Complex (Organic) Molecules in the ALMA and SKA era: data needs

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Some COMs falling into the ALMA (84-950Ghz) and (up to 14 GHz) frequency ranges

Glycolaldehyde	CH_2OHCHO	SgrB2, YSOs
Acetic acid	CH_3COOH	SgrB2, YSOs
Methyl formate	$HCOOCH_3$	SgrB2, YSOs, CC
Formamide	CH_3NO	SgrB2, YSOs
Amino acetonitrile	H_2NCH_2CN	SgrB2
iso-Propyl Cyanide	C_4H_7N	SgrB2
Acetone	$(CH_3)_2CO$	SgrB2, Orion KL
Acetaldehyde	CH_3CHO	SgrB2, evolved stars
Ethyl Formate	C_2H_5OCHO	SgrB2, Orion KL
Methoxy	CH_3O	CC
Triacarbon monoxide	C_3O	CC?
cyanamide	NH_2CN	SgrB2, Extragal
Dymethyl ether	CH_3OCH_3	Orion
Propanal	CH_3CH_2CHO	SgrB2
Propene	CH_3CHCH_2	CC
Glycolic acid	$HOCH_2COOH$	SgrB2
Ethyl alcohol	CH_3CH_2OH	SgrB2
Formic acid	$HCOOH$	SgrB2, CC, YSO
Hydroxylamine	NH_2OH	not yet detected
glycine	H_2NCH_2COOH	not yet detected
ketenimine	CH_2CNH	SgrB2

YSO: young stellar objects
CC: cold core

IMPORTANCE OF COMs

- Their detection is a confirmation of the high density cores where stars form
- COMs are now known to be present in cold gas in pre-stellar cores e.g. propylene (Marcelino et al. 2007)
- Some believe that formation of aminoacids may have occurred in the ISM and comets (e.g. Glavin et al. 2006; Elsila et al. 2009)

Intensity of the line → Column density of the transition – **assuming LTE and temperature**

However, we are often not in LTE environments and/or we do not know the temperature of the gas → need collisional coefficients to solve the radiative tranfer equations and obtain best gas density and temperature (e.g. with RADEX)

BUT:

1. **For none of the COMs listed a full set of collisional coefficients is available, apart from methyl formate and only within a certain range of temperatures (Faure et al. 2014)**
2. Collisional coefficients are important for some COMs with transitions with small dipole strengths (Beltran et al. 2009)
3. For SKA the need for collisional coefficients is even more important as it has been shown that a lower frequencies NLTE effects are more important (Faure et al. 2014, apj)

What about rest frequencies?
E.g. Massive star forming regions: the big problem of line confusion in the submm
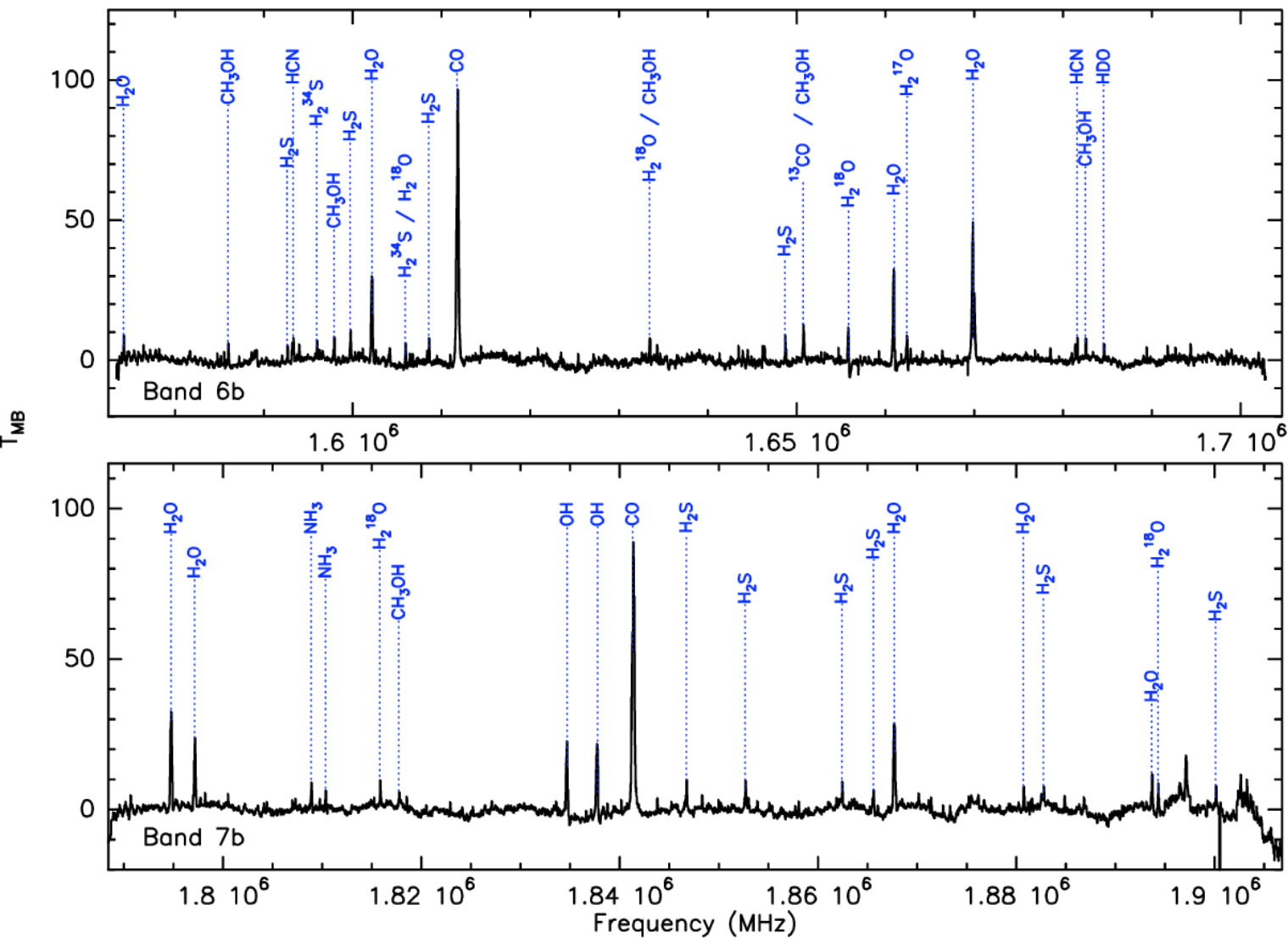
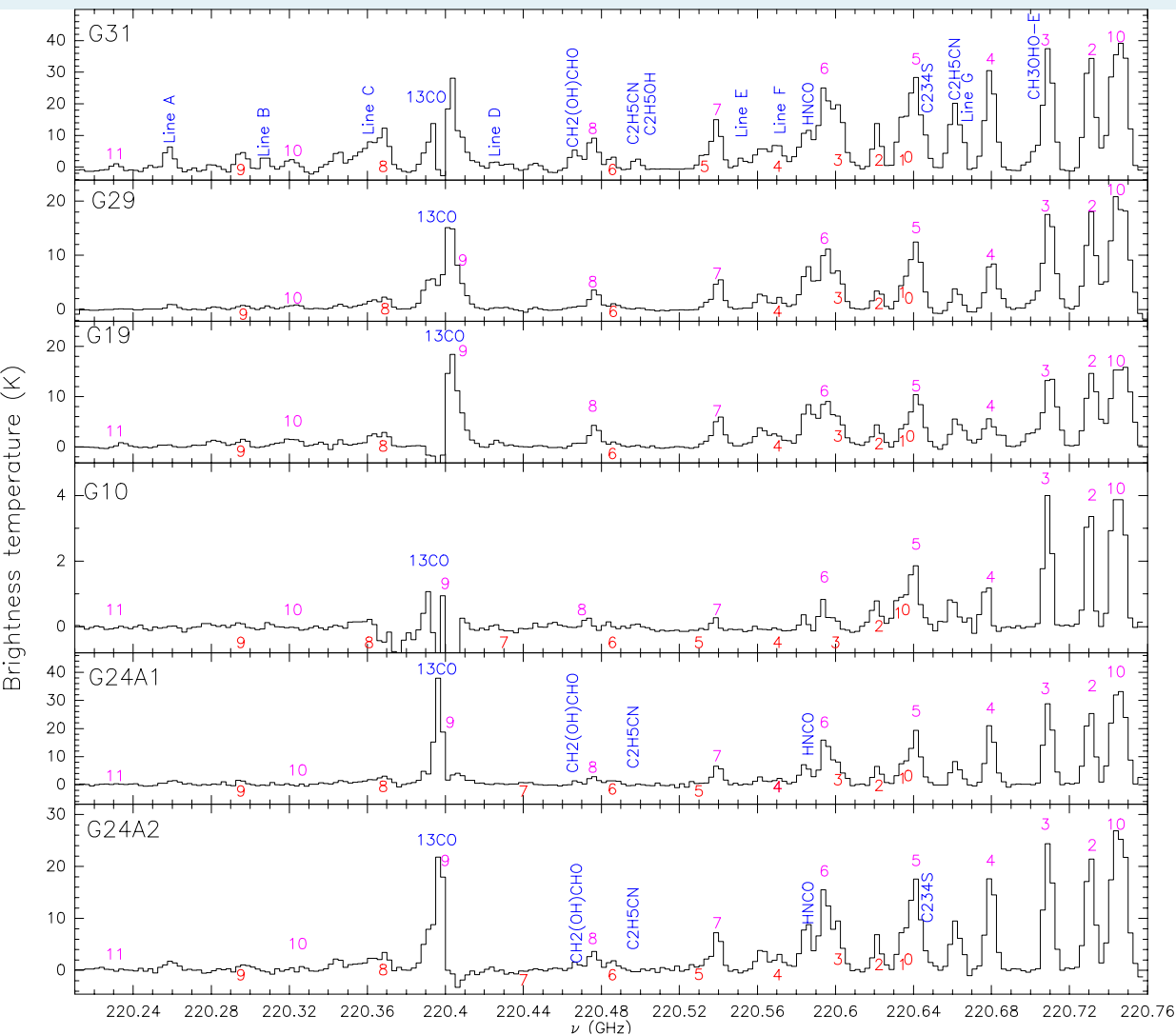Crockett et al. (2010), Orion KL observed with HIFI on Herschel
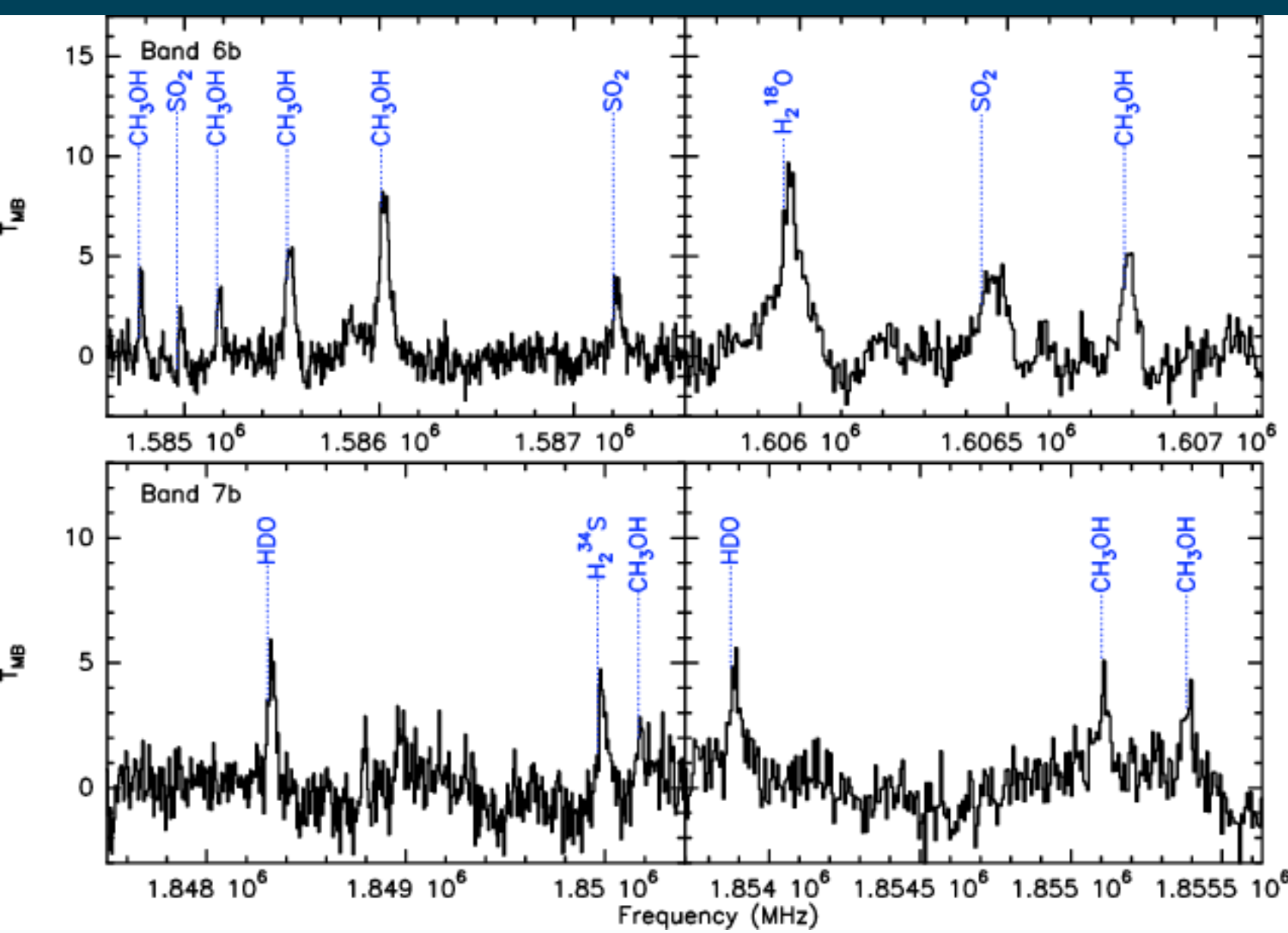
If one zooms in…..

More is less……

line confusion due to:
- Richness of the spectrum
- Blending (due to large linewidths)
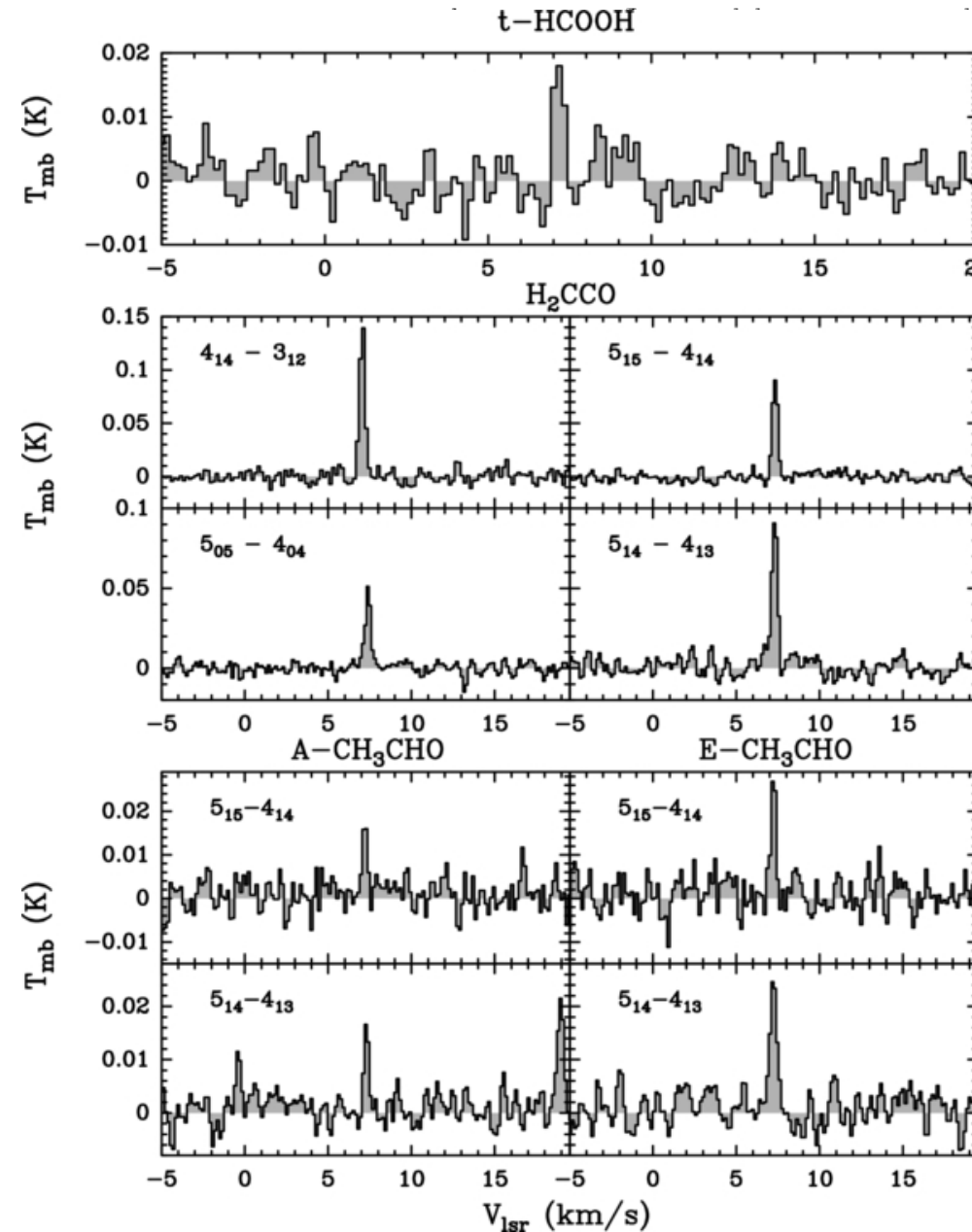- **Uncertainties in the lab rest frequencies as well as in the observations**

↓

This leads to only tentative detections in most cases (e.g. glycolaldehyde @ 220.4 GHz may be acetone instead!)

Calcutt et al. 2014

In solar-type stars, similar problems because linewidth is very small (~0.1 MHz)

Table 1

...ward L1544 and Results from the Line Gaussian Fits

A_{ij} (s^{-1})	rms (mK)	T_{mb} (mK)	FWHM (km s^{-1})	V_{LSR} (km s^{-1})
2.05×10^{-5}	3.5	36.8 ± 3.5	0.39 ± 0.04	7.04 ± 0.0
2.82×10^{-5}	6.1	...	...	...
3.77×10^{-5}	4.9	...	...	...
2.53×10^{-5}	3.5	17.8 ± 3.4	0.33 ± 0.07	7.20 ± 0.0
2.84×10^{-5}	5.9	25.6 ± 3.6	0.81 ± 0.13	7.35 ± 0.0
2.99×10^{-5}	2.7	17.2 ± 2.6	0.31 ± 0.05	7.30 ± 0.0
2.53×10^{-5}	3.9	29.3 ± 3.8	0.33 ± 0.05	7.23 ± 0.0
2.84×10^{-5}	5.8	50.5 ± 8.4	0.24 ± 0.05	7.20 ± 0.0
2.99×10^{-5}	3.2	24.7 ± 2.4	0.49 ± 0.05	7.23 ± 0.0
6.35×10^{-6}	3.4	19.9 ± 3.3	0.34 ± 0.07	7.17 ± 0.0
5.33×10^{-6}	5.8	147.2 ± 5.6	0.38 ± 0.02	7.05 ± 0.0
1.03×10^{-5}	4.2	95.5 ± 3.7	0.39 ± 0.02	7.32 ± 0.0
1.10×10^{-5}	3.5	49.1 ± 3.0	0.42 ± 0.03	7.39 ± 0.0
1.09×10^{-5}	5.3	95.3 ± 4.5	0.41 ± 0.02	7.30 ± 0.0
1.70×10^{-6}	3.8	70.8 ± 3.4	0.46 ± 0.03	7.18 ± 0.0
1.95×10^{-6}	3.6	740.8 ± 15.9	0.43 ± 0.01	7.18 ± 0.0
2.03×10^{-6}	3.6	740.2 ± 10.3	0.46 ± 0.01	7.18 ± 0.0
3.16×10^{-6}	4.4	61.1 ± 3.5	0.46 ± 0.03	7.40 ± 0.0
3.46×10^{-6}	4.4	612.6 ± 10.6	0.47 ± 0.01	7.38 ± 0.0
3.56×10^{-6}	4.5	632.4 ± 10.8	0.47 ± 0.01	7.38 ± 0.0
1.97×10^{-6}	4.1	18.9 ± 4.0	0.37 ± 0.09	7.12 ± 0.0
2.55×10^{-6}	6.8	805.0 ± 6.0	0.38 ± 0.01	7.24 ± 0.0
3.40×10^{-6}	6.1	95.8 ± 5.7	0.34 ± 0.02	7.25 ± 0.0
1.47×10^{-5}	8.1	195.2 ± 7.1	0.34 ± 0.01	7.33 ± 0.0
2.38×10^{-6}	6.8	20.1 ± 6.0	0.45 ± 0.15	7.02 ± 0.0
3.40×10^{-6}	6.6	1047.5 ± 6.1	0.39 ± 0.01	7.24 ± 0.0
2.62×10^{-6}	5.6	21.8 ± 5.7	0.29 ± 0.09	7.27 ± 0.0
3.06×10^{-6}	4.4	22.3 ± 3.5[a]	0.41 ± 0.08	7.45 ± 0.0
3.17×10^{-6}	6.6	25.9 ± 6.1	0.40 ± 0.15	7.23 ± 0.0

Notes. The rms on a 50 kHz frequency bin was computed over a range of 45 km s^{-1}. The error in the main-beam temperature T_{mb} does not include the calibration... Note that the A and E forms for CH_3OH are taken from the CASSIS database. The line labeled a is in absorption.

Vastel et al. 2014

Catalogues disagree in some rest frequencies!

Some examples:

- Glycolaldehyde: some low J transitions within Band 3 and 4 of ALMA disagreement up to 0.3 MHz.
- Acetic Acid: only one source of frequencies (LOVAS) with errors > 0.1 MHz

→ **We do not have a systematic database of transitions for which rest frequencies are needed.**

Partition functions: how accurate are these for COMs?

Examples:

- For Acetic Acid SPLATALOGUE does not report any partition function (now estimated/calculated by several groups (eg Calcutt et al. 2015))
- For methyl formate: SPLATALOGUE/JPL has two contributions for the partition functions which seem to differ by over an order of magnitude at high (300K) temperatures.

How do the non-experts choose?