ISMS conference

The pure rotational spectrum of hydroxymethyl radical reinvestigated to enable its interstellar detection

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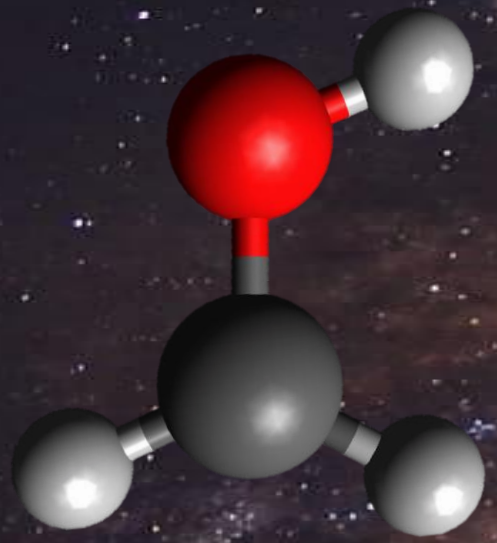
Olivia Chitarra | ***June 23, 2021***

CH_2OH: a missing link in interstellar chemistry?



- Hydrogen, Carbon and Oxygen containing species

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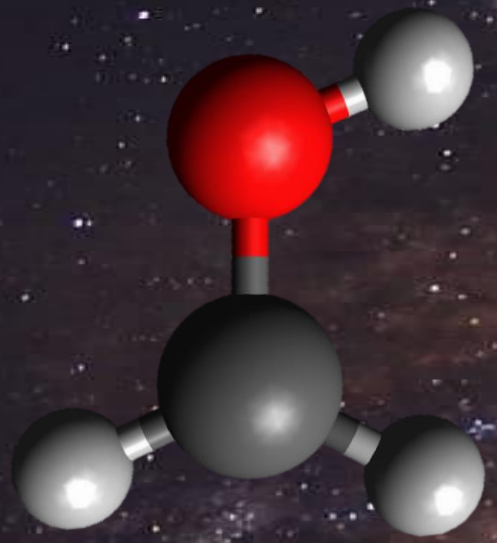


- Hydrogen, Carbon and Oxygen containing species
- Potentially produced from methanol (ice and/ or gas phase)

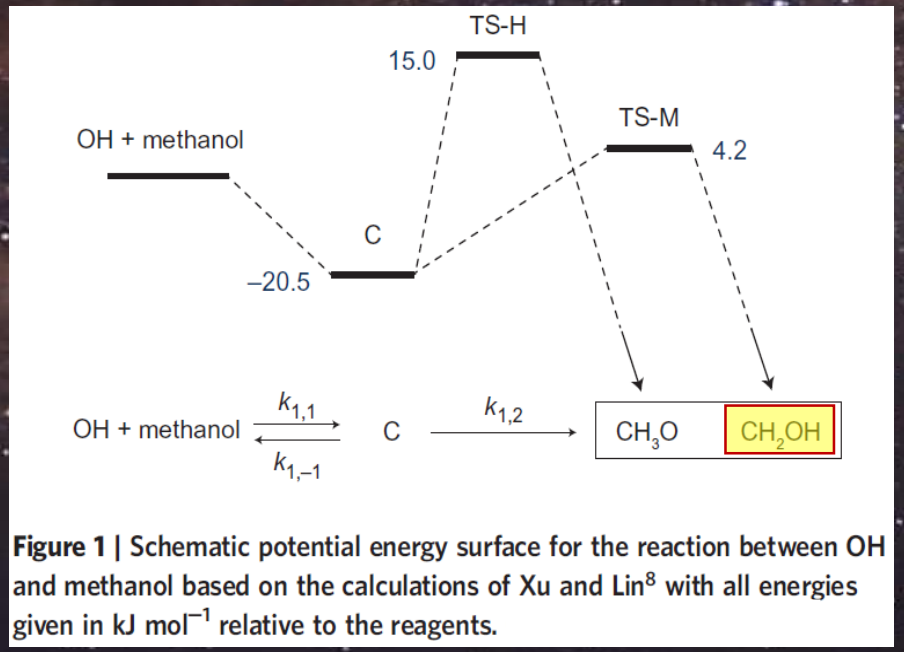
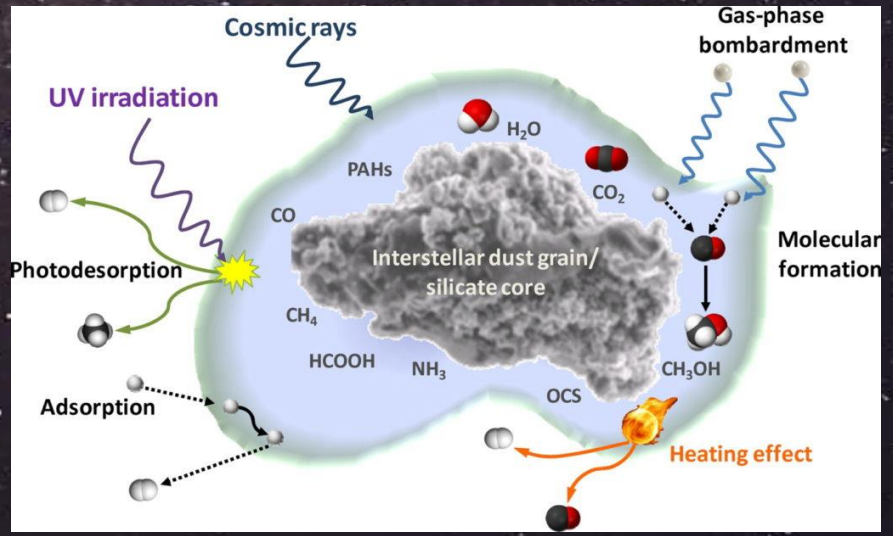


Figure 1 | Schematic potential energy surface for the reaction between OH and methanol based on the calculations of Xu and Lin[8] with all energies given in kJ mol^{-1} relative to the reagents.



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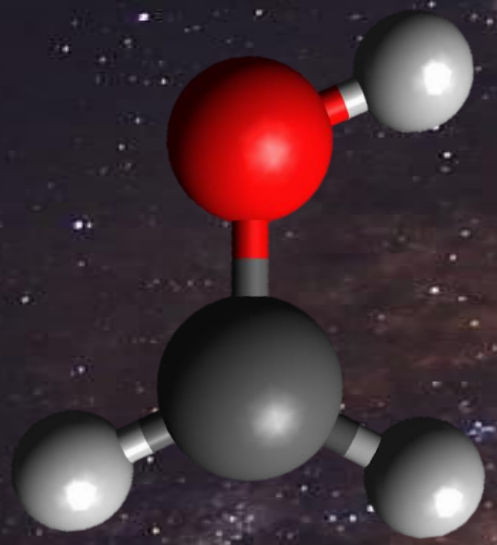
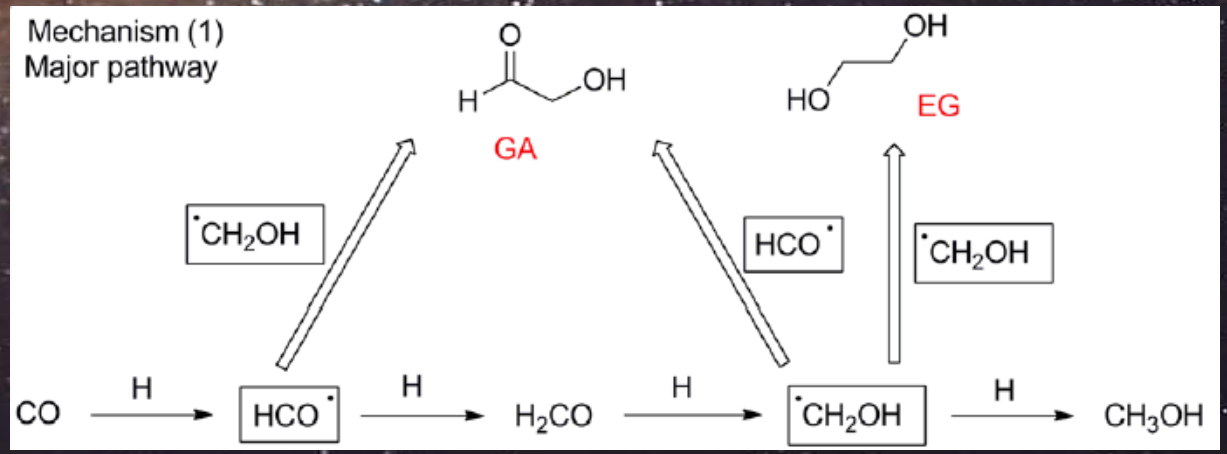


- Hydrogen, Carbon and Oxygen containing species
- Potentially produced from methanol (ice and/ or gas phase)
- Precursor of Complex Organic Molecules (COMs)



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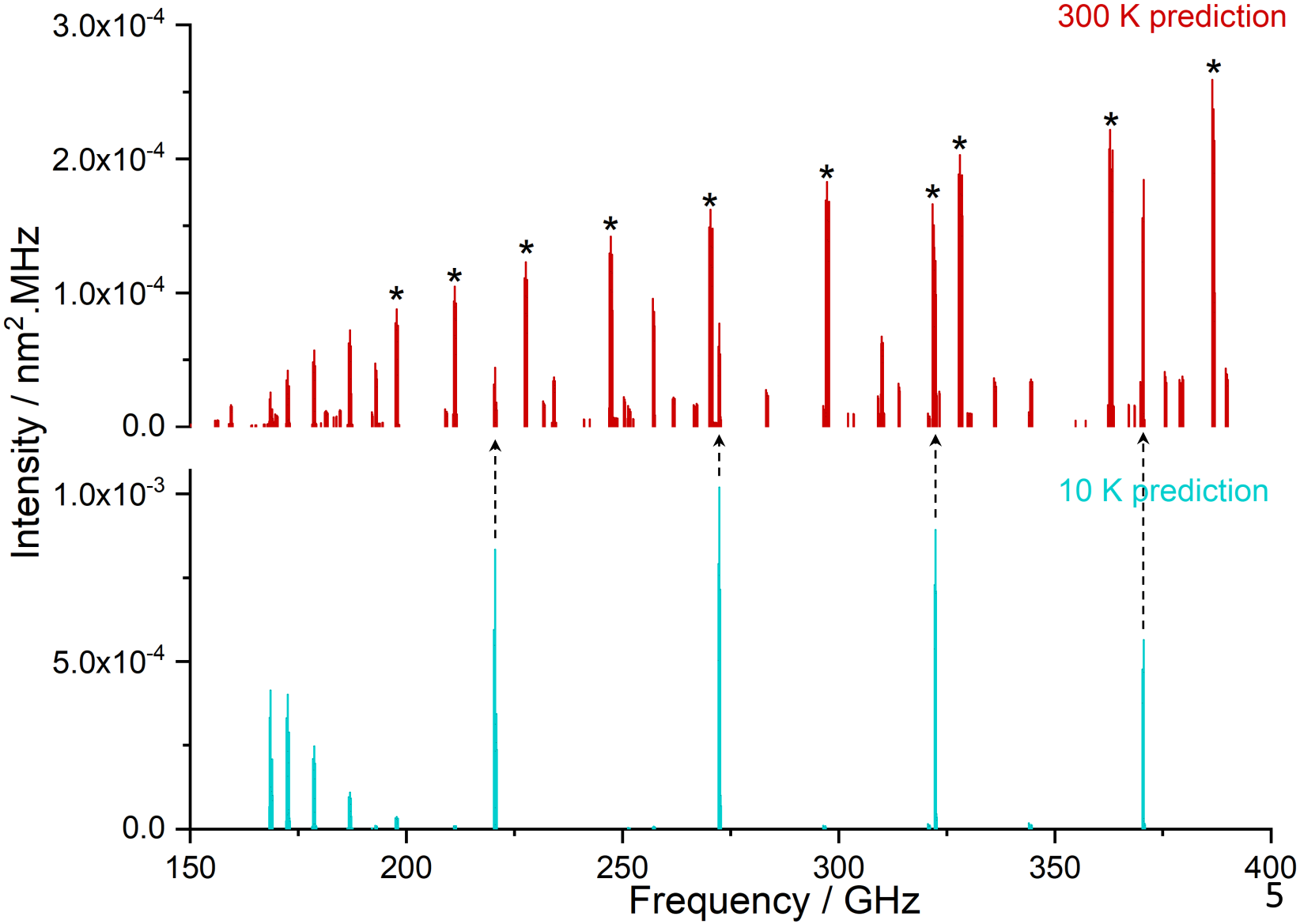
CH_2OH: laboratory challenge

❑ Ro-vibration studies

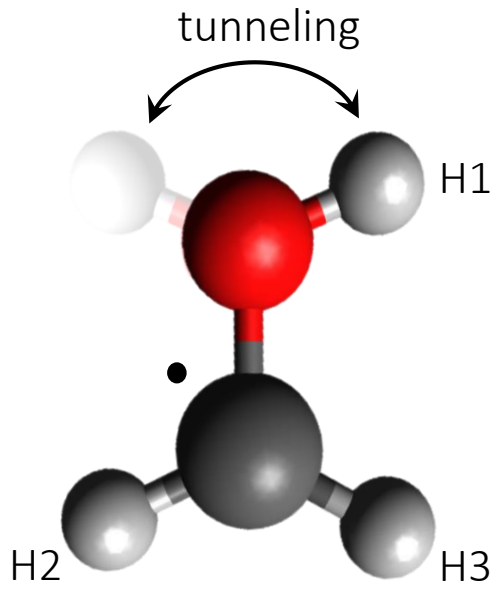
- Infrared spectral region
- Supersonic jet
- Roberts M. A. *et al.*, *The Journal of Physical Chemistry*, **117**, 7042-7049, 2013
- Schuder M. D. et al., *The Journal of Chemical Physics*, **146**, 194307, 2017

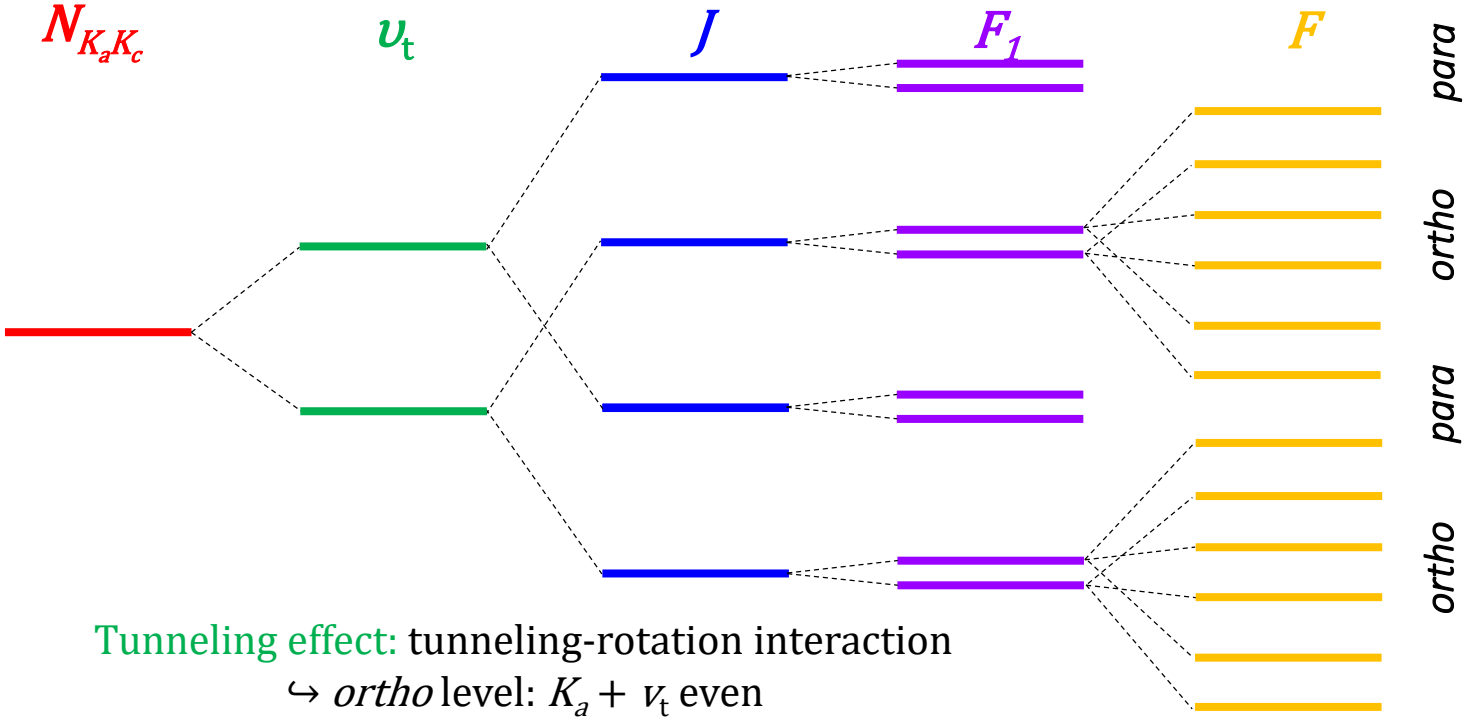
❑ Rotational study

- Millimeter-wave spectral region
- First observation of the rotational-tunneling spectrum
- Bermudez C. *et al.*, *Astronomy & Astrophysics*, **598**, A9, 2017



Spectroscopy





- ❑ Asymmetric top molecule
- ❑ Planar in $v = 0$
  - ➢ One unpaired electron
  - ➢ 3 H (of non-zero nuclear spin)
  - ➢ Tunneling of H1

Tunneling effect: tunneling-rotation interaction
↪ *ortho* level: $K_a + v_t$ even
↪ *para* level: $K_a + v_t$ odd

Fine structure: spin-rotation interaction
↪ $\boldsymbol{J = N + S}$

Hyperfine Structure: hydroxyl hydrogen nucleus interaction
↪ $\boldsymbol{F_1 = J + I_{H_1}}$

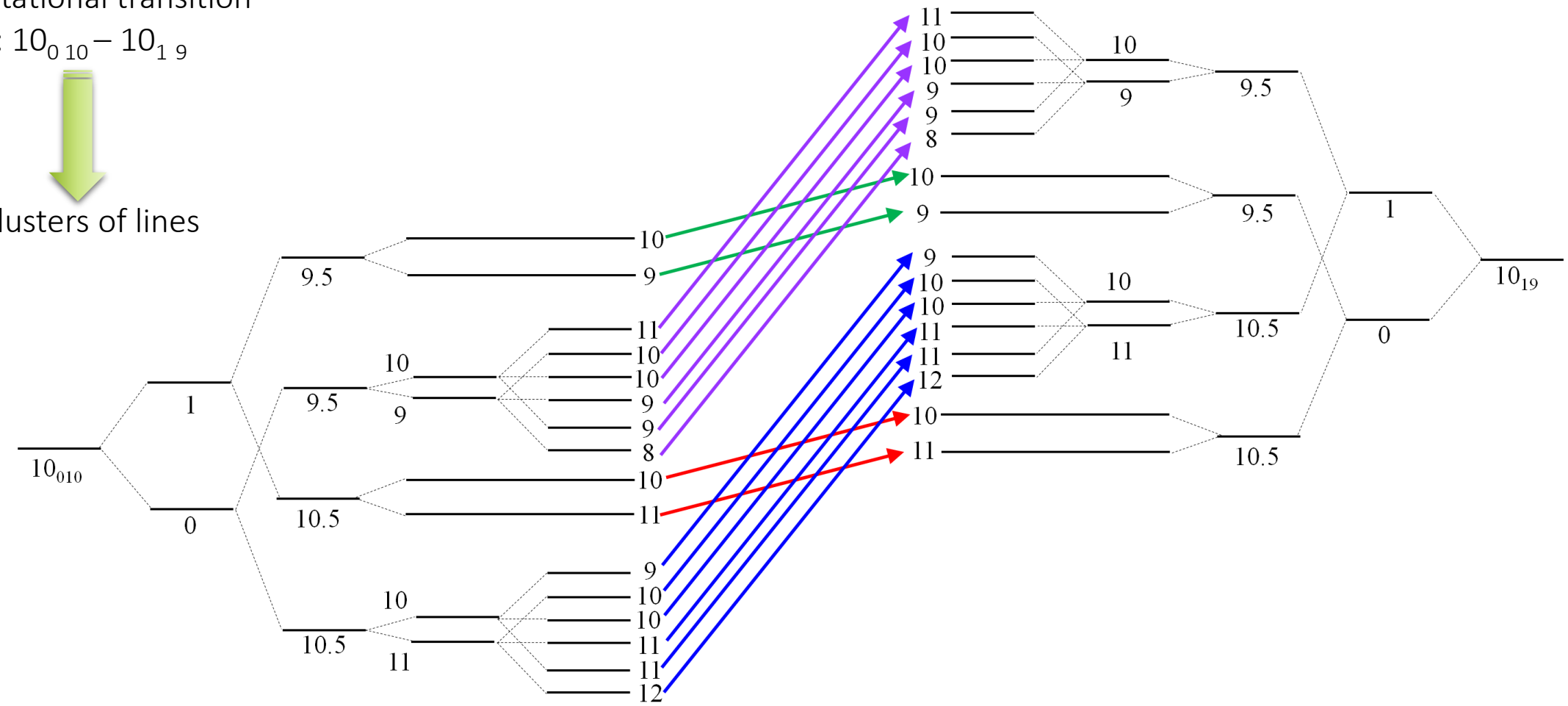
Hyperfine Structure: equivalent methylenic hydrogen nucleus interaction
↪ $\boldsymbol{F = J + I_{H_2} + I_{H_3}}$

Spectroscopy

One rotational transition

ex: $10_{0\,10} - 10_{1\,9}$

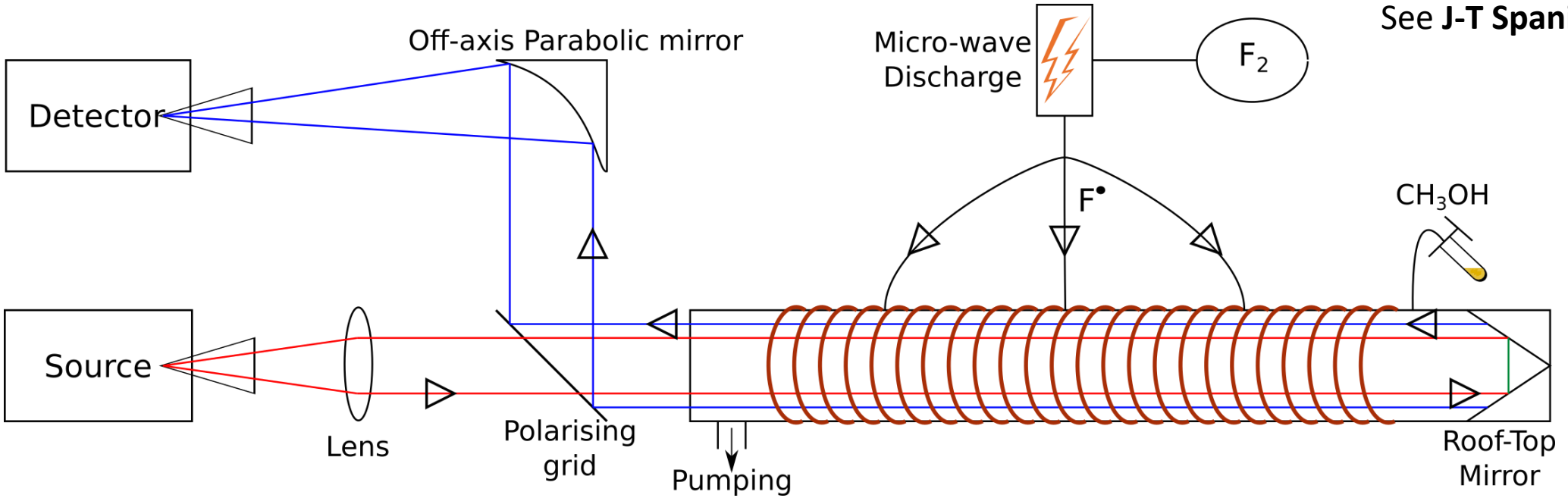
4 clusters of lines



Systematic measurements compulsory

Experimental methods

See **J-T Spaniol's talk** (TI05)



Production

Hydrogen abstraction from methanol by fluorine atom

Acquisition

Frequency multiplication chain spectrometer:

140-900 GHz

Magnetic Field Modulation to distinguish paramagnetic lines

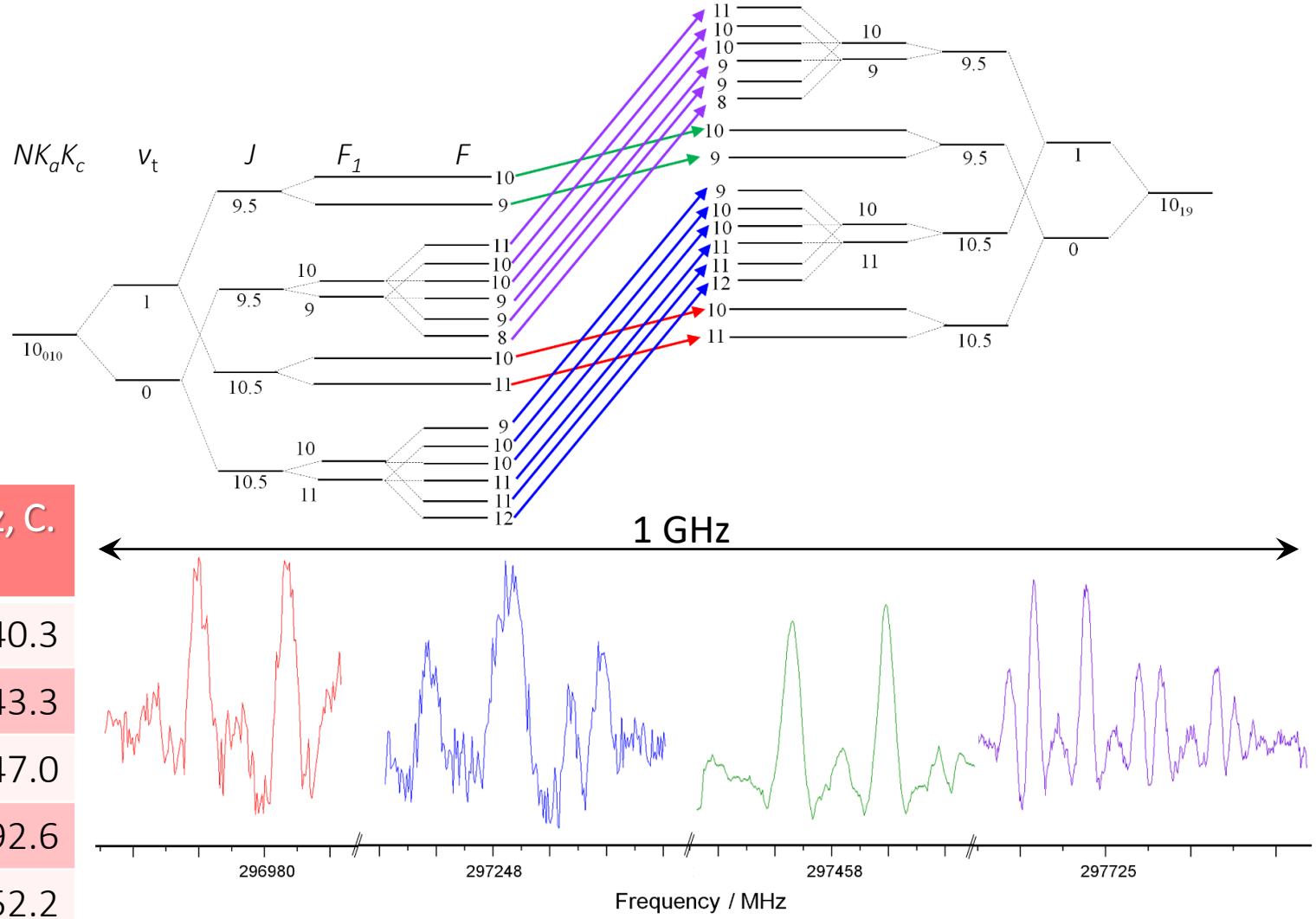
Results and discussion

Experimental measurements

- 676 mmw lines recorded + 96 from Bermudez et al. (2017)
- Freq. accuracies: from 50 to 800 kHz
- $^{r}R_{1\text{-}2}(1\text{-}15)$, $^{r}Q_{1\text{-}2}(1\text{-}16)$ and $^{p}R_{0\text{-}1}(6\text{-}17)$ transitions

Reliable and **constrained** fit

Parameters (MHz)	Present	Chitarra, O. et al.	Bermudez, C. et al.
A	194536.5	194535.4	194540.3
B	28869.5	29843.4	29843.3
C	26921.5	25947.5	25947.0
D_{NK} x 10^3	593.7	584.7	792.6
a_F(H)	-54.0	-54.4	-52.2
RMS	0.409	0.081	0.077



See **L Coudert's talk** (FC12)

Results and discussion

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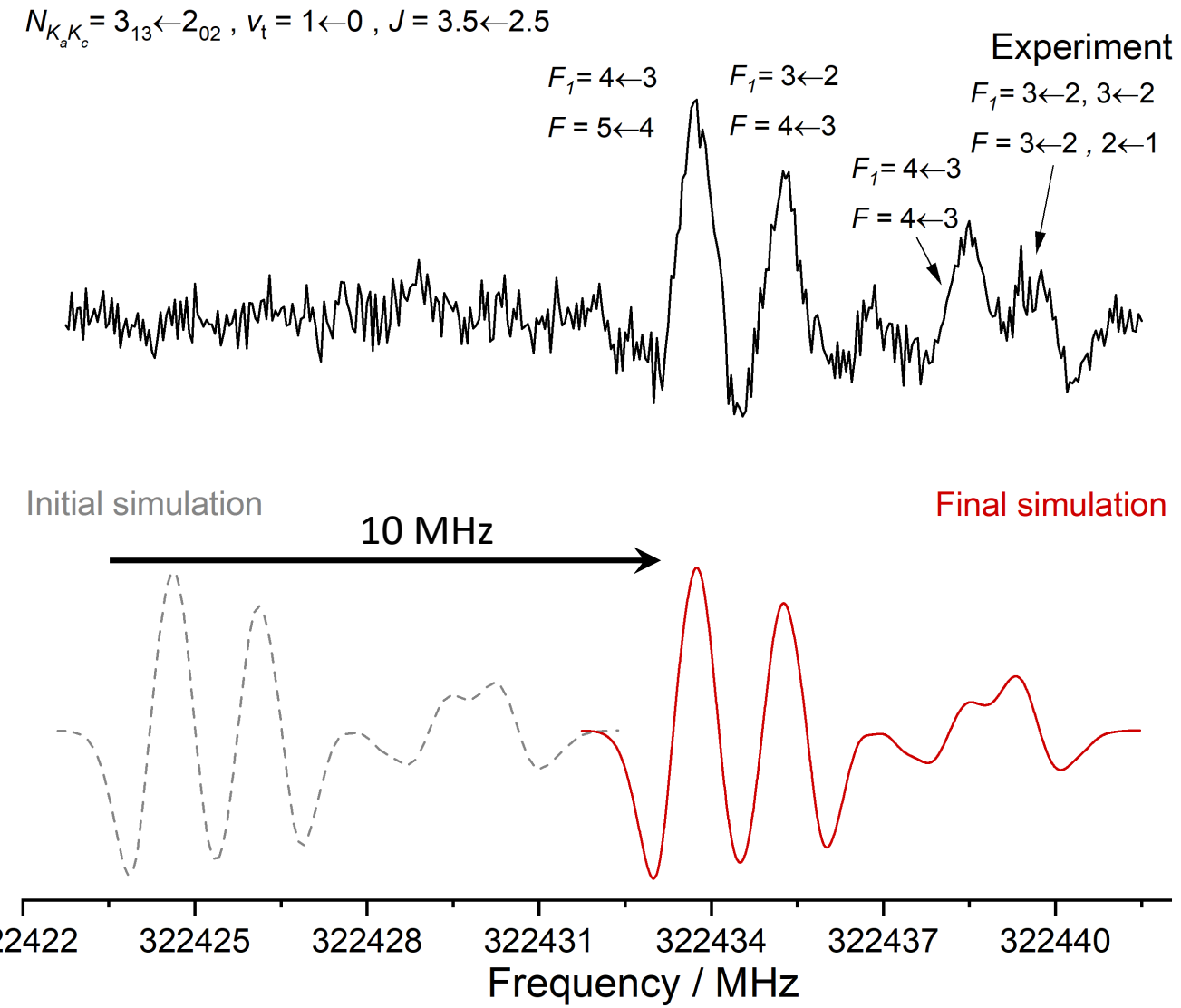

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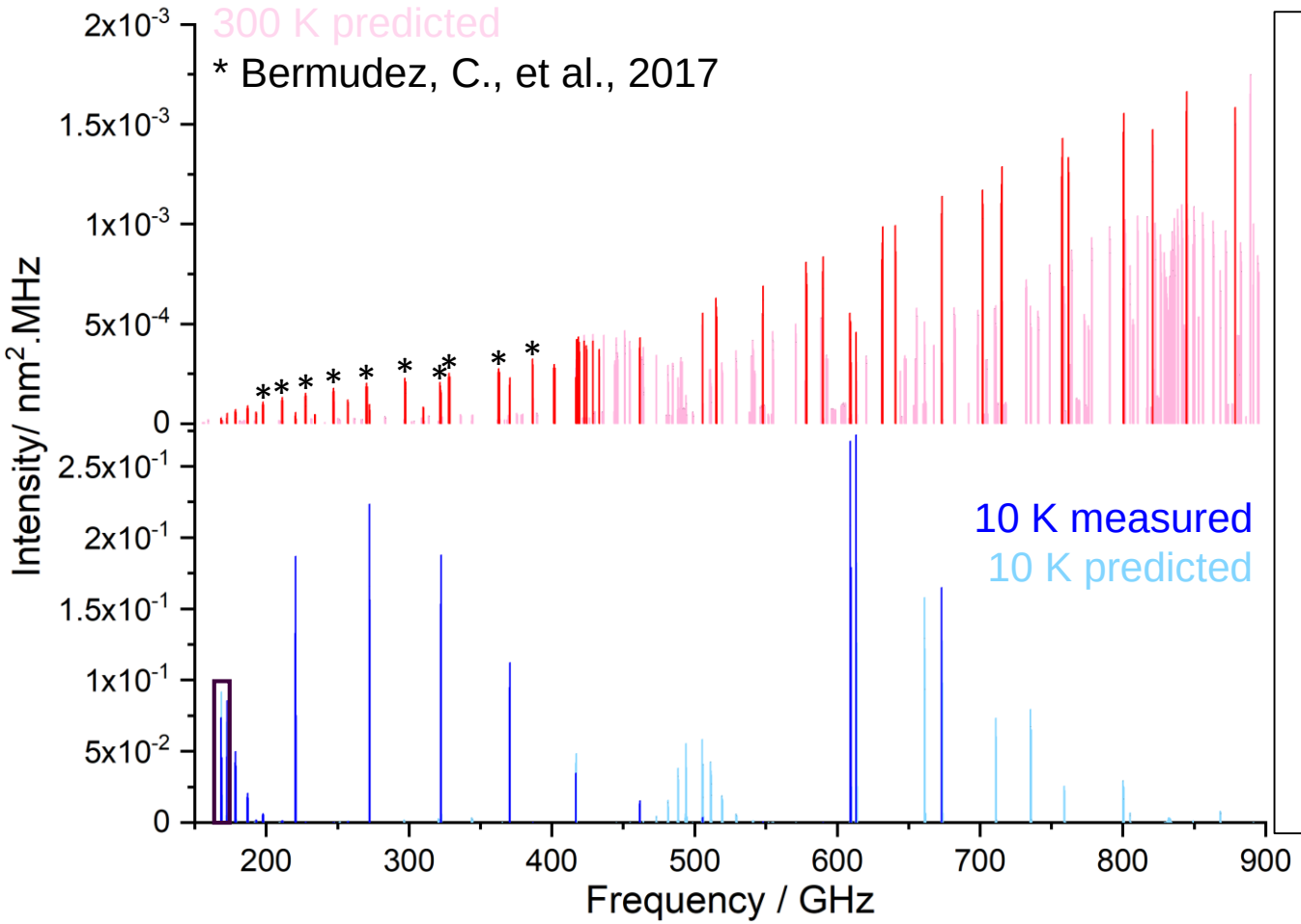
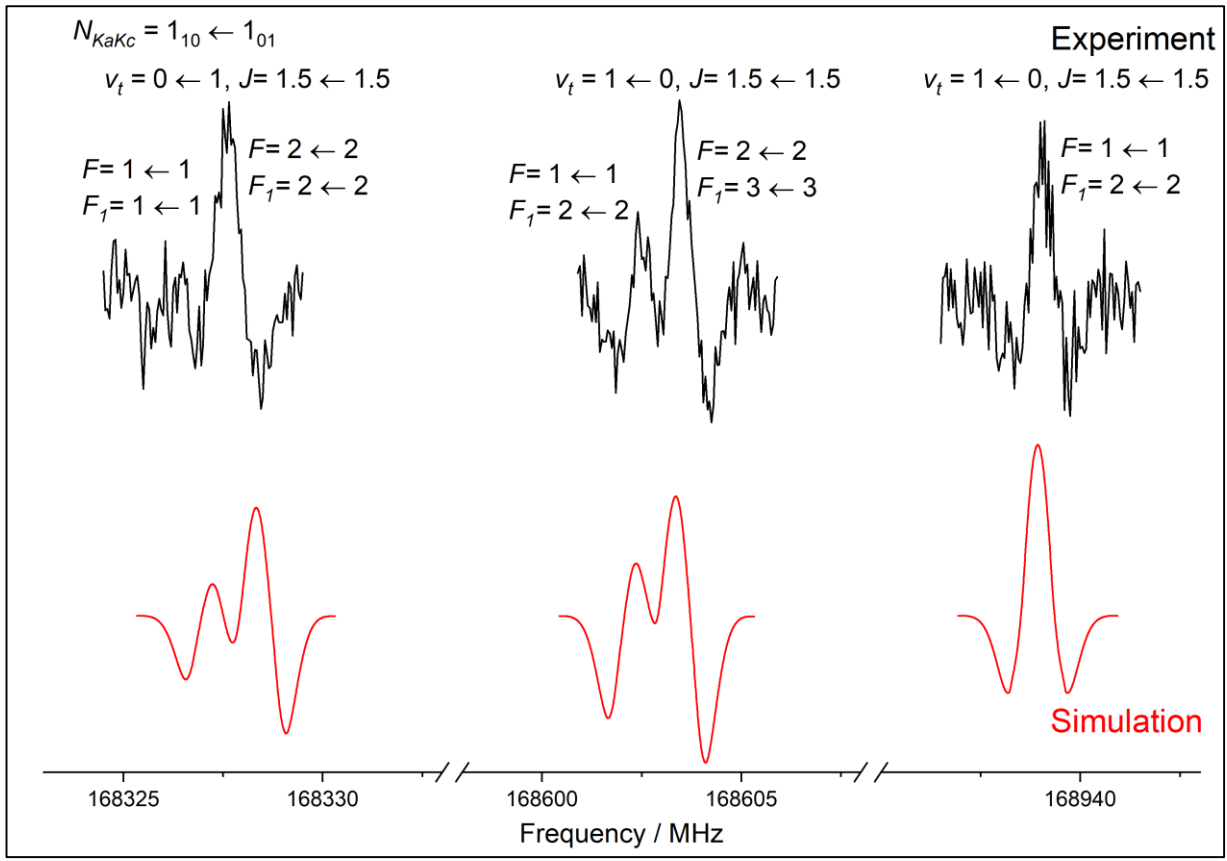
Results and discussion

Astrophysical relevant transitions





Perspectives

Our work

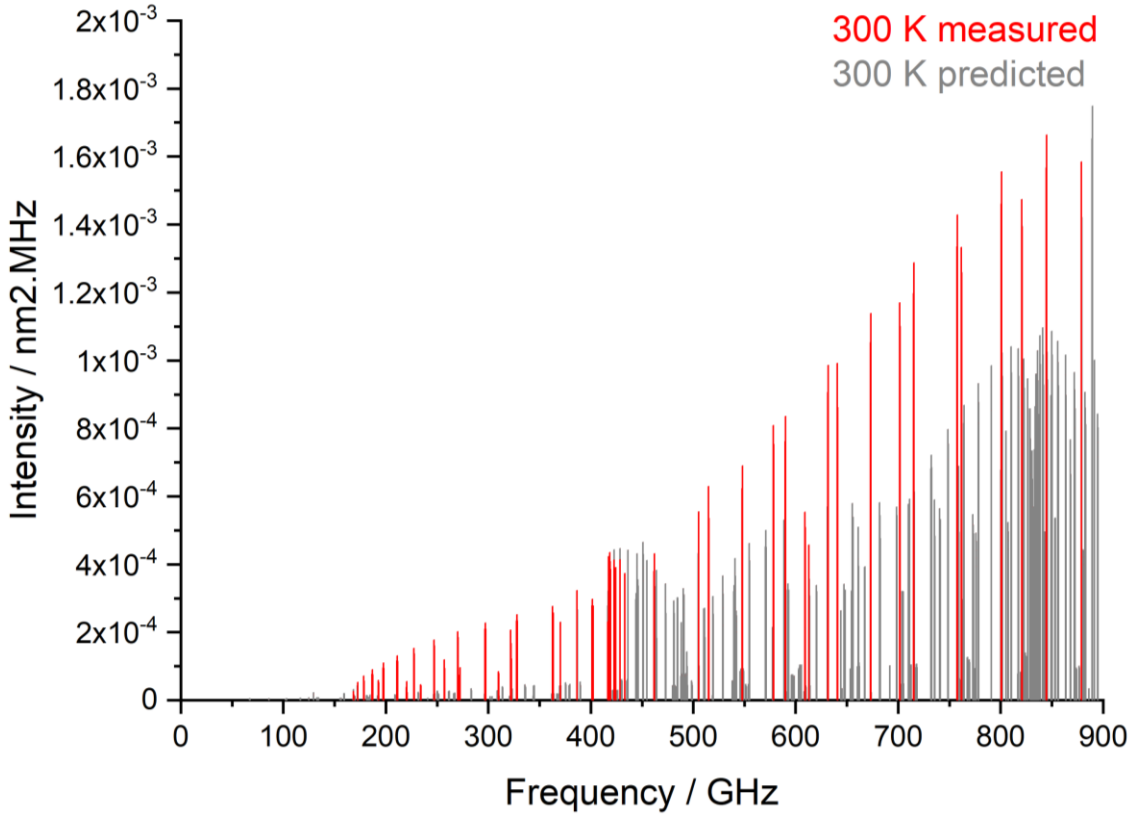
- More constrained set of rotational parameters

Consequences

- Better predictions of line positions

Perspectives

- Toward a more suitable model



Perspectives

Our work

- ❑ More constrained set of rotational parameters
- ❑ Measurement of astrophysical relevant transitions

Consequences

- ❑ Better predictions of line positions
- ❑ Confident search of the CH_2OH radical in the ISM

  Ongoing observations (30m IRAM telescope)

Perspectives

- ❑ Toward a more suitable model
- ❑ Confirmation or modification of astrophysical models

Acknowledgments

Collaborators

Institut des Sciences Moléculaires d'Orsay (France)

Olivier Pirali
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Thomas Hearne
Jean-Thibaut Spaniol

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Jean-Christophe Loizon

Max-Planck-Institut für extraterrestrische Physik (Germany)

Silvia Spezzano
Valerio Lattanzi

I. Physikalisches Institut (Germany)

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