Complex Molecules in Space: Present Status and Prospects with ALMA
8–11 May 2006, Fuglsøcentret, Denmark

The Cologne Database for Molecular Spectroscopy, and Requirements of Laboratory Spectroscopy for ALMA

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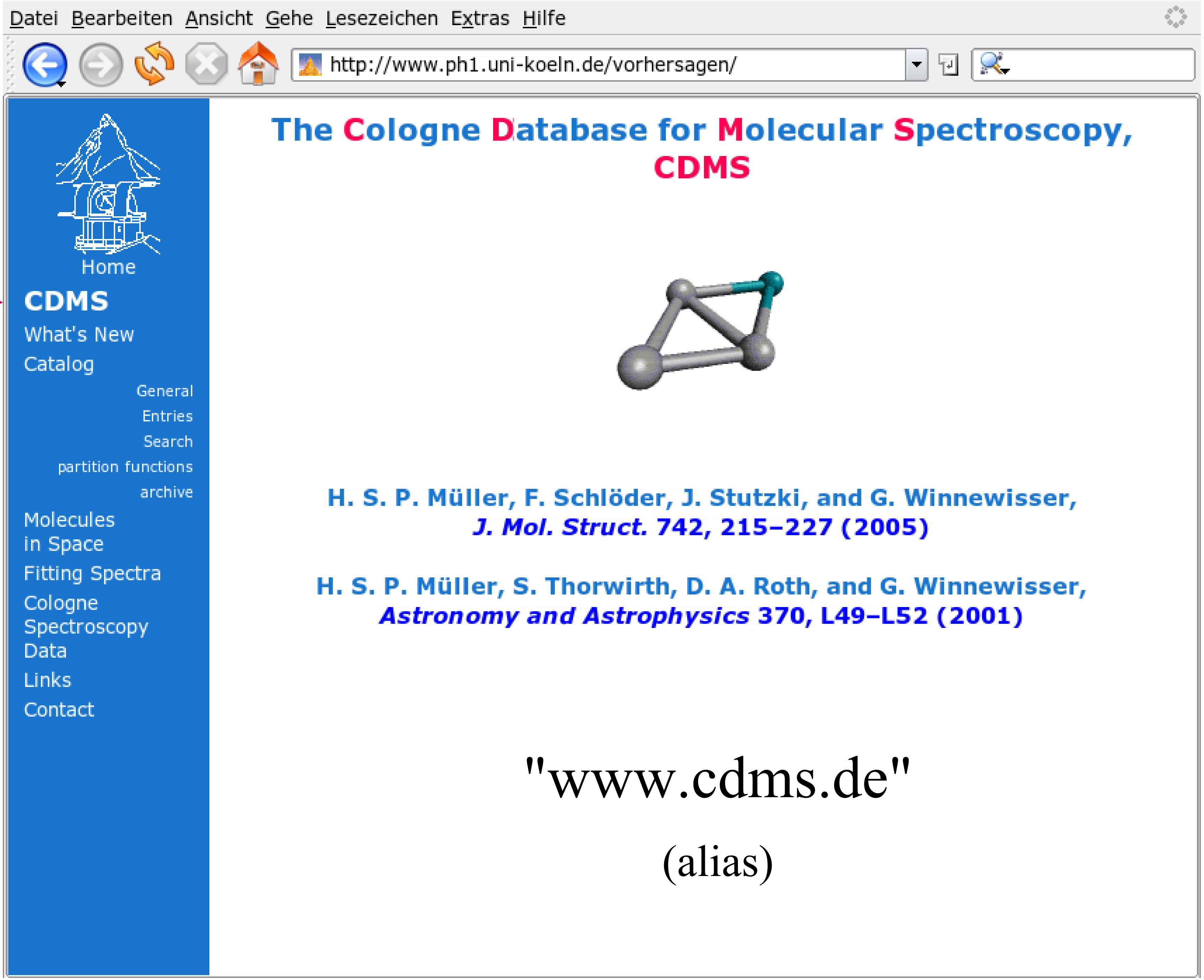


The Cologne Database for Molecular Spectroscopy, CDMS

H. S. P. Müller, F. Schlöder, J. Stutzki, and G. Winnewisser,
J. Mol. Struct. 742, 215–227 (2005)

H. S. P. Müller, S. Thorwirth, D. A. Roth, and G. Winnewisser,
Astronomy and Astrophysics 370, L49–L52 (2001)

"www.cdms.de"

(alias)

CDMS Catalog: Basic Facts

- line lists for molecules of astrochemical and astrophysical interest
  not restricted to observed species
- separate entries for different molecules, isotopic species, vibrational states
- entries created from fitting existing (laboratory) data
- only such catalog publically available – besides that from JPL
- entries for 372 species – 179+ have been detected
- ~ 5 – 10 new or updated entries each month
- important source of spectroscopic information for many web tools

What Do We Want from Laboratory Spectroscopists ?

- experimental line lists – in particular also for IR data

- evaluate uncertainties critically – and state them

- electronic files can be helpful

- publication of predictions not necessary for standard problems

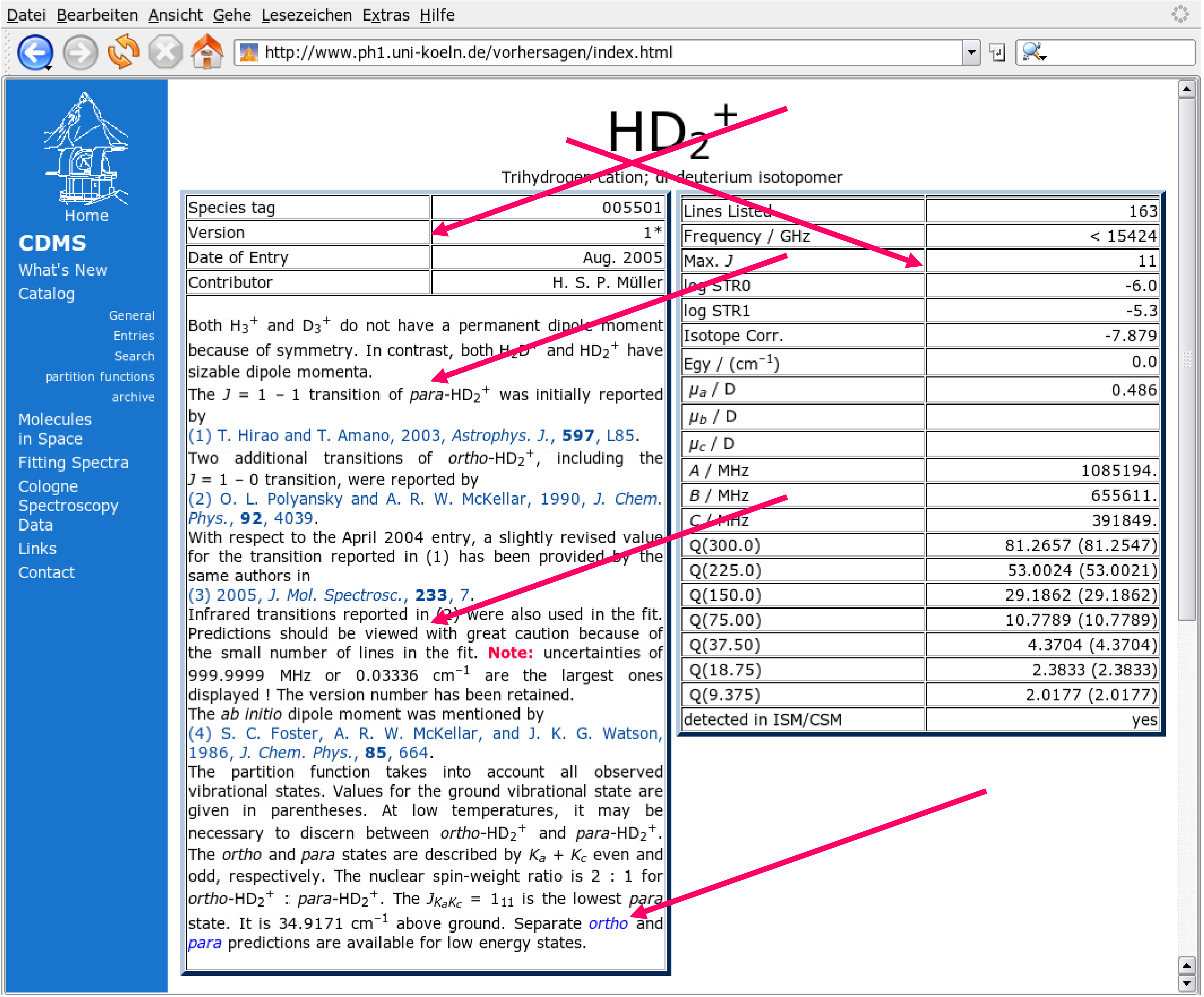
- in case of predictions for non-standard problems
  - consider sufficient quantum number range
  - provide info. on I, $S\mu^2$, or A
  - provide info. on Q (including treatment of spin-statistic)

What Do We Want from Observers ?

- which molecule needs attention
- which isotopic species need consideration
- some indications on the quantum number range (including that for vibrations)

What Do We Offer ?

- transition frequencies with uncertainties
- I @ 300 K (or selected other Ts) or $S\mu^2$ or A
- quantum numbers
- E_{lower}, g_{up} etc.
- background information on species



http://www.ph1.uni-koeln.de/vorhersagen/index.html

HD_2^+

Trihydrogen cation; di-deuterium isotopomer

Species tag	005501
Version	1*
Date of Entry	Aug. 2005
Contributor	H. S. P. Müller

Both H_3^+ and D_3^+ do not have a permanent dipole moment because of symmetry. In contrast, both H_2D^+ and HD_2^+ have sizable dipole momenta.
The $J = 1 - 1$ transition of *para*-HD_2^+ was initially reported by
(1) T. Hirao and T. Amano, 2003, *Astrophys. J.*, **597**, L85.
Two additional transitions of *ortho*-HD_2^+, including the $J = 1 - 0$ transition, were reported by
(2) O. L. Polyansky and A. R. W. McKellar, 1990, *J. Chem. Phys.*, **92**, 4039.
With respect to the April 2004 entry, a slightly revised value for the transition reported in (1) has been provided by the same authors in
(3) 2005, *J. Mol. Spectrosc.*, **233**, 7.
Infrared transitions reported in (2) were also used in the fit. Predictions should be viewed with great caution because of the small number of lines in the fit. **Note:** uncertainties of 999.9999 MHz or 0.03336 cm^{-1} are the largest ones displayed ! The version number has been retained.
The *ab initio* dipole moment was mentioned by
(4) S. C. Foster, A. R. W. McKellar, and J. K. G. Watson, 1986, *J. Chem. Phys.*, **85**, 664.
The partition function takes into account all observed vibrational states. Values for the ground vibrational state are given in parentheses. At low temperatures, it may be necessary to discern between *ortho*-HD_2^+ and *para*-HD_2^+. The *ortho* and *para* states are described by $K_a + K_c$ even and odd, respectively. The nuclear spin-weight ratio is 2 : 1 for *ortho*-HD_2^+ : *para*-HD_2^+. The $J_{K_aK_c} = 1_{11}$ is the lowest *para* state. It is 34.9171 cm^{-1} above ground. Separate *ortho* and *para* predictions are available for low energy states.

Lines Listed	163
Frequency / GHz	< 15424
Max. J	11
log STR0	-6.0
log STR1	-5.3
Isotope Corr.	-7.879
Egy / (cm^{-1})	0.0
μ_a / D	0.486
μ_b / D	
μ_c / D	
A / MHz	1085194.
B / MHz	655611.
C / MHz	391849.
Q(300.0)	81.2657 (81.2547)
Q(225.0)	53.0024 (53.0021)
Q(150.0)	29.1862 (29.1862)
Q(75.00)	10.7789 (10.7789)
Q(37.50)	4.3704 (4.3704)
Q(18.75)	2.3833 (2.3833)
Q(9.375)	2.0177 (2.0177)
detected in ISM/CSM	yes

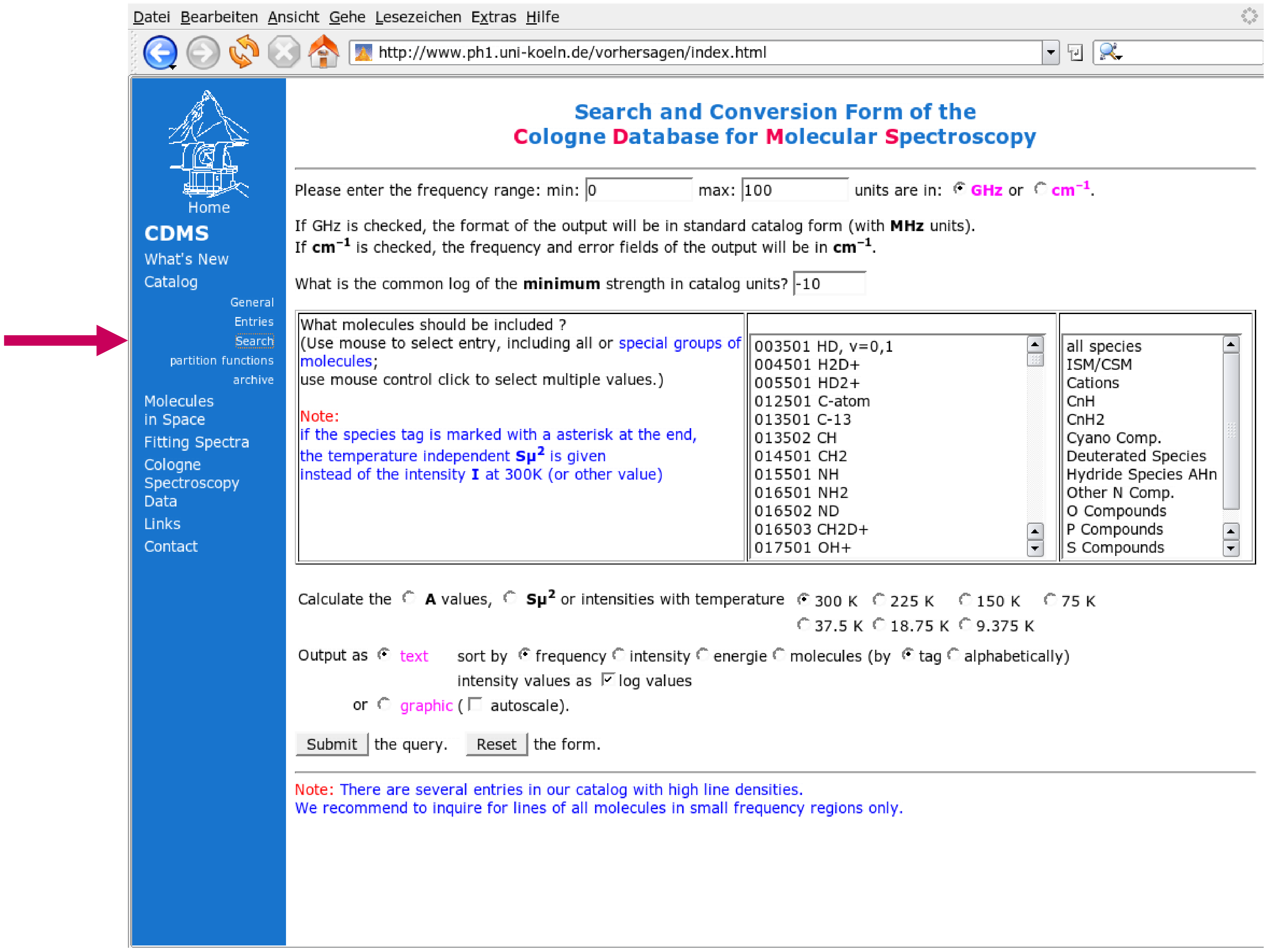
Remark on *ortho* and *para* Conversion

Obviously, *ortho*-*para* conversion can be neglected? **NO !!**

Matrix elements exist usually which will cause *ortho*-*para* conversion.
(Exception: nuclei on symmetry axis)

Effects of small matrix elements may be enhanced
through appropriately interacting energy levels.
E.g. $\boldsymbol{C_{ab}}$ in $\mathbf{AH_2}$ molecules

Larger matrix elements may exits for radicals;
e.g. $\boldsymbol{T_{ab}}$ in $\mathbf{NH_2}$.
Largest effect between levels $\mathbf{1_{11}}$ and $\mathbf{1_{01}}$!



Search and Conversion Form of the Cologne Database for Molecular Spectroscopy

Please enter the frequency range: min: 0 max: 100 units are in: ● GHz or ○ cm^{-1}.

If GHz is checked, the format of the output will be in standard catalog form (with **MHz** units).
If $\mathbf{cm^{-1}}$ is checked, the frequency and error fields of the output will be in $\mathbf{cm^{-1}}$.

What is the common log of the **minimum** strength in catalog units? -10

What molecules should be included ?
(Use mouse to select entry, including all or special groups of molecules;
use mouse control click to select multiple values.)

Note:
if the species tag is marked with a asterisk at the end,
the temperature independent $\mathbf{S\mu^2}$ is given
instead of the intensity **I** at 300K (or other value)

003501 HD, v=0,1
004501 H2D+
005501 HD2+
012501 C-atom
013501 C-13
013502 CH
014501 CH2
015501 NH
016501 NH2
016502 ND
016503 CH2D+
017501 OH+

all species
ISM/CSM
Cations
CnH
CnH2
Cyano Comp.
Deuterated Species
Hydride Species AHn
Other N Comp.
O Compounds
P Compounds
S Compounds

Calculate the ○ **A** values, ○ $\mathbf{S\mu^2}$ or intensities with temperature ● 300 K ○ 225 K ○ 150 K ○ 75 K ○ 37.5 K ○ 18.75 K ○ 9.375 K

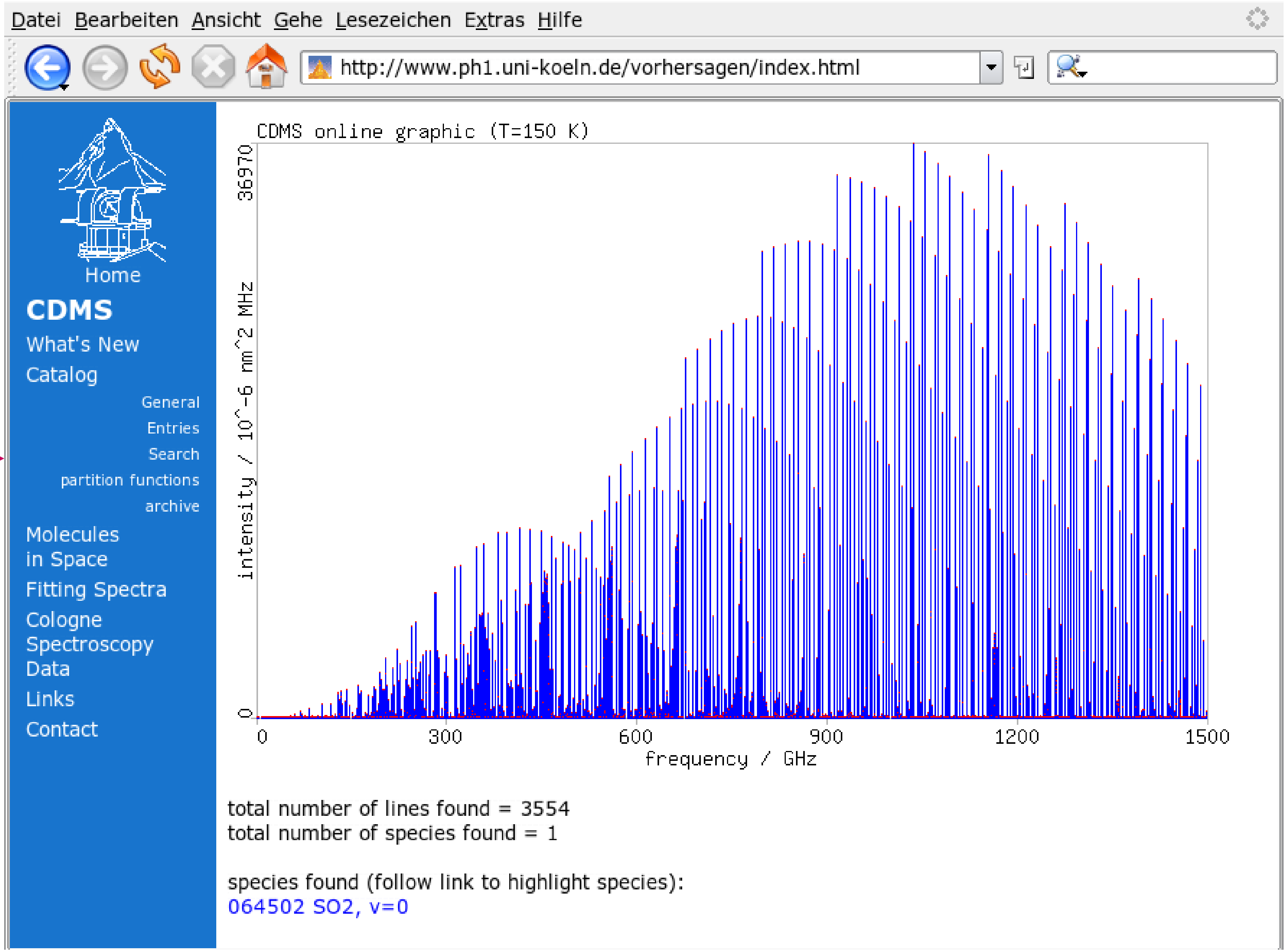
Output as ● text sort by ● frequency ○ intensity ○ energie ○ molecules (by ● tag ○ alphabetically)
intensity values as ☑ log values
or ○ graphic (☐ autoscale).

the query.

the form.

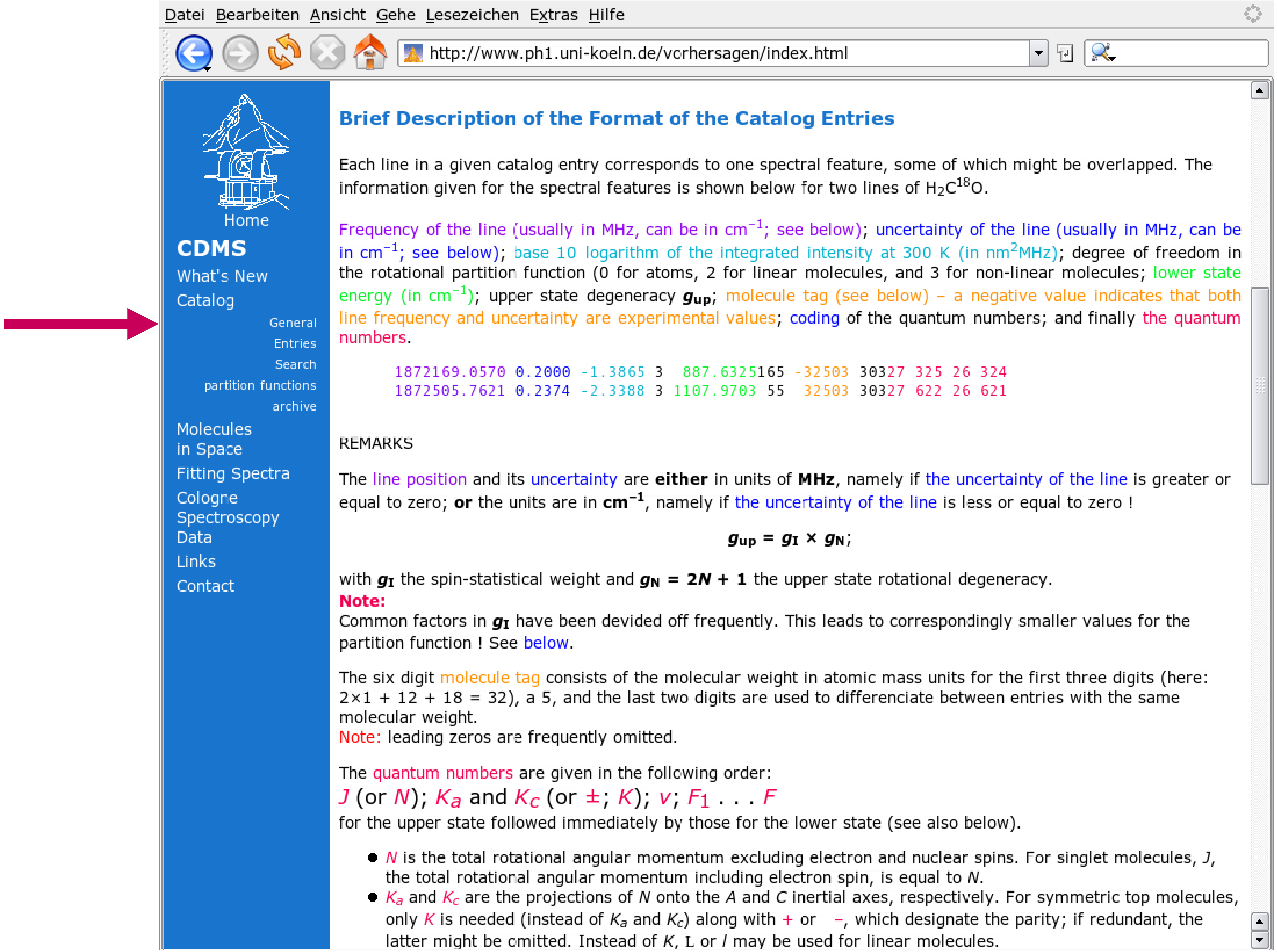
Note: There are several entries in our catalog with high line densities.
We recommend to inquire for lines of all molecules in small frequency regions only.

Graphic Output for SO_2 at 150 K



total number of lines found = 3554
total number of species found = 1

species found (follow link to highlight species):
064502 SO2, v=0



Brief Description of the Format of the Catalog Entries

Each line in a given catalog entry corresponds to one spectral feature, some of which might be overlapped. The information given for the spectral features is shown below for two lines of $H_2C^{18}O$.

Frequency of the line (usually in MHz, can be in cm^{-1}; see below); uncertainty of the line (usually in MHz, can be in cm^{-1}; see below); base 10 logarithm of the integrated intensity at 300 K (in nm^2MHz); degree of freedom in the rotational partition function (0 for atoms, 2 for linear molecules, and 3 for non-linear molecules; lower state energy (in cm^{-1}); upper state degeneracy g_{up}; molecule tag (see below) – a negative value indicates that both line frequency and uncertainty are experimental values; coding of the quantum numbers; and finally the quantum numbers.

```
1872169.0570 0.2000 -1.3865 3  887.6325165 -32503 30327 325 26 324
1872505.7621 0.2374 -2.3388 3 1107.9703 55  32503 30327 622 26 621
```

REMARKS

The line position and its uncertainty are **either** in units of **MHz**, namely if the uncertainty of the line is greater or equal to zero; **or** the units are in $\mathbf{cm^{-1}}$, namely if the uncertainty of the line is less or equal to zero !

$$g_{up} = g_I \times g_N;$$

with g_I the spin-statistical weight and $g_N = 2N + 1$ the upper state rotational degeneracy.

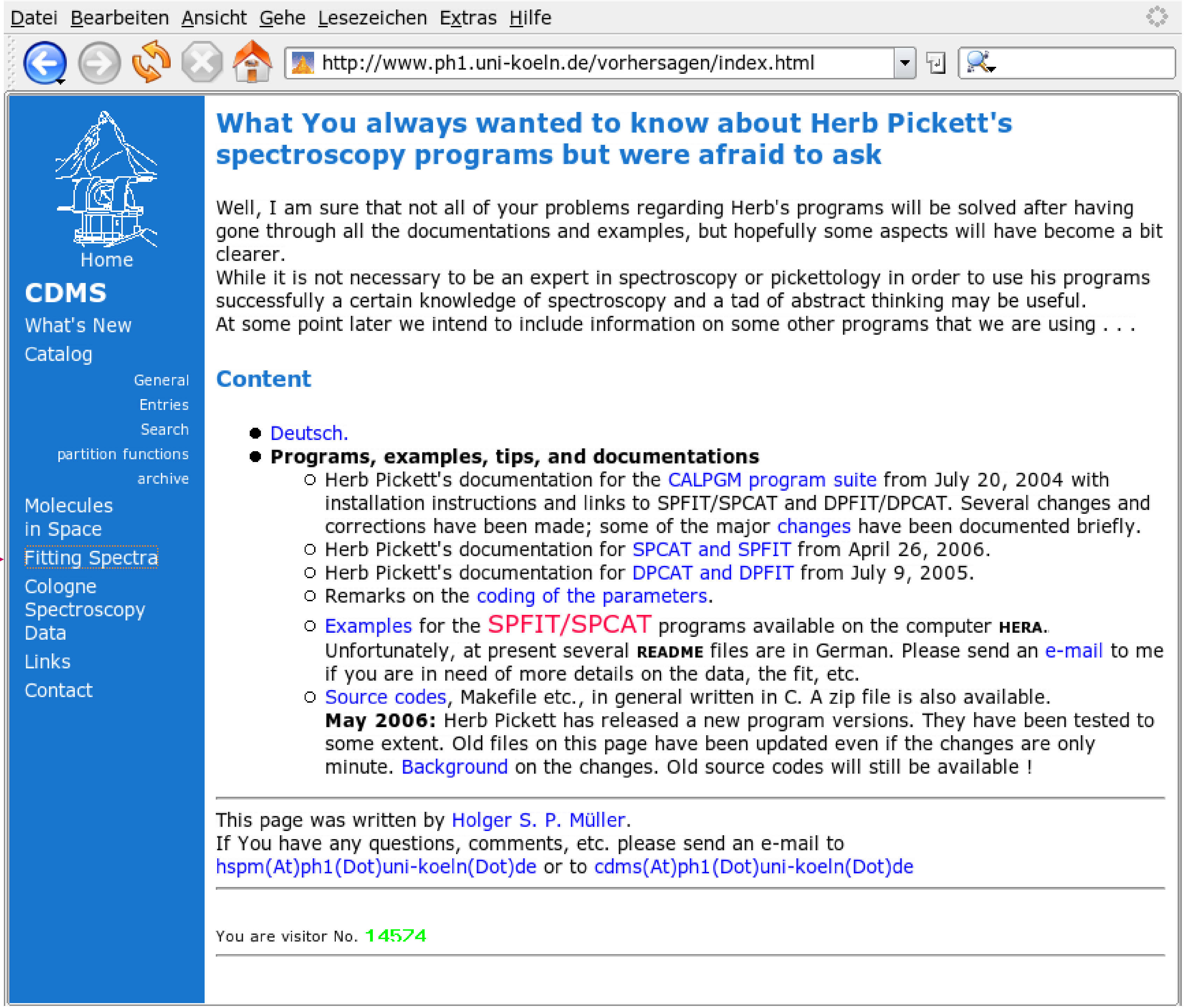
Note:

Common factors in g_I have been devided off frequently. This leads to correspondingly smaller values for the partition function ! See below.

The six digit molecule tag consists of the molecular weight in atomic mass units for the first three digits (here: 2×1 + 12 + 18 = 32), a 5, and the last two digits are used to differenciate between entries with the same molecular weight.
Note: leading zeros are frequently omitted.

The quantum numbers are given in the following order:
J (or N); K_a and K_c (or ±; K); v; F_1 . . . F
for the upper state followed immediately by those for the lower state (see also below).

- N is the total rotational angular momentum excluding electron and nuclear spins. For singlet molecules, J, the total rotational angular momentum including electron spin, is equal to N.
- K_a and K_c are the projections of N onto the A and C inertial axes, respectively. For symmetric top molecules, only K is needed (instead of K_a and K_c) along with + or −, which designate the parity; if redundant, the latter might be omitted. Instead of K, Λ or l may be used for linear molecules.



What You always wanted to know about Herb Pickett's spectroscopy programs but were afraid to ask

Well, I am sure that not all of your problems regarding Herb's programs will be solved after having gone through all the documentations and examples, but hopefully some aspects will have become a bit clearer.
While it is not necessary to be an expert in spectroscopy or pickettology in order to use his programs successfully a certain knowledge of spectroscopy and a tad of abstract thinking may be useful.
At some point later we intend to include information on some other programs that we are using . . .

Content

- Deutsch.
- **Programs, examples, tips, and documentations**
  - Herb Pickett's documentation for the CALPGM program suite from July 20, 2004 with installation instructions and links to SPFIT/SPCAT and DPFIT/DPCAT. Several changes and corrections have been made; some of the major changes have been documented briefly.
  - Herb Pickett's documentation for SPCAT and SPFIT from April 26, 2006.
  - Herb Pickett's documentation for DPCAT and DPFIT from July 9, 2005.
  - Remarks on the coding of the parameters.
  - Examples for the SPFIT/SPCAT programs available on the computer **HERA**. Unfortunately, at present several **README** files are in German. Please send an e-mail to me if you are in need of more details on the data, the fit, etc.
  - Source codes, Makefile etc., in general written in C. A zip file is also available. **May 2006:** Herb Pickett has released a new program versions. They have been tested to some extent. Old files on this page have been updated even if the changes are only minute. Background on the changes. Old source codes will still be available !

This page was written by Holger S. P. Müller.
If You have any questions, comments, etc. please send an e-mail to
hspm(At)ph1(Dot)uni-koeln(Dot)de or to cdms(At)ph1(Dot)uni-koeln(Dot)de

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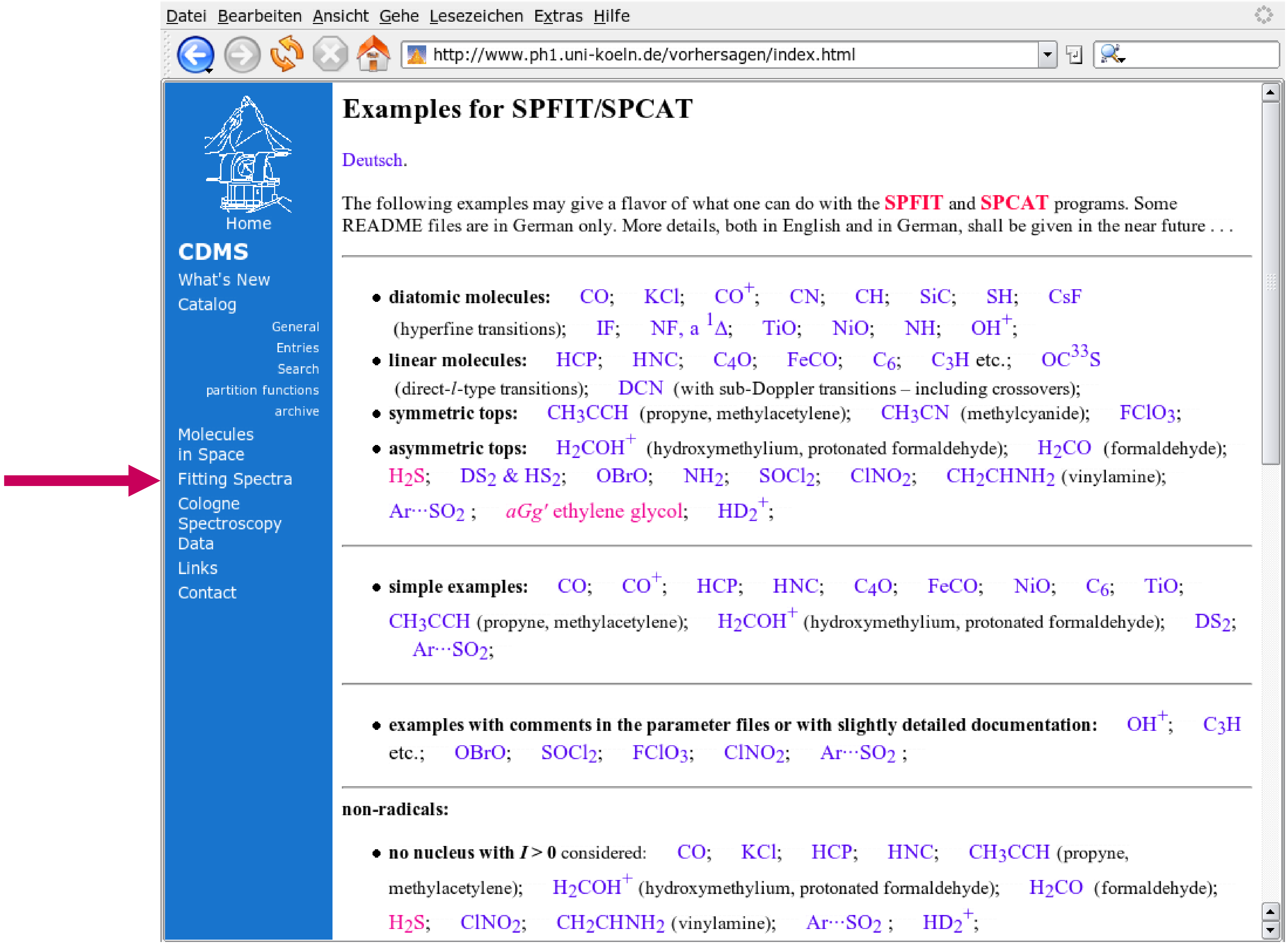
You are visitor No. 14574



Examples for SPFIT/SPCAT

Deutsch.

The following examples may give a flavor of what one can do with the **SPFIT** and **SPCAT** programs. Some README files are in German only. More details, both in English and in German, shall be given in the near future . . .

- **diatomic molecules:** CO; KCl; CO^+; CN; CH; SiC; SH; CsF (hyperfine transitions); IF; NF, a $^1\Delta$; TiO; NiO; NH; OH^+;
- **linear molecules:** HCP; HNC; C_4O; FeCO; C_6; C_3H etc.; $OC^{33}S$ (direct-l-type transitions); DCN (with sub-Doppler transitions – including crossovers);
- **symmetric tops:** CH_3CCH (propyne, methylacetylene); CH_3CN (methylcyanide); $FClO_3$;
- **asymmetric tops:** H_2COH^+ (hydroxymethylium, protonated formaldehyde); H_2CO (formaldehyde); H_2S; DS_2 & HS_2; OBrO; NH_2; $SOCl_2$; $ClNO_2$; CH_2CHNH_2 (vinylamine); $Ar\cdots SO_2$; *aGg′* ethylene glycol; $HD_2{}^+$;

- **simple examples:** CO; CO^+; HCP; HNC; C_4O; FeCO; NiO; C_6; TiO; CH_3CCH (propyne, methylacetylene); H_2COH^+ (hydroxymethylium, protonated formaldehyde); DS_2; $Ar\cdots SO_2$;

- **examples with comments in the parameter files or with slightly detailed documentation:** OH^+; C_3H etc.; OBrO; $SOCl_2$; $FClO_3$; $ClNO_2$; $Ar\cdots SO_2$;

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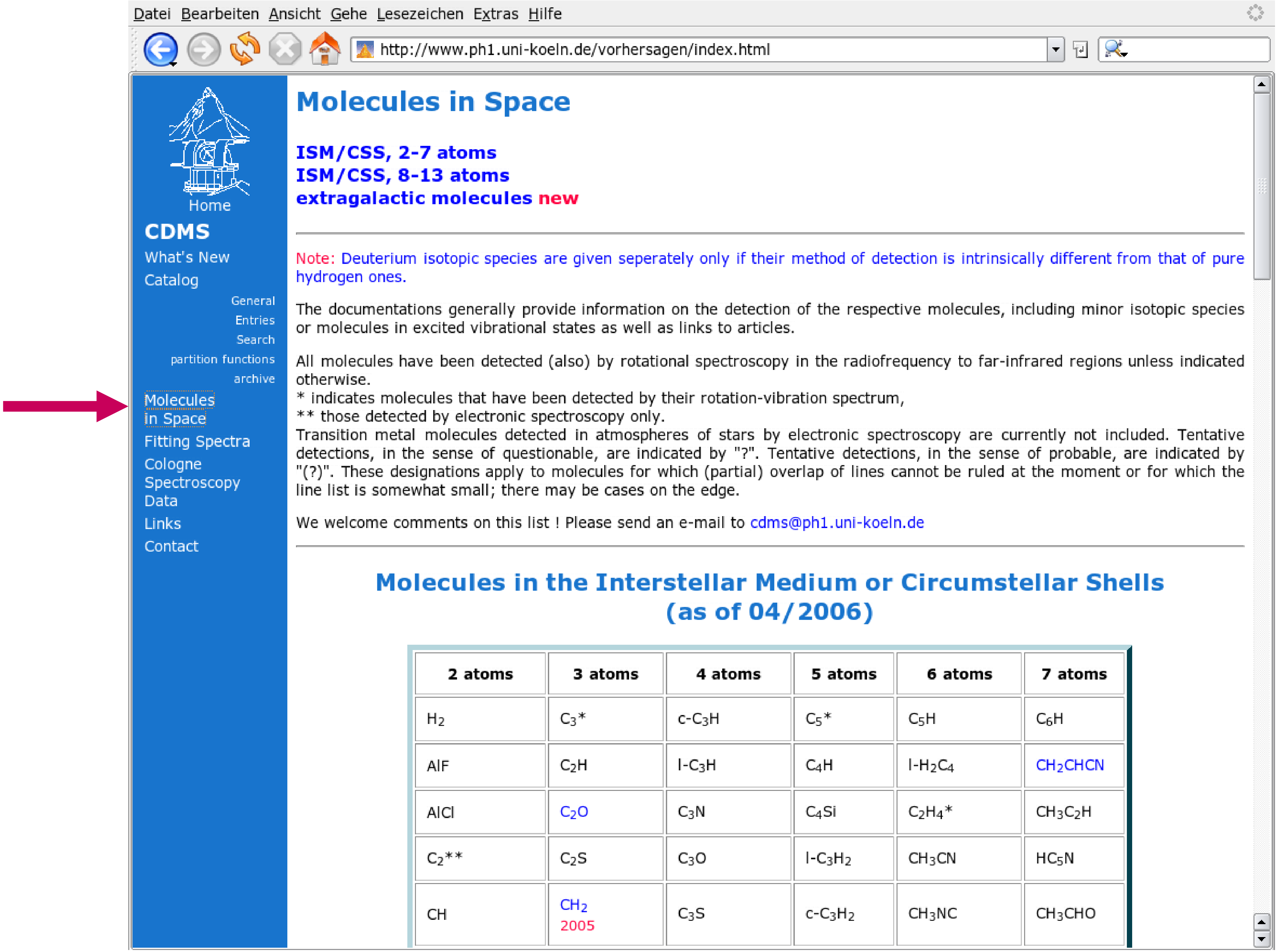
non-radicals:

- **no nucleus with $I > 0$** considered: CO; KCl; HCP; HNC; CH_3CCH (propyne, methylacetylene); H_2COH^+ (hydroxymethylium, protonated formaldehyde); H_2CO (formaldehyde); H_2S; $ClNO_2$; CH_2CHNH_2 (vinylamine); $Ar\cdots SO_2$; $HD_2{}^+$;



Molecules in Space

ISM/CSS, 2-7 atoms
ISM/CSS, 8-13 atoms
extragalactic molecules new

Note: Deuterium isotopic species are given seperately only if their method of detection is intrinsically different from that of pure hydrogen ones.

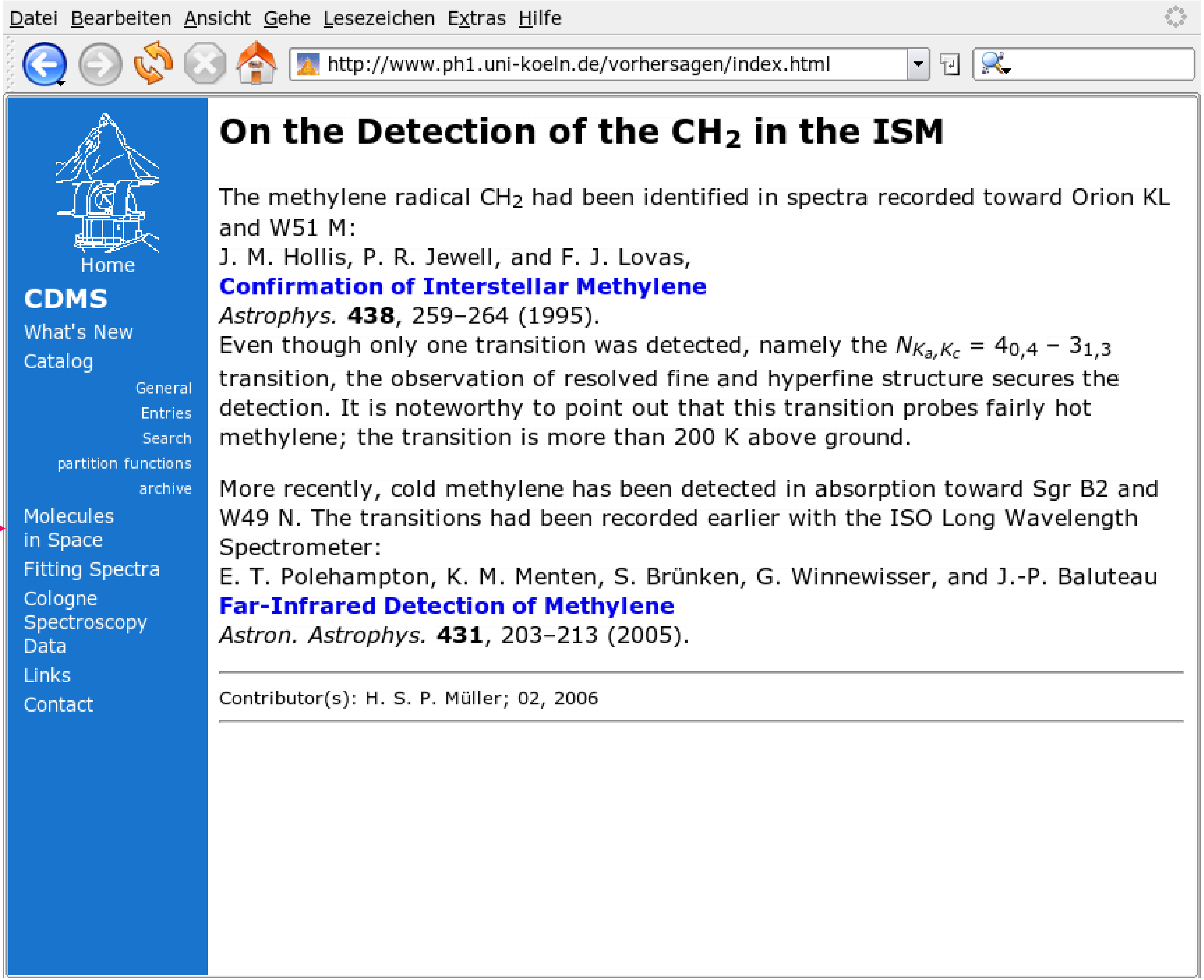
The documentations generally provide information on the detection of the respective molecules, including minor isotopic species or molecules in excited vibrational states as well as links to articles.

All molecules have been detected (also) by rotational spectroscopy in the radiofrequency to far-infrared regions unless indicated otherwise.
* indicates molecules that have been detected by their rotation-vibration spectrum,
** those detected by electronic spectroscopy only.
Transition metal molecules detected in atmospheres of stars by electronic spectroscopy are currently not included. Tentative detections, in the sense of questionable, are indicated by "?". Tentative detections, in the sense of probable, are indicated by "(?)". These designations apply to molecules for which (partial) overlap of lines cannot be ruled at the moment or for which the line list is somewhat small; there may be cases on the edge.

We welcome comments on this list ! Please send an e-mail to cdms@ph1.uni-koeln.de

Molecules in the Interstellar Medium or Circumstellar Shells (as of 04/2006)

2 atoms	3 atoms	4 atoms	5 atoms	6 atoms	7 atoms
H_2	C_3*	c-C_3H	C_5*	C_5H	C_6H
AlF	C_2H	l-C_3H	C_4H	l-H_2C_4	CH_2CHCN
AlCl	C_2O	C_3N	C_4Si	C_2H_4*	CH_3C_2H
C_2**	C_2S	C_3O	l-C_3H_2	CH_3CN	HC_5N
CH	CH_2 2005	C_3S	c-C_3H_2	CH_3NC	CH_3CHO

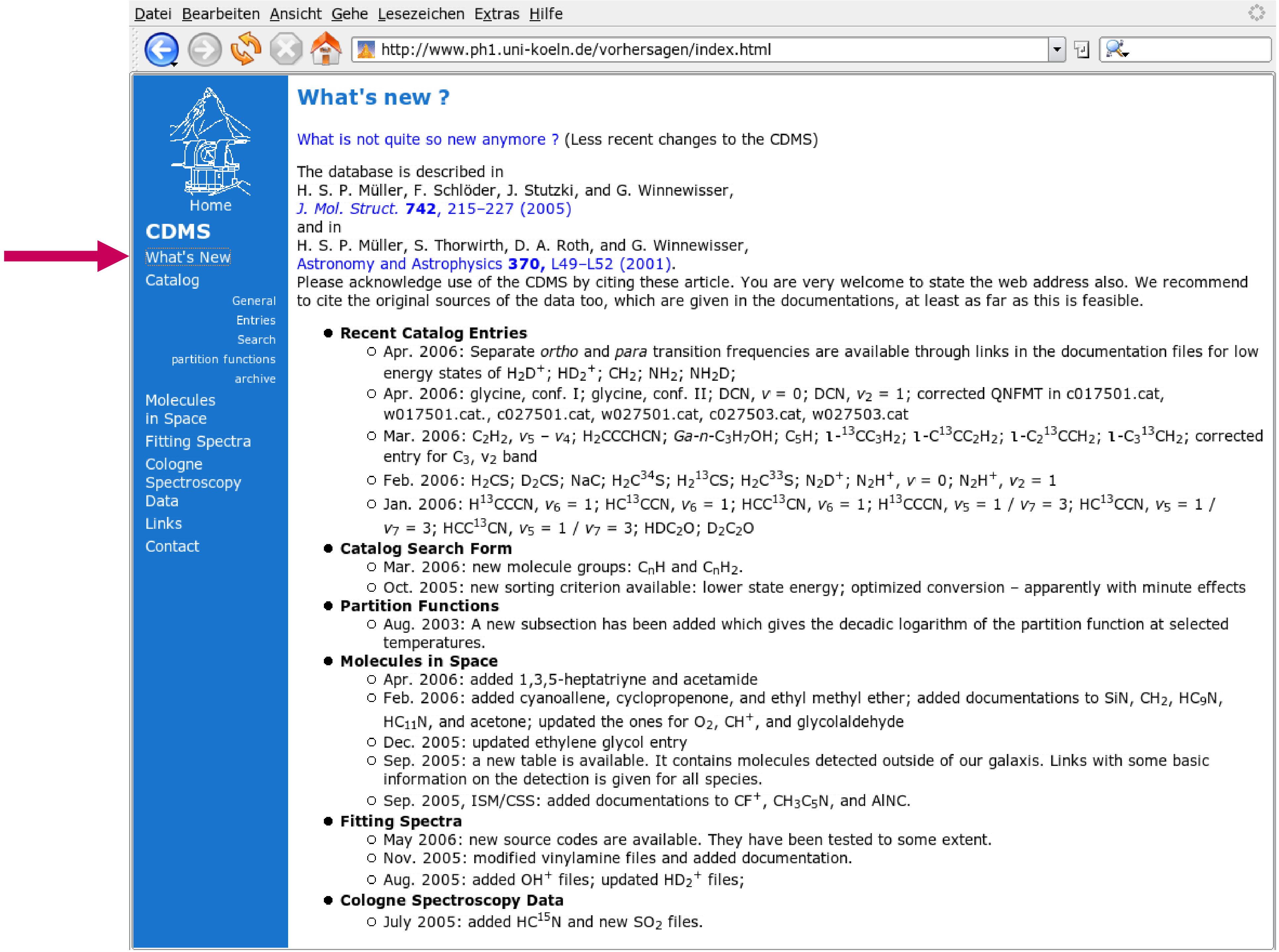


On the Detection of the CH_2 in the ISM

The methylene radical CH_2 had been identified in spectra recorded toward Orion KL and W51 M:
J. M. Hollis, P. R. Jewell, and F. J. Lovas,
Confirmation of Interstellar Methylene
Astrophys. **438**, 259–264 (1995).
Even though only one transition was detected, namely the $N_{K_a,K_c} = 4_{0,4} - 3_{1,3}$ transition, the observation of resolved fine and hyperfine structure secures the detection. It is noteworthy to point out that this transition probes fairly hot methylene; the transition is more than 200 K above ground.

More recently, cold methylene has been detected in absorption toward Sgr B2 and W49 N. The transitions had been recorded earlier with the ISO Long Wavelength Spectrometer:
E. T. Polehampton, K. M. Menten, S. Brünken, G. Winnewisser, and J.-P. Baluteau
Far-Infrared Detection of Methylene
Astron. Astrophys. **431**, 203–213 (2005).

Contributor(s): H. S. P. Müller; 02, 2006



What's new ?

What is not quite so new anymore ? (Less recent changes to the CDMS)

The database is described in
H. S. P. Müller, F. Schlöder, J. Stutzki, and G. Winnewisser,
J. Mol. Struct. **742**, 215–227 (2005)
and in
H. S. P. Müller, S. Thorwirth, D. A. Roth, and G. Winnewisser,
Astronomy and Astrophysics **370,** L49–L52 (2001).
Please acknowledge use of the CDMS by citing these article. You are very welcome to state the web address also. We recommend to cite the original sources of the data too, which are given in the documentations, at least as far as this is feasible.

- **Recent Catalog Entries**
  - Apr. 2006: Separate *ortho* and *para* transition frequencies are available through links in the documentation files for low energy states of H_2D^+; HD_2^+; CH_2; NH_2; NH_2D;
  - Apr. 2006: glycine, conf. I; glycine, conf. II; DCN, $v = 0$; DCN, $v_2 = 1$; corrected QNFMT in c017501.cat, w017501.cat., c027501.cat, w027501.cat, c027503.cat, w027503.cat
  - Mar. 2006: C_2H_2, $v_5 - v_4$; $H_2CCCHCN$; *Ga-n*-C_3H_7OH; C_5H; l-$^{13}CC_3H_2$; l-$C^{13}CC_2H_2$; l-$C_2{}^{13}CCH_2$; l-$C_3{}^{13}CH_2$; corrected entry for C_3, v_2 band
  - Feb. 2006: H_2CS; D_2CS; NaC; $H_2C^{34}S$; $H_2{}^{13}CS$; $H_2C^{33}S$; N_2D^+; N_2H^+, $v = 0$; N_2H^+, $v_2 = 1$
  - Jan. 2006: $H^{13}CCCN$, $v_6 = 1$; $HC^{13}CCN$, $v_6 = 1$; $HCC^{13}CN$, $v_6 = 1$; $H^{13}CCCN$, $v_5 = 1 / v_7 = 3$; $HC^{13}CCN$, $v_5 = 1 / v_7 = 3$; $HCC^{13}CN$, $v_5 = 1 / v_7 = 3$; HDC_2O; D_2C_2O
- **Catalog Search Form**
  - Mar. 2006: new molecule groups: C_nH and C_nH_2.
  - Oct. 2005: new sorting criterion available: lower state energy; optimized conversion – apparently with minute effects
- **Partition Functions**
  - Aug. 2003: A new subsection has been added which gives the decadic logarithm of the partition function at selected temperatures.
- **Molecules in Space**
  - Apr. 2006: added 1,3,5-heptatriyne and acetamide
  - Feb. 2006: added cyanoallene, cyclopropenone, and ethyl methyl ether; added documentations to SiN, CH_2, HC_9N, $HC_{11}N$, and acetone; updated the ones for O_2, CH^+, and glycolaldehyde
  - Dec. 2005: updated ethylene glycol entry
  - Sep. 2005: a new table is available. It contains molecules detected outside of our galaxis. Links with some basic information on the detection is given for all species.
  - Sep. 2005, ISM/CSS: added documentations to CF^+, CH_3C_5N, and AlNC.
- **Fitting Spectra**
  - May 2006: new source codes are available. They have been tested to some extent.
  - Nov. 2005: modified vinylamine files and added documentation.
  - Aug. 2005: added OH^+ files; updated HD_2^+ files;
- **Cologne Spectroscopy Data**
  - July 2005: added $HC^{15}N$ and new SO_2 files.

Complex Molecules in the CDMS Catalog

c-C_2H_4O
c-C_2H_4NH
c-H_2C_3O
c-$H_2C_3CH_2$
c-C_6H_4

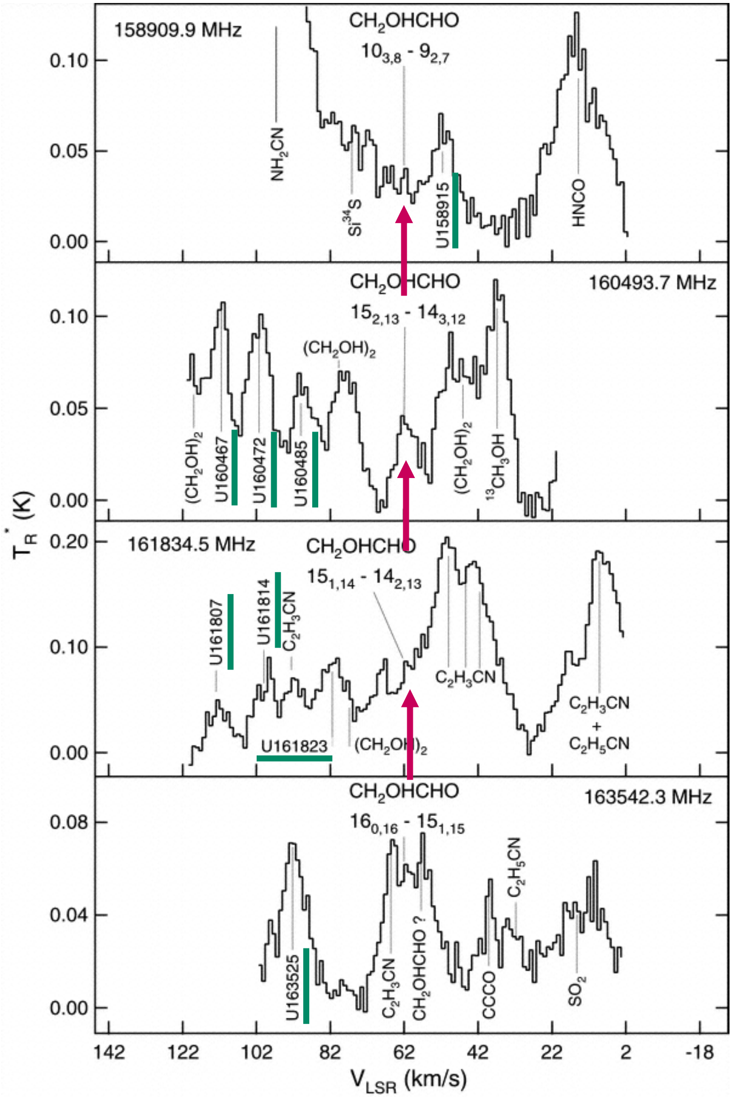
$C_2H_3NH_2$
C_2H_3OH
C_2H_3CCH
C_3H_3CN
n-C_3H_7OH

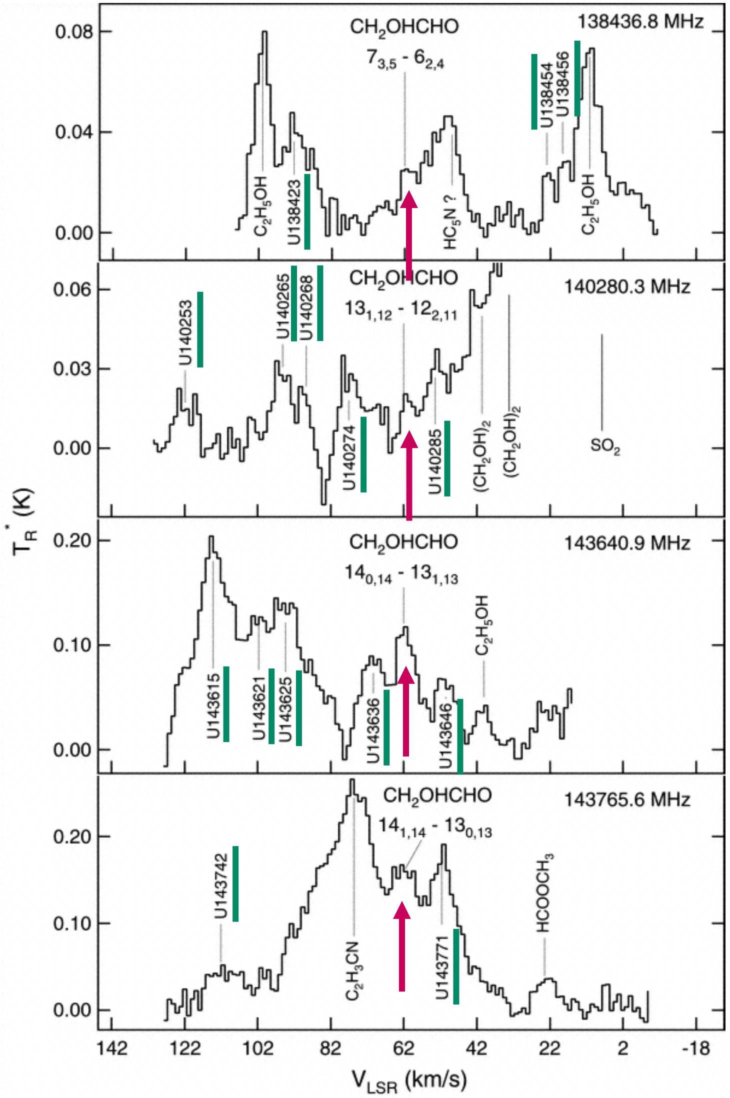
glycolaldehyde
ethylene glycol
diethyl ether
glycine

species detected in ISM/CSS

plus many more large molecules

The Quest for Complex Molecules, e.g. CH_2OHCHO





is often hampered by **U-lines**, D. T. Halfen *et al.*, ApJ 639 (2006) 237

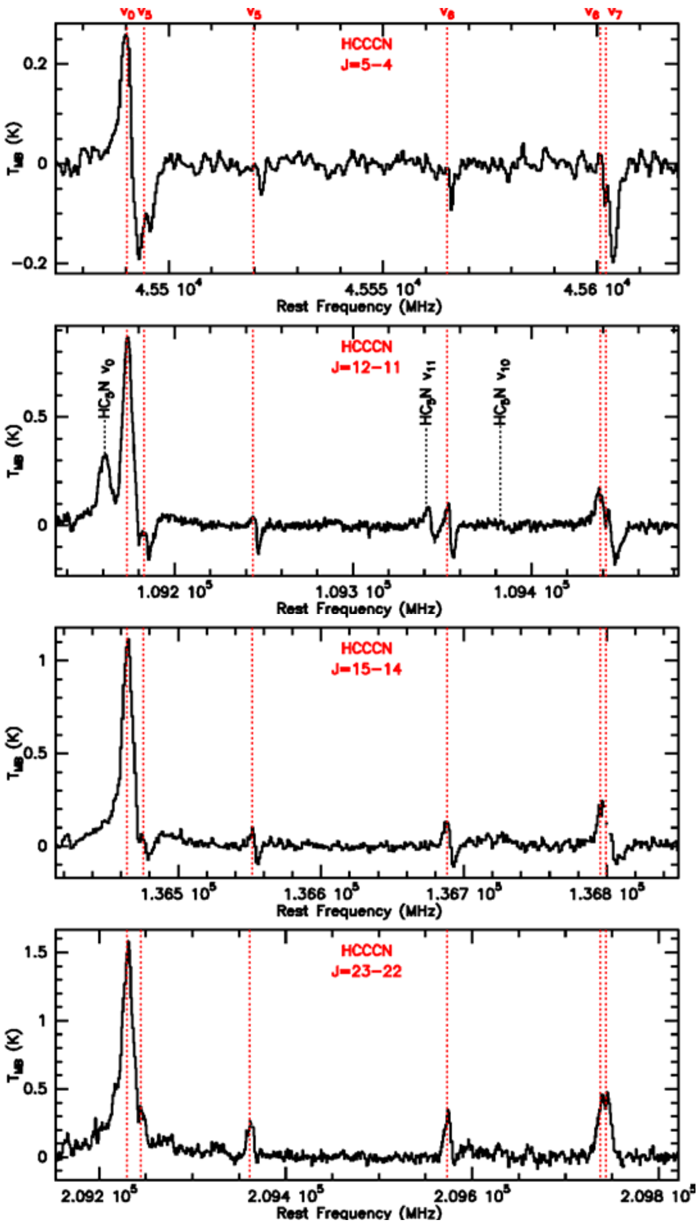
The U-line Issue

- already many detected in surveys with IRAM 30 m, Odin, CSO etc.

- desired line may be overlapped by U-line
  (e.g. O_2 @ 424763 MHz obs. with SWAS ?)

- U-lines may be due to
  - high r or v lines of known compounds, e.g. CH_3OH
  - isotopic species of known molecules, e.g. CH_3OH
  - new, maybe exotic species

Do we have to consider vibrational satellites as weed only ?



The case of HC_3N in CRL 618

– several states ≤ 1100 cm $^{-1}$ ≅ 1600 K

– plus ^{13}C data

⇒ physical model of CRL 618

F. Wyrowski *et al.*, *ApJ* **586** (2003) 344

similar study on HC_3N in CRL 618:

J. R. Pardo *et al.*, *ApJ* **615** (2004) 495

vibrationally excited HC_3N toward hot cores

e.g. F. Wyrowski, *A&A* **341** (1999) 882

What do we need to know? Selected case studies

- alcohols: CH_3OH, C_2H_5OH, *n,i*-C_3H_7OH
- ethers: CH_3OCH_3, $C_2H_5OCH_3$, $C_2H_5OC_2H_5$
- sat. cyanides: CH_3CN, C_2H_5CN, *n,i*-C_3H_7CN

(CH_3CHO, CH_3OCHO)

(frequency limits **not** restricted to ALMA)

Methanol, CH_3OH, I

- CH_3OH
  - needed: $\upsilon_t \geq 3$; $\nu >> 2$ THz
  - available: $\upsilon_t \leq 4$ (soon; new, unpubl. data from JPL)
- $^{13}CH_3OH$
  - needed: $\upsilon_t \geq 2$; $\nu >> 1$ THz
  - available: $\upsilon_t \leq 2$ (3 or 4), $\nu \leq 0.5$ THz + FIR
- $CH_3{}^{18}OH$
  - needed: $\upsilon_t \geq 1$; $\nu >> 1$ THz
  - available: $\upsilon_t \leq 1$ (3), $\nu \leq 0.2$ THz + FIR
- $CH_3{}^{17}OH$
  - needed: $\upsilon_t \leq 1$; $\nu >> 1$ THz
  - available: $\upsilon_t = 0$, just a few lines
- $^{13}CH_3{}^{18}OH$
  - needed: $\upsilon_t = 0$; $\nu >> 1$ THz ?
  - available: $\upsilon_t = 0$ a few lines (?)
- CH_3OD
  - needed: $\upsilon_t \geq 1$; $\nu >> 1$ THz
  - available: $\upsilon_t \leq 2$, $\nu \leq 0.5$ THz + FIR

Methanol, CH_3OH, II

• CH_2DOH	needed: $\upsilon_t \geq 1$; $\nu >> 1$ THz available: $\upsilon_t = 0$, some ≤ 0.7 THz (+ unpubl. data from JPL)
• CHD_2OH	needed: $\upsilon_t = 0$; $\nu \leq 1$ THz available: $\upsilon_t = 0$, just a few lines (+ unpubl. OSU lines ?)
• CH_2DOD	needed: $\upsilon_t = 0$; $\nu \leq 1$ THz available: $\upsilon_t = 0$, just a few lines
• CD_3OH	needed: $\upsilon_t = 0$; $\nu \leq 1$ THz available: $\upsilon_t \leq 1$, $\nu \leq 0.18$ THz (+ FIR ?)
• CD_3OD	needed: $\upsilon_t = 0$; $\nu \leq 1$ THz available: $\upsilon_t \leq 1$, $\nu \leq 0.9$ THz (+ unpubl. FIR)

also needed: $^{13}CH_2DOH$, $^{13}CH_3OD$, CHD_2OD, $\upsilon_t = 0$; $\nu \leq 1$ THz

Ethanol, C_2H_5OH (1 + 2 conf.: $a + g\pm$)

- needed for C_2H_5OH: $\upsilon_t \geq 1$; $\nu >> 1$ THz
- available for $\upsilon_t = 0$: $\nu \leq 0.5$ THz; soon more from JPL
- available for $\upsilon_t > 0$: some lines ≤ 60 GHz

- needed for C_2H_5OH-$^{13}C_1$: $\upsilon_t \geq 0$; $\nu >> 1$ THz
- available for $\upsilon_t = 0$: some lines ≤ 60 GHz (in part from PhD thesis)

- are $^{13}C_2$, ^{18}O, or D_1 species needed ?

n,*i*-Propanol, C_3H_7OH (2 isom., several conf.)

- needed: $\upsilon_t = 0$; $\nu \approx 1$ THz for 2 isom., lowest conf.

- available: $\nu \leq 0.35$ THz for *Ga*-conf. of *n*-isom.

- more to come from OSU

Butanol, C_4H_9OH (4 isomers . . .)

not (urgently) needed

Dimethyl ether, CH_3OCH_3

- CH_3OCH_3

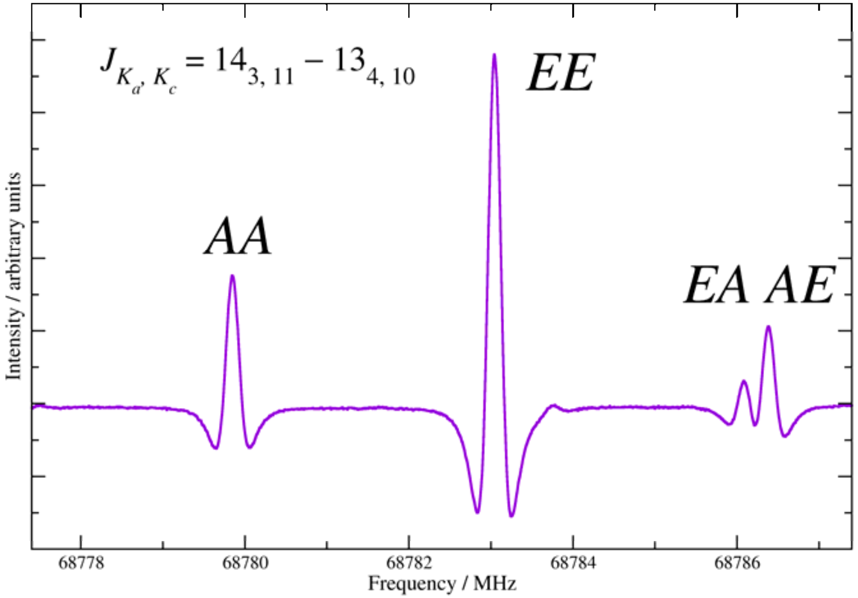
needed: $\upsilon_t >> 1$; $\nu >> 2$ THz
available: $\upsilon_t = 0$; $\nu \leq 0.55$ THz; some lines for higher υ

- CH_3OCH_3-$^{13}C_1$

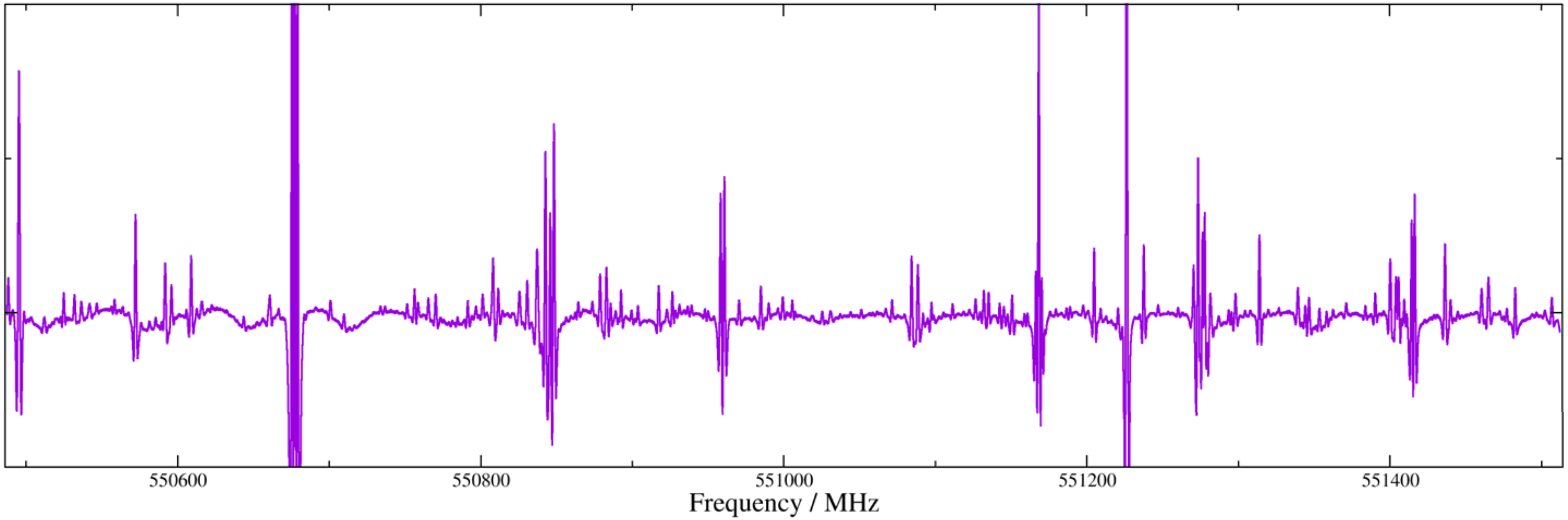
needed: $\upsilon_t \geq 0$; $\nu >> 1$ THz
available: $\upsilon_t = 0$; some MW lines

maybe not needed: ^{18}O (?), $^{13}C_2$, D_1 (?)

Ongoing investigations of CH_3OCH_3



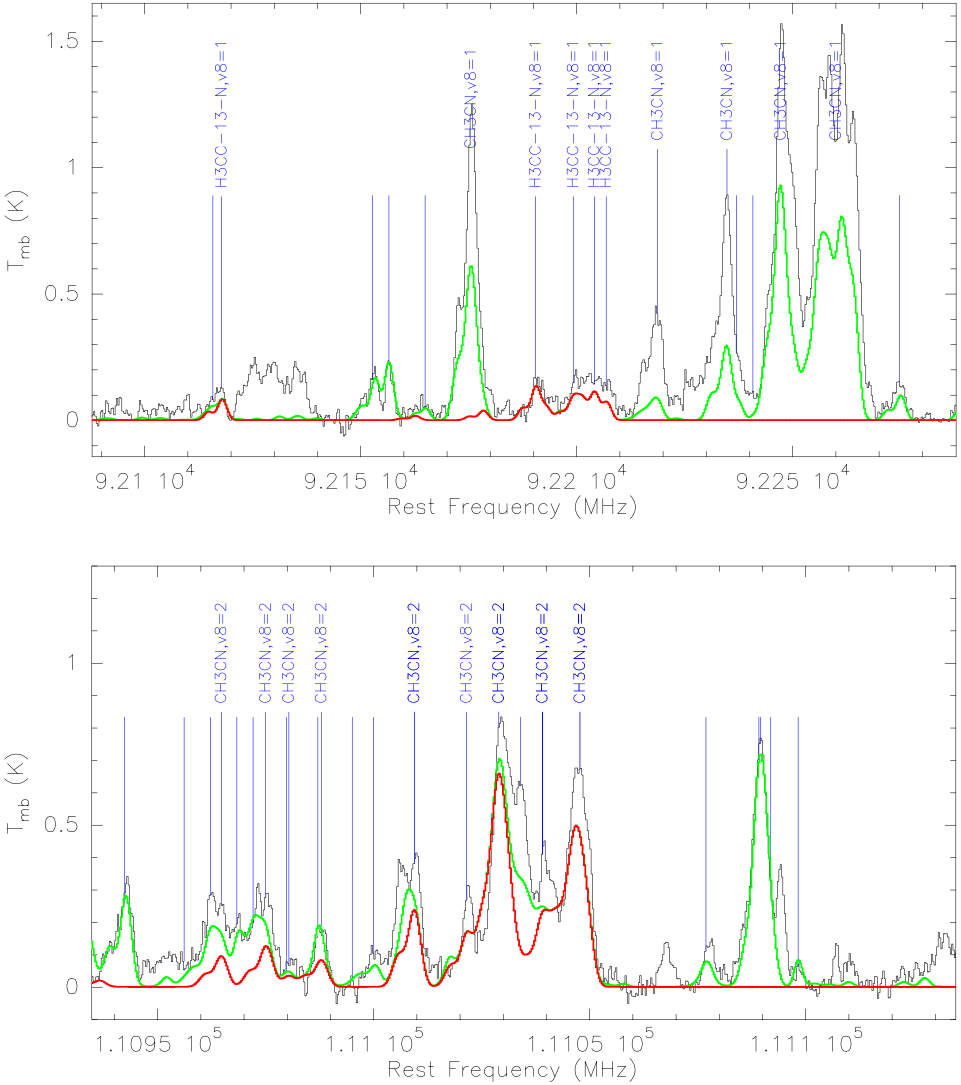
- measurements at Köln and at JPL
- main species: $\upsilon = 0$ ready soon !?
- higher υ to follow
- $^{13}C_1$: $\upsilon = 0$ intended
- maybe torsional bands



Ethyl methyl ether (EME) and diethyl ether (DEE)

- EME
  - needed: $\upsilon_t \geq 0$; $v > 1$ THz
  - available: $\upsilon_t = 0$; $v \leq 0.35$ THz;
  - higher v in Köln (?)
- DEE
  - needed: $\upsilon_t = 0$; $v \approx 1$ THz for *aa*-conf.
  - available: $\upsilon_t = 0$; $v \leq 0.35$ THz for *aa*- and *ag*-conf.

Methyl cyanide, CH_3CN



in Sgr B2(N)

- CH_3CN

  needed: $v_8 \geq 3$; $\nu \geq 1.5$ THz

  available: $v_8 = 2$; $\nu \leq 1.3$ THz

  $v_4 = 1$; $\nu \leq 0.46$ THz

- CH_3CN-$^{13}C_1$

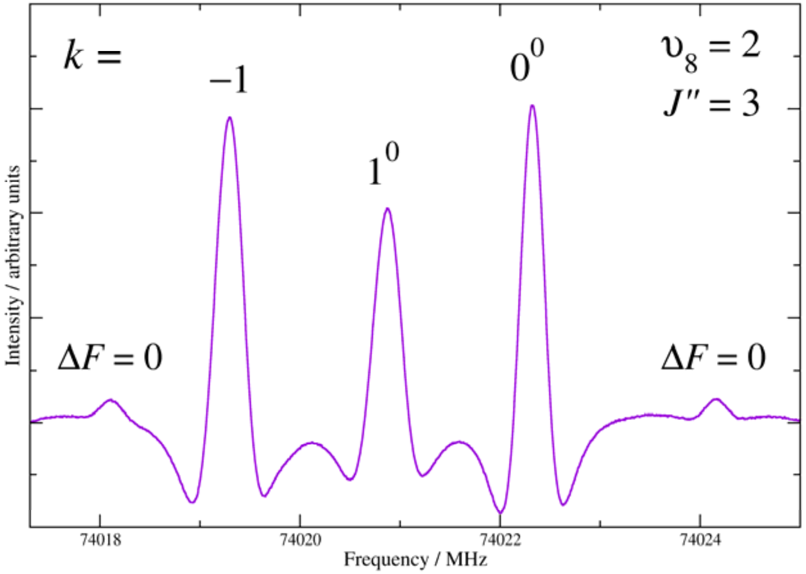
  needed: $v_8 \geq 2$; $\nu \geq 1.5$ THz

  available: $v = 0$; $\nu \leq 0.6$ THz

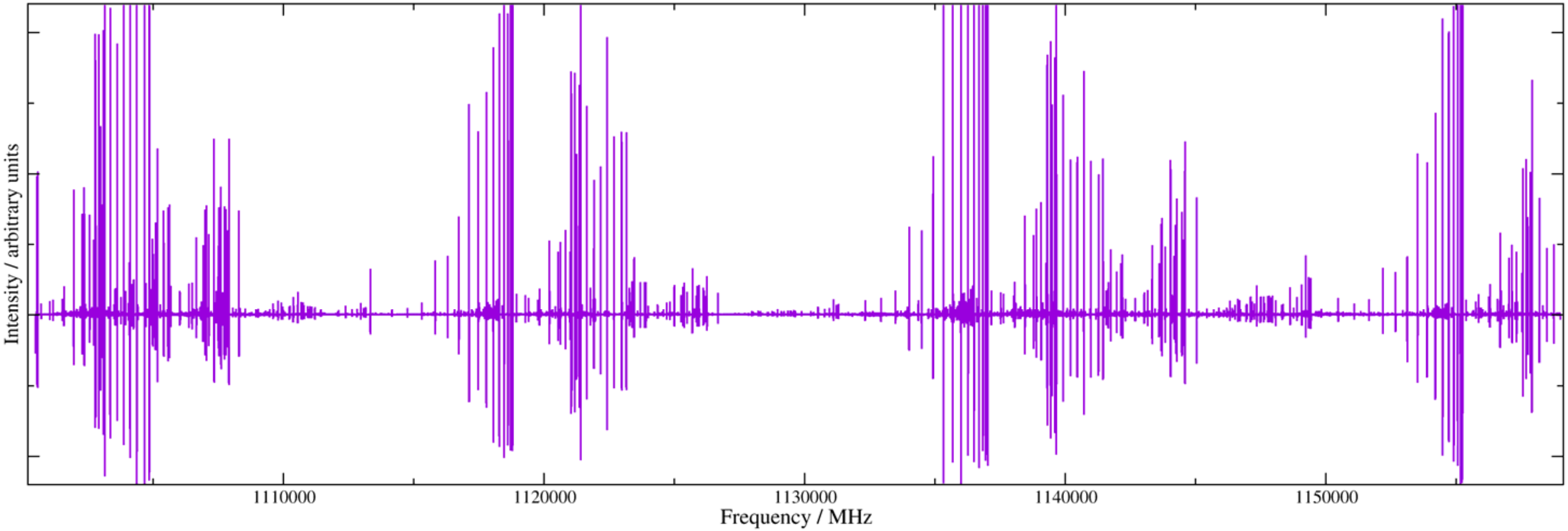
  $v_8 = 2$; $\nu \leq 80$ GHz

also needed: $^{13}C_2$, ^{15}N, D_1
known up to 80, 600, 470 GHz

Ongoing investigations of CH_3CN



- measurements at Köln and at JPL
- CH_3CN: $\upsilon_8 \geq 3$
- $^{13}C_1$: $\upsilon_8 = 2$ (?)
- ^{15}N: $\upsilon_8 = 0$ or 1
- D_1 (?)
- $^{13}C_2$?



Ethyl cyanide, C_2H_5CN

• C_2H_5CN	needed: $\upsilon_{13} + \upsilon_{21} \geq 2$; $\nu \approx 1$ THz available: $\upsilon = 0$; $\nu \leq 0.6$ THz; soon: $\upsilon_{13} + \upsilon_{21} = 1$
• $C_2H_5CN\text{-}^{13}C_1$	needed: $\upsilon_{13} + \upsilon_{21} \geq 1$; $\nu \approx 1$ THz available: $\upsilon = 0$, just a few lines
• $C_2H_5CN\text{-}^{13}C_2$	needed: $\upsilon_{13} + \upsilon_{21} \geq 0$; $\nu \approx 1$ THz available: nothing

maybe not needed: D_1 (??), ^{15}N (?), $^{13}C_3$

n,*i*-Propyl cyanide, C_3H_7CN

- $\upsilon = 0$; $v \leq 0.3$ THz known for *a*- and *g*-conformers of *n*-isomer

- just some MW lines known for conformers of *i*-isomer

Acetaldehyde, CH_3CHO

- CH_3CHO

needed: $\upsilon_t \geq 0$; $\nu > 1$ THz (?)
available: $\upsilon_t \leq 4$; $\nu \leq 0.25$ THz + FIR
new measurements at JPL

also needed: $\upsilon_t = 0$ for $^{13}C_1$, D_1, ^{18}O, . . .
available: just a few lines each

Available for methyl formate, CH_3OCHO

- CH_3OCHO, $\upsilon_t = 0$: $\nu \leq 0.6$ THz
  $\upsilon_t = 1$: $\nu \leq 0.2$ THz

- $CH_3O^{13}CHO$, $\upsilon_t = 0$: $\nu \leq 0.6$ THz

- CH_3OCDO, $\upsilon_t = 0$: $\nu \leq 0.4$ THz

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