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The Cologne Database for Molecular Spectroscopy, CDMS

H. S. P. Müller, S. Thorwirth, D. A. Roth, and G. Winnewisser

I. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany

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Abstract. The computer-accessible Cologne Database for Molecular Spectroscopy (CDMS) contains a catalog of radio frequency and microwave to far-infrared spectral lines of atomic and molecular species that (may) occur in the interstellar or circumstellar medium or in planetary atmospheres. The catalog is continuously updated and is primarily intended to supplement existing data bases such as the JPL or NIST catalogs. Presently it contains entries for 111 species. Other sections of the database include information on the programs used for fitting spectra and creating the catalog entries, along with detailed information on some spectroscopy projects performed at the university of Cologne and a list of known inter- and circumstellar molecules. The database can be accessed online free of charge via `http://www.ph1.uni-koeln.de/vorhersagen/` or alternatively via the short-cut `http://www.cdms.de`.

Key words. line: identification – molecular data – ISM: molecules – radio lines: ISM – catalogs

1. Introduction

Ever since molecular lines have been detected from interstellar and circumstellar sources, their unequivocal assignment was substantially dependent on the availability of appropriately precise laboratory data. However, the availability of laboratory rest frequencies depends to a large extent on the frequency region of interest. Above 500 GHz the number density of measured transitions decreases fast. But, for example, around 663 GHz strong features of molecules as heavy as CH_3CN and even SO_2 reveal strong features towards the Orion A molecular cloud (Belov et al. 1998). More recently, Herpin & Cernicharo (2000) detected interstellar lines of CO, ^{13}CO, HCN, HNC, H_2O, and OH between 80 and 197 μm, which is equivalent to 4.2 and 1.7 THz, respectively. These observations were performed towards CRL 618 using the long wavelength spectrometer of the *Infrared Space Observatory*, ISO. Accurate rest frequencies up to ≈2 THz for the first four species were provided by our laboratory (Winnewisser et al. 1997; Klapper et al. 2000; Maiwald et al. 2000; Thorwirth et al. 2000).

In addition to the more familiar pure rotational transitions, also vibration rotation transitions originating predominantly from low-lying bending modes of, e.g., carbon chain molecules can be detected in the far-infrared region, as demonstrated for the ν_2 mode of the C_3 molecule (origin at 63.4 cm^{-1} or 1.9 THz) by Cernicharo et al. (2000) towards Sgr B2. Very recently, improved rest frequencies have been obtained by Giesen et al. (2001). Future missions such as the Stratospheric Observatory For Infrared Astronomy (SOFIA) and the Herschel Space Observatory, formerly known as FIRST, will extend high frequency observations by a substantial amount. This offers not only the possibility to observe (new) species at terahertz frequencies but also affords the knowledge of accurate rest frequencies.

One major goal of the Cologne Database for Molecular Spectroscopy (CDMS), which we have started to build recently, is to provide a catalog of pure rotational and ro-vibrational transition frequencies of atomic and molecular species from the radio frequency and microwave to the far-infrared regions (i.e. frequencies up to 14.3 THz or wavelengths longer than 21 μm). This section is called New Line Predictions. In addition, information on programs to fit and predict spectra, on spectroscopic data obtained in the Cologne laboratories, and on recent changes in the CDMS along with a list of known inter- and circumstellar molecules is available in separate sections of the CDMS. These sections are called Fitting Spectra, Cologne Spectroscopy Data, What's New, and Molecules in Space.

2. New line predictions section

Currently, the catalog contains pure rotational transition frequencies of atomic and molecular species. Vibration-rotation spectral information in the far infrared region, such as the bending mode of C_3 mentioned above, will be included shortly. This section of the CDMS is intended to be used as a planning guide or to facilitate the identification and analysis of observed spectral features in the interstellar and circumstellar region as well as in planetary atmospheres.

Send offprint requests to: H. S. P. Müller,
e-mail: `hspm@ph1.uni-koeln.de`

Table 1. Species in the CDMS catalog as of January 2001

Tag[a]	Name	Tag[a]	Name	Tag[a]	Name	Tag[a]	Name
012501	C-atom	040502[b]	CH_3CCH	049504	C_4H, $v_7 = 1$	060501	$CH_2(OH)CHO$
013501	^{13}C-atom	040503	KH	049505	C_4H, $v_7 = 2^0$	062501	l-H_2C_5
013502[b]	CH	042501[b]	H_2C_2O	049506	C_4H, $v_7 = 2^2$	063501	l-HC_4N
016501[b]	NH_2	043501	CP	049507	MgCCH	064501	c-SiC_3
024501	NaH	043502[c]	c-C_2H_4NH	050501	^{34}SO	064502[b]	SO_2, $v = 0$
025501	CCH	043503	MgF	050502	$S^{18}O$	064503[b]	SO_2, $v_2 = 1$
026501	CCD	043504	$C_2H_3NH_2$	050503	l-C_4H_2	064504	TiO
026502	^{13}CCH	044501	CS, $v = 0, 1$	050504[c]	MgNC, $v = 0$	064505	l-SiC_3
026503	$C^{13}CH$	044502	HCP, $v = 0$	050505	MgNC, $v_2 = 1$	065501	$^{33}SO_2$
027501[b]	HCN, $v = 0$	044503	HCP, $v_2 = 1$	050506	C_4D	065502[c]	$SO^{17}O$
027502[b]	HNC, $v_2 = 0, 1$	044504	c-C_2H_4O	051501	HCCCN, (0000)	065503	CH_3C_3N
028501[b,c]	$H^{13}CN$	044505	SiO, $v = 0 - 6$	051502	HCCCN, (0001)	066501[b]	$^{34}SO_2$
028502	H_2CN	045501	^{13}CS, $v = 0, 1$	051503	HCCCN, (0002)	066502	$SO^{18}O$
028503[b]	CO, $v = 0$	045502	$C^{33}S$, $v = 0, 1$	051504	HCCCN, (0010)	066503	CaNC
029501[b]	^{13}CO	045503	DCP	051505	HCCCN, (0011)	068501	FeC
030501	H_2CO	045504	^{29}SiO, $v = 0 - 3$	051506	HCCCN, (1000)	068502	HCCCP
031501	HDCO	046501	$C^{34}S$, $v = 0, 1$	051507	HCCCN, (1001)	069501	NCCP
031502[b]	$^{13}C^{18}O$	046502	^{30}SiO, $v = 0 - 3$	051508	HCCCN, (0100)/(0003)	074501	C_5N
031503	$H_2^{13}CO$	046502	$Si^{18}O$, $v = 0 - 3$	051509	HCCCN, (1002)/$(0200)^{0e}$	074502	l-H_2C_6
031504	H_2COH^+	047501	$^{13}C^{34}S$	051510	KC	076501	NC_3NC
031505	CF	048501	SO, $v = 0$	052501	CCCO	076502	SiC_4
032501[b]	PH	048502	SO, $v = 1$	052502	^{36}SO	085501	C_7H
032502	D_2CO	048503	$C^{36}S$	052503	HC_3NH^+	088501	SiC_5
032503	$H_2C^{18}O$	048504	SO, $^1\Delta$, $v = 0, 1$	052504	KCH	097501	C_8H
036501	NaCH	048505	NaCCH	053501[c]	AlNC	100501	SiC_6
038501	l-C_3H_2	049501	^{33}SO	054501	SiCN	109501	C_9H
039501	HCCN	049502	$S^{17}O$	056501	HCCP	121501	$C_{10}H$
040501	SiC, $v = 0$	049504	C_4H, $v = 0$	059501[c]	MgCl		

[a] The six digit tag consists of the molecular weight in atomic mass units for the first three digits, of a 5, and of two counting numbers to distinguish between entries with the same molecular weight.

[b] Entry also available in units of cm^{-1}.

[c] Entry also available with/without hyperfine splitting.

Because of the great number of astrochemically and – physically relevant species and the various isotopomers as well as vibrationally excited states, the focus is presently on supplementing existing databases such as the Jet Propulsion Laboratory (JPL) catalog (Pickett et al. 1998) and the NIST recommended rest frequencies database (Lovas 1992). Currently, there are 111 atomic and molecular species in the CDMS catalog which are presented in Table 1. The majority of these are species that have been detected recently during astronomical or laboratory investigations. However, several entries are also present in one of the catalogs mentioned above, but generally with a less extensive data set.

The catalog part consists of three subsections: the new line predictions main page, the catalog entries page, and the catalog search page.

Some general information is given on the catalog main page. It includes a brief, color-coded description of the structure of the entries including units as well as some useful equations.

The catalog entries page gives the six-digit molecule tag **tttttt**, which is the sorting criterion, the chemical formula or name, the number of lines for this entry, the current version number, the catalog entry file having the name **cttttttt.cat**, the documentation file called **ettttttt.cat**, and the date of the generation of the current entry version. The six-digit tag consists of the molecular weight in atomic mass units for the first three digits, a 5, and two digits for counting species with the same molecular weight.

The catalog entry itself has one line of 80 characters for each spectral feature as demonstrated in Table 2 for a detail of the $H_2^{13}CO$ entry. The intensity $I(T)$ of the spectral feature is calculated according to

$$I(T) = (8\pi^3/3hc)\,\nu\,S_g\,\mu_g^2\,(\mathrm{e}^{-E''/kT} - \mathrm{e}^{-E'/kT})/Q_{\mathrm{rs}}(T), \quad (1)$$

(e.g. Pickett et al. 1998) where ν and S_g are line frequency and strength, respectively, μ_g is the dipole moment along the molecular g-axis, E'' and E' are the lower and upper state energy, respectively, and Q_{rs} is the rotation-spin partition function at the temperature T. The default temperatur in the catalog is 300 K, but other temperatures may be requested in the catalog search form, see below. Additional equations relating I to the absorption cross

Table 2. Explanation of catalog entry, format (in parentheses), and units using the example of $H_2^{13}CO$

```
Frequency^a  | Uncert.^b | Intensity^c |D^d| E_lower^e  |g_up^f| Tag^g |QnF^h|   Qn'^i    |   Qn"^k
031503 H2C-13-O
. . .
 1845136.0780  0.2500 -2.2680 3 1064.3477 53 -31503 30326 621      25 620
 1845148.7520  0.2500 -2.2680 3 1064.3484 53 -31503 30326 620      25 619
 1845226.6490  0.1000 -1.3157 3  844.7128159 -31503 30326 324      25 323
 1848201.2566  0.0330 -1.5964 3  975.1317159  31503 30326 522      25 521
 1848551.4238  0.0330 -1.5963 3  975.1567159  31503 30326 521      25 520
 1851234.8117  0.0312 -1.9146 3  902.3434 53  31503 30326 423      25 422
 1855045.8383  0.0087 -3.6914 3  142.4349 63  31503 30310 3 8      10 1 9
. . .
```

[a] Calculated or experimental frequency in MHz (F13.4) or in cm^{-1} (F13.6), see b and g. Vertical lines show how far the respective field extends.

[b] Calculated or experimental uncertainty of line in MHz (F8.4) if ≥ 0 or in cm^{-1} (F8.5) if ≤ 0, see also g.

[c] Base 10 logarithm of the integrated intensity at 300 K in nm^2 MHz (F8.4); see Eq. (1).

[d] Degree of freedom (I2) in the rotational partition function (0 for atoms, 2 for linear molecules, 3 for nonlinear molecules).

[e] Lower state energy in cm^{-1} (F10.4) relative to the lowest energy level in the ground vibronic state.

[f] Upper state degeneracy; $g_{\mathrm{up}} = g_{\mathrm{I}} \times g_{\mathrm{N}}$ (I3); with g_{I} the spin-statistical weight and $g_{\mathrm{N}} = 2N + 1$ the rotational degeneracy.

[g] Molecule tag (I7); see Table 1 or text. A negative value indicates that both frequency and uncertainty are experimental values.

[h] Coding for the format of the quantum numbers (I4). $QnF = 100 \times Q + 10 \times H + N_{Qn}$; N_{Qn} is the number of quantum numbers for each state; H indicates the number of half integer quantum numbers; Qmod5, the residual when Q is devided by 5, gives the number of principal quantum numbers (without the spin designating ones). Thus, Q is 0 for atoms, 1 for linear molecules in Σ states, 2 for symmetric rotors or linear molecules in states other than Σ. Add 11 if several states, e.g. vibrational, are fit together; add 20 if two spins are coupled to $\mathrm{I}_{\mathrm{tot}}$; and add 40 if aggregate quantum number is used because otherwise more than 6 quantum numbers would be needed. In the present case, 303 indicates that there are three principal quantum numbers and a total of three quantum numbers for each state with no quantum number being half integer.

[i] Quantum numbers for the upper state (6×I2): N; K_a, K_c or parity&K; v; F_1, . . . F, as far as applicable. Half integer quantum numbers are rounded up. Here the three quantum numbers are $N = J$ (26, 26, 26, etc.), because there are no unpaired electrons present in the molecule; K_a (6, 6, 3, etc.); and K_c (21, 20, 24, etc.).

[k] Quantum numbers for the lower state (6×I2) as in i.

section σ, the A-value, or other quantities can be found, for example, on the catalog main page or in Pickett et al. (1998).

The catalog entries have been generated by least-squares fitting of published spectral lines to accepted spectroscopic models. The predicted line frequencies and their uncertainties are derived from the resulting fitted parameters and their covariance. For the sake of transferability and comparability, mostly the same programs are used for the CDMS as for the JPL catalog (Pickett 1991), therefore, both formats are identical in general. As a consequence, most of the description of the JPL catalog given by Pickett et al. (1998) applies also to the catalog section of the CDMS.

The documentation gives the tag number, chemical formula, frequently the proper chemical name along with trivial names, the electronic or vibrational state, in particular if it is not a singlet state with $v = 0$, the version number and the name of the creator of the entry, some information on the data used for the fit including special considerations. Furthermore, values for the number of lines, the highest frequency and J quantum numbers, the rotational constants, dipole components, the partition function at certain temperatures, intensity cut-offs, the energy of the state, and the (terrestrial) isotopic correction for the intensity are listed in the documentation.

The partition function (Q_{rs}) in the documentation takes into account rotation, splitting caused by the electron or nuclear spin, and spin statistics. Care is taken to ensure proper calculation of the partition function even at high temperatures. Vibrational or electronic corrections are generally not considered mainly because of lacking data; exceptions are noted. For heavier molecules, the vibrational corrections to the partition function may be substantial even at fairly low temperatures. Thus, neglect of vibrational corrections to the partition function constitutes a possible major source of error in the calculation of the intensities. Additional large errors may stem from the fact that the dipole components or their centrifugal distortion corrections are not or only with moderate precision known experimentally.

Finally, a search form offers the opportunity to scan for transition frequencies of certain species (including all) in desired frequency ranges. The output can be displayed in tabular or graphic form. In addition, intensities may be recalculated for temperatures of 225, 150, 75, 37.5, 18.75,

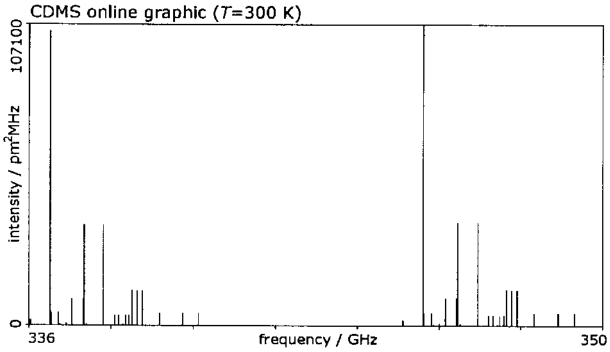

Fig. 1. Graphic output of a search for transitions of all available vibrational states of HCCCN between 336 and 350 GHz at 300 K

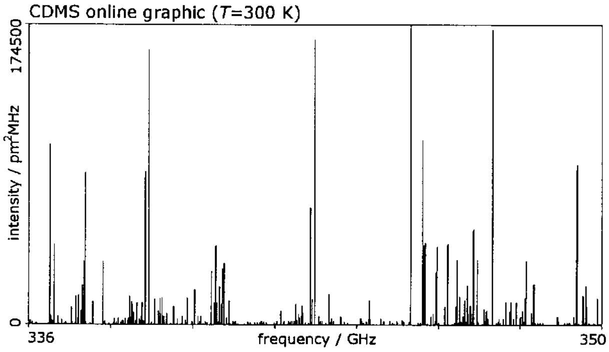

Fig. 2. Graphic output of a search for transitions of all species contained in the CDMS between 336 and 350 GHz at 300 K

and 9.375 K besides the default temperature of 300 K. Currently we are working on an option to calculate A-values instead of intensities. Figures 1 and 2 show graphic outputs for all available vibrational states of HC_3N and all molecules contained in the catalog, respectively, between 336 and 350 GHz at 300 K. It is intended to include online labeling of the graphic output.

3. Fitting spectra section

Another section of the CDMS gives information and examples to the programs that are used to fit spectra and to generate predictions of transition frequencies. At present, information is available only on the JPL spectroscopy programs (Pickett 1991). The examples include diatomics as well as linear, symmetric, and asymmetric polyatomic molecules. Singlet, doublet, and triplet molecules are included. For linear molecules, the different electronic states Σ, Π, and Δ are covered. Simple examples include CO ($^1\Sigma^+$), CO^+ ($^2\Sigma^+$), C_4O ($^3\Sigma^-$), NF (a $^1\Delta$), TiO ($^3\Delta$), the symmetric top molecule CH_3CCH, the asymmetric H_2S, H_2CO, H_2COH^+, and the asymmetric radical DSS. More complicated examples with nuclear ($SOCl_2$) or with electron spin interaction, such as SiC ($^3\Pi_i$), or both, e.g. CH ($^2\Pi_r$), NH_2 ($^2B_1$), and OBrO ($^2B_1$), are also included as are examples with vibration rotation interaction, such as $ClNO_2$, C_3H, and CH_2CHNH_2.

Information on additional programs will be available in the future.

4. Cologne spectroscopy data section

Details related to spectroscopic projects performed in the Cologne laboratories are presented in this section for the convenience of other spectroscopists. Information that is too extensive to be published fully in a refereed journal can be included, for example the output of a fitting procedure which includes the full correlation matrix among other details.

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