001	S2	174
29004	HCO	2454	46007	N2O-18	88	64002	SO2	13573
29005	NNH+	34	46008	CH3OCH3	21735	64003	AlCl-37	11326
29006	CO-17	50	46009	AlF	1188	G1004	C4O	535
29007	HOC+	40	46010	NS	2402	64005	S02-V2	9225
30001	CO- 18	60	46011	DOCO+	G77	65001	S-33-02	19048
30002	HC-13-O+	31	46012	HOC-13-O+	1735	G6001	COF2	23090
30003	1) O+	41	46013	o- 18-CO	91	GG002	S-3.1-02	1189-1
30001	H2CO	611	47001	H2C-13-S	110	66003	CaNC	259
30005	C-13-H2NH	439	47002	HC-13-OOH	1194	66004	SOO-18	9758
30006	CH2N-15-H	440	47003	DCOOH	628	(7001	OCl-35-O	57232
30007	CH2ND	1834	47004	HCOOD	612	68001	CCCS	99
30008	NO	1909	47005	[O t v= 0-4	239	69001	O(T-37-o	49388
30009	NND+	41	47006	PO	743	69002	C3H7CN	131319

Table 1: List of Species in the Catalog (con.)

Tag	Name	lines	Tag	Name	lines	Tag	Name	lines
30010	HOC-13+	40	48001	SO	330	70001	CCCS-3I	99
30011	NO+	154	48002	SO-v1	261	73001	C6H	3031
30012	DOC+	40	48003	H2CS-3I	111	74001	KCl	99
31001	HCO-18+	34	4800-1	O3	7089	74002	C2H5OOCH	60671
31002	112(3 -13-0	601	48005	O3-v2	4947	75001	HCCCCCN	99
31003	HDCO	4204	48006	O3-v1,3	9685	75002	H2NCH2COOH I	27217
31004	HO-18-C+	40	48007	O3-2v2	3031	75003	H2NCH2COOH II	26544
31005	HNO	10293	48008	O3-v1,3+v2	10912	76001	HCCCC-13-N	99
32001	O2	237	48009	NS-34	2364	76002	HCCCC-13-CN	99
32002	O2-v1	237	48010	so+	194	76003	HCCC-13-CCN	99
32003	CH3OH	709	49001	O3-sym-O-17	26092	76004	HCC-13-CCCN	99
32004	H2CO-18	449	49002	O3-asym-O-17	52613	76005	HC-13-CCCN	99
32005	O2-snglt-dlta	67	49003	C4H	742	76006	HCCCCCN- 15	99
32006	D2CO	3682	49004	MgCCH	274	76007	DCCCCCN	99
32007	DNO	14739	50001	S-34-O	280	76008	KCl-37	99
33001	H02	21954	50002	SO-18	179	76009	C4Si	229
33002	O-17-0	10787	50003	O3-sym-O-18	3184	76010	C5O	99
33003	SH v=0,1	646	50004	O3-asym-O-18	7304	79001	HOONO2	50775
34001	O-18-0	400	50005	O3-s- O18-v2	2387	80001	HBr-79	143
34002	H2S	1525	50006	O3-a-O18-v2	4213	81001	Cl-35-NO2	3520
34003	PH3	728	50007	CH3Cl-35	6372	82001	HBr-81	143
34004	H2O2	38357	50008	C3N	1351	88001	C6O	567
34005	SD	1125	50009	MgCN	273	89001	Sr-88-H	391
35001	HDS	1138	50010	MgNC	269	90001	Sr-88-D	922
36001	HCl	137	51001	HCCCN	139	92001	C5S	99
37001	DCl	228	51002	ClO	2585	94001	C5-34-S	99
37002	C3H	4990	51003	ClO-v1	2112	95001	Br-79-O	1892
37003	C-C3H	2973	51004	HCCNC	563	96001	HOBBr-79	9898
38001	HCl-37	137	51005	HCCNC-V7	291	97001	Br-81-O	1892
38002	c-C3H2	30436	51006	HCCNC-v6	291	97002	Cl-35-ONO2	78323
38003	C3D	1560	51007	HCCNC-v5	278	98001	H2S04	5690
38004	C- CCC-13-H	6541	51008	HNCCC	574	98002	HOBBr-81	9920
38005	c-C-13-CCH	9753	52001	HCCC-13-N	152	99001	Cl-37-ONO2	49505
38006	c-C3D	6001	52002	HCC-13-CN	146	99002	HC7N	518
39001	c-HC-13-CCH	17768	52003	HC-13-CCN	144	100001	C7O	99
39002	C- HCC-13-CH	6892	52004	HCCCN-15	99	102001	ClOOC1	17266
39003	c-C3HD	21610	52005	DCCCN	156	104001	Cl-37-OOC1	17482
39004	I) Cl-37	228	52006	HOCl	6929	111001	OBr-79-O	52631
40001	CH3CCH	813	52007	SiCC	30.1	112001	SC-80-02	7484
40002	NaOH	91	52008	CCCO	99	112002	C80	644
40003	SiC	982	52009	CH3Cl-37	6403	113001	OBr-81-O	52840
40004	SiC-v1	703	52010	CH2F2	11942	123001	HC9N	99
40005	KH	40	52011	CH2F2-v4	7808	124001	C9O	100
40006	C2O	354	52012	DNCCC	3098	147001	HC11N	99
40007	MgO v=0,1	88						