Rotational spectroscopy of *normal*-propanol: *Aa* and *Ag* conformers

by

Oliver Zingsheim

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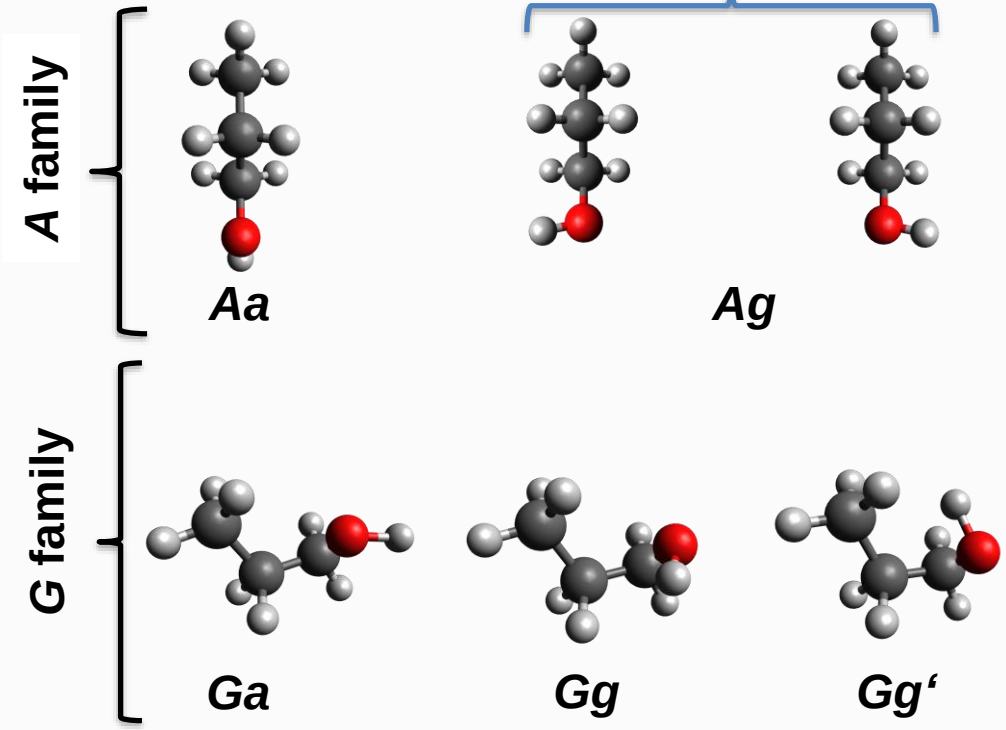
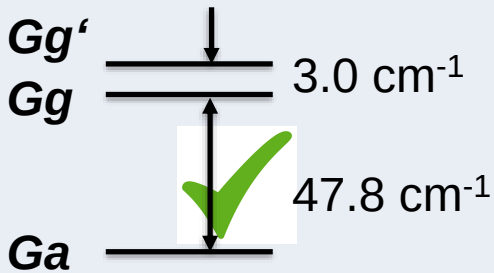
22.06.2022

ISMS 2022 – WF11

Molecule of interest: *normal*-Propanol

„Mirror images“
Low barrier/ Tunneling:
Ag⁺ and Ag⁻



*.cat file	3-state analysis
X	X
✓	
Ref. [4b]	Ref. [4b]

Selected studies on *normal*-propanol:
[1] Abdurakhmanov *et al.*: several studies (1967-1987)
[2] H. Dreizler & F. Scappini, *Z. Naturforsch. A* **36** (1981) 1187
[3] Kahn & Bruice**,** *Chem.Phys.Chem.* **6** (2005) 487
[4a] Z. Kisiel et al., Talk RI14 @ 61st ISMS (2006)
[4b] Z. Kisiel et al., *Phys. Chem. Chem. Phys.* **12** (2010) 8329
and references therein

Our Work:
A&A accepted (2022) - doi: 10.1051/0004-6361/202243571

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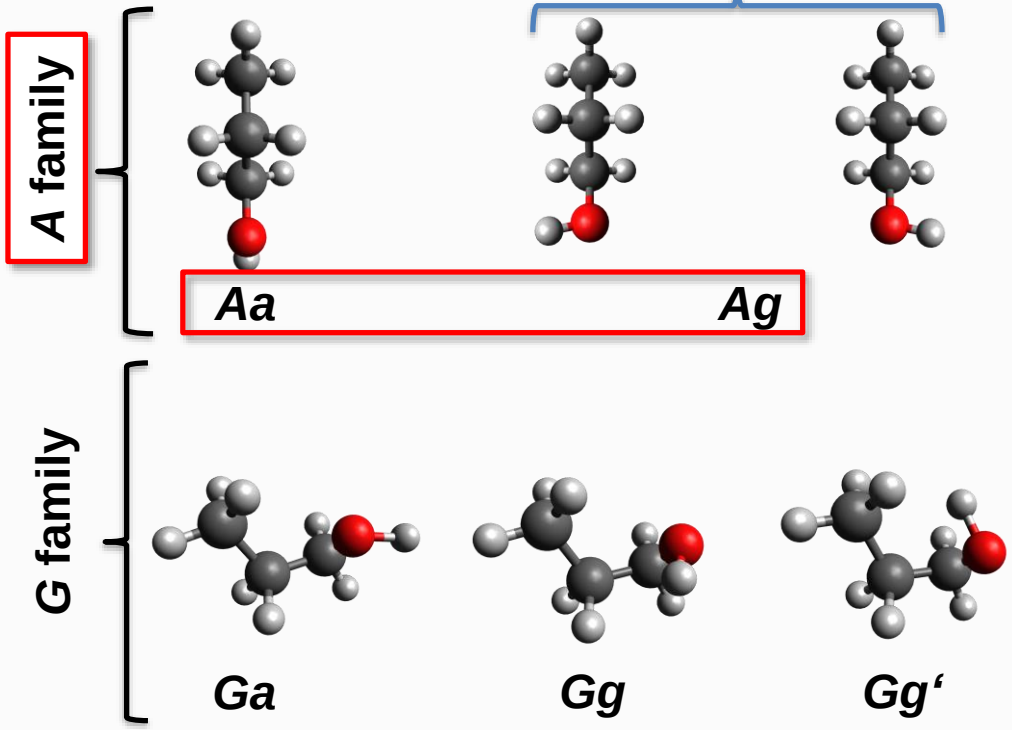

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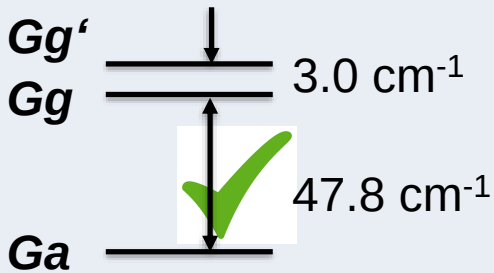
✓	
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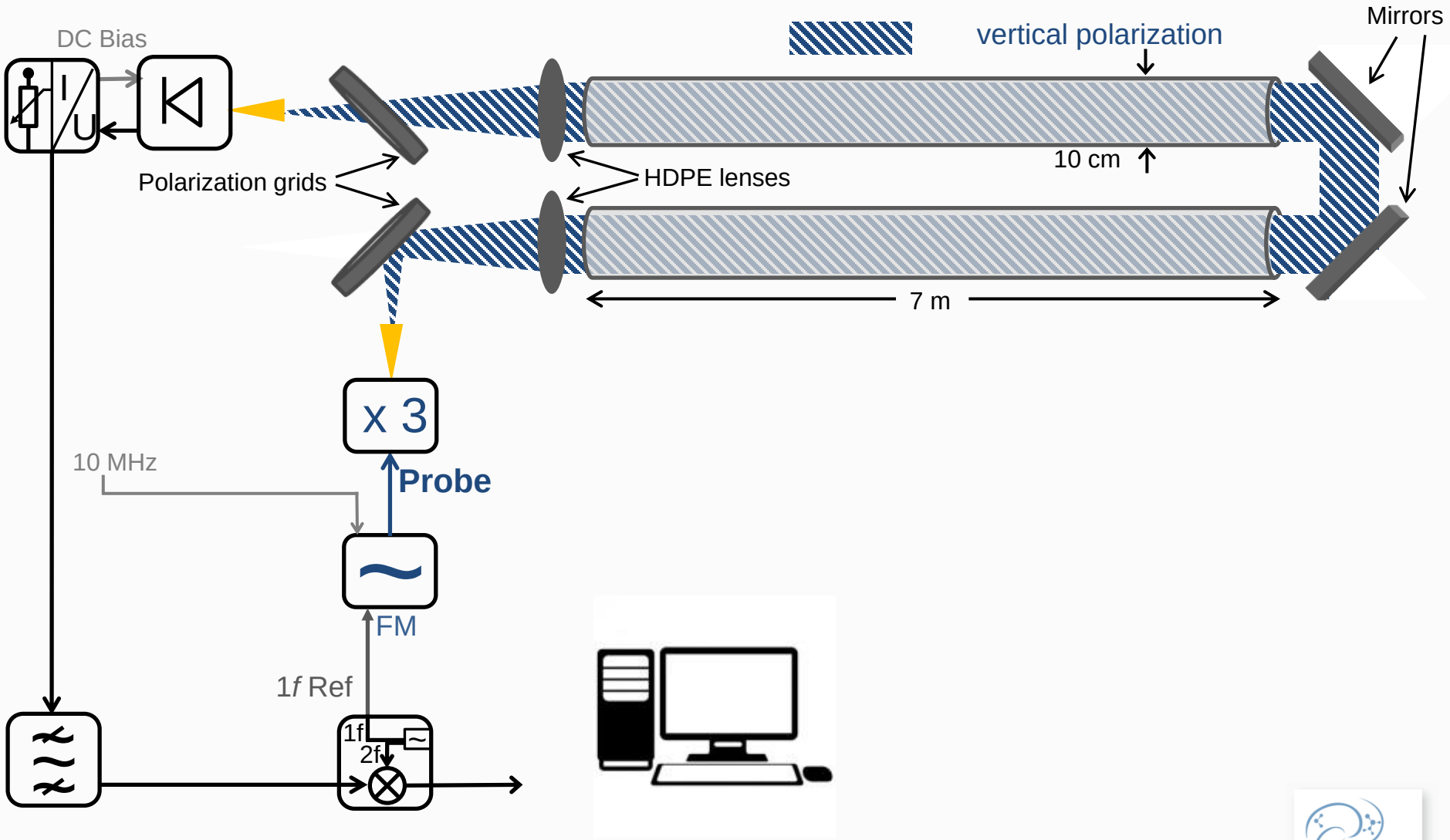
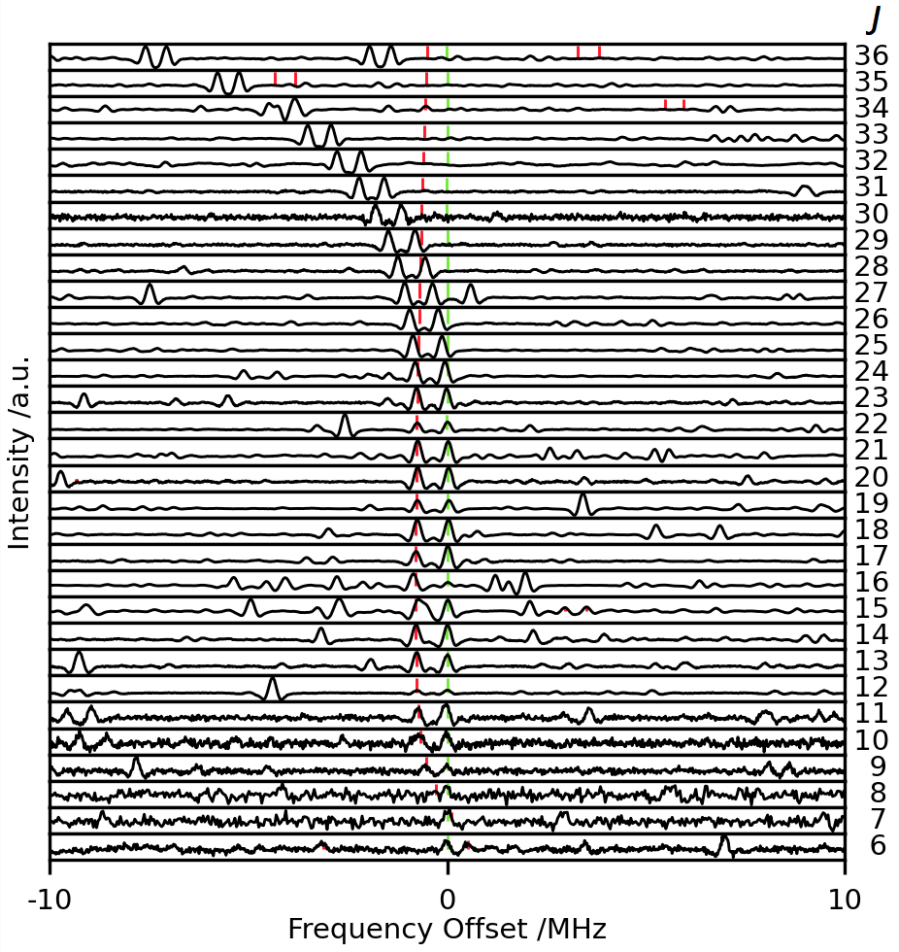
Rotational Spectroscopy: Experimental Setup



Loomis-Wood plot: *Aa n*-propanol

b-type transition:

$J_{Ka;Kc} = J_{3;J-3} \leftarrow J_{2;J-2}$



- Transitions assigned:

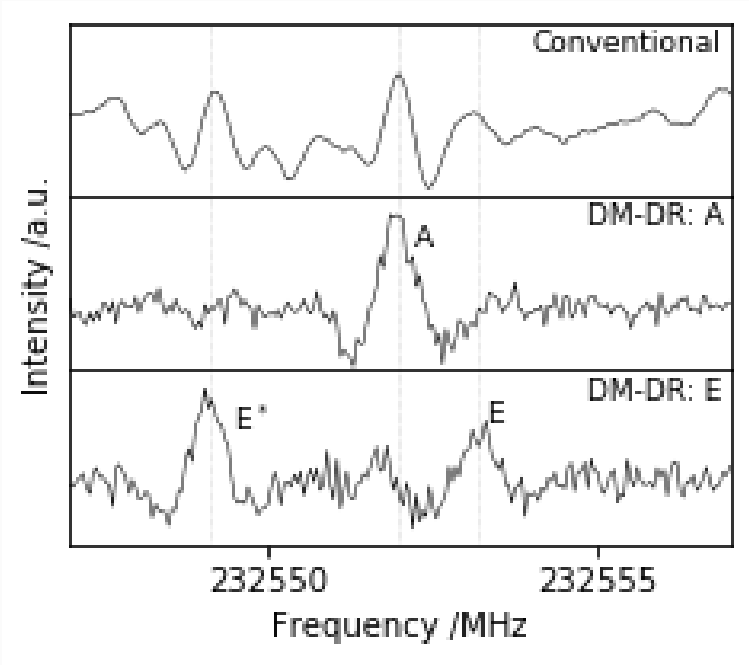
up to J = 41 ($\Delta\nu$ = 90 MHz)

- Transitions fit:

up to J = 22

Double-Modulation Double-Resonance (DM-DR) spectroscopy

DM-DR: O. Zingsheim et al., *Journal of Molecular Spectroscopy* **381** (2021) 111519



Aa n-propanol:

$J_{Ka;Kc} = 10_{4;6} \leftarrow 9_{3;7}$

- DM-DR: Baseline- and confusion-free spectroscopy
- Assignments of internal rotation components A and E are verified
- Shifted (or perturbed) transitions can unambiguously be assigned
- DM-DR technique is applicable at higher frequencies than W-band

Spectroscopic parameters: *Aa n*-propanol

Theory | Experiment

Parameter	Ref. [1]	Ref. [2]	Ref. [3]	Ref. [3]	Our Work
A /MHz	26579	26401.671(50)	26401.5164(50)	26422.79(91)	26401.4395(40)
B /MHz	3784	3802.154(11)	3802.15219(57)	3802.3984(63)	3802.16025(39)
C /MHz	3532	3549.543(20)	3549.46158(60)	3549.4244(18)	3549.45427(33)
No. of transitions		113	(232)		928
rms /kHz		195	110	Not presented	48
wrms					1.07

We were not aware of this ISMS talk

[1] Z. Kisiel et al., *Phys. Chem. Chem. Phys.* **12** (2010) 8329
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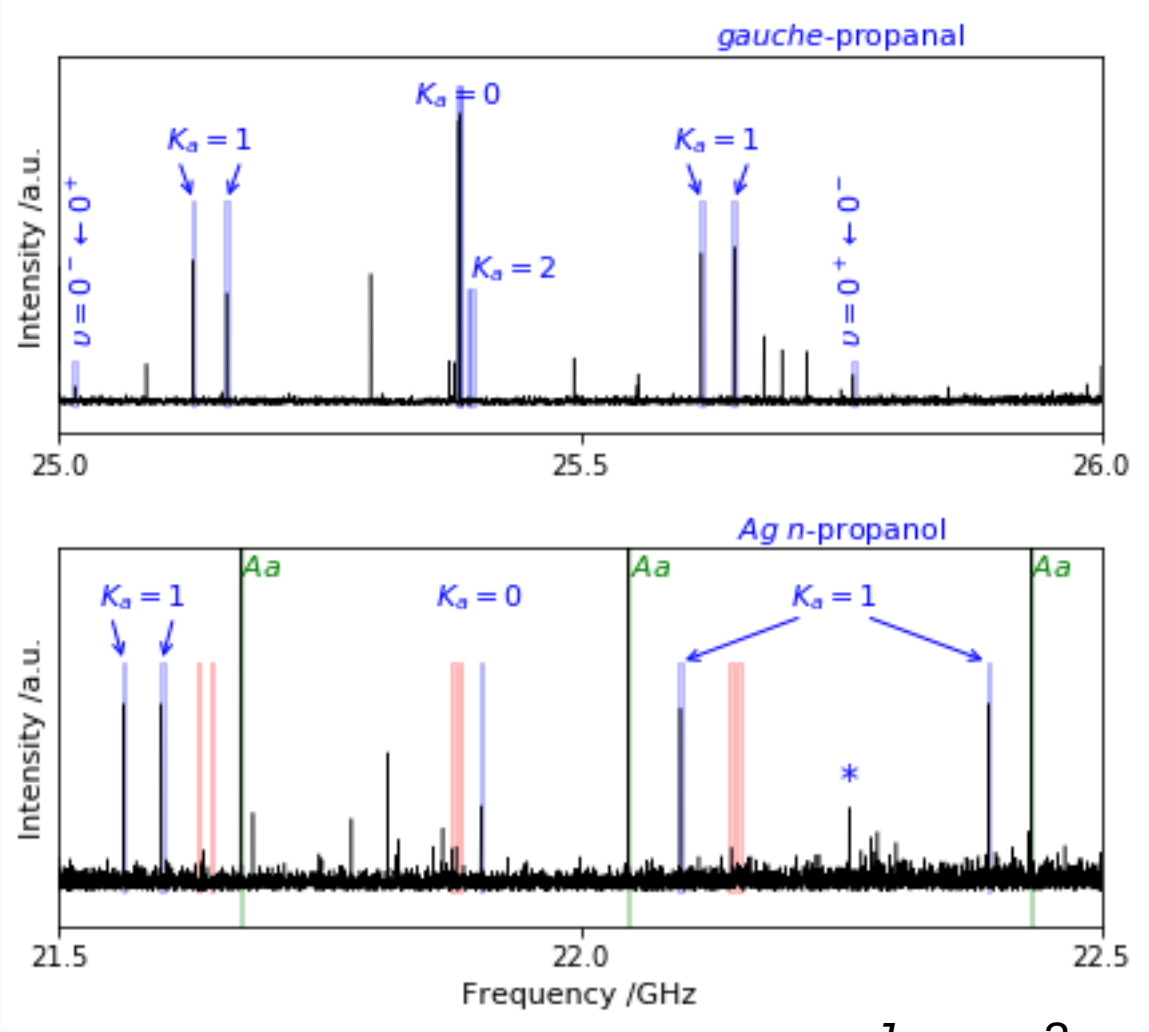
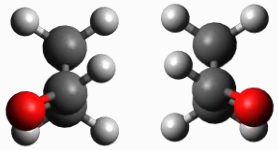
MW spectrum: Chirped-pulse experiment

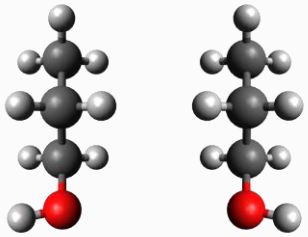


➢ *gauche*-propanol



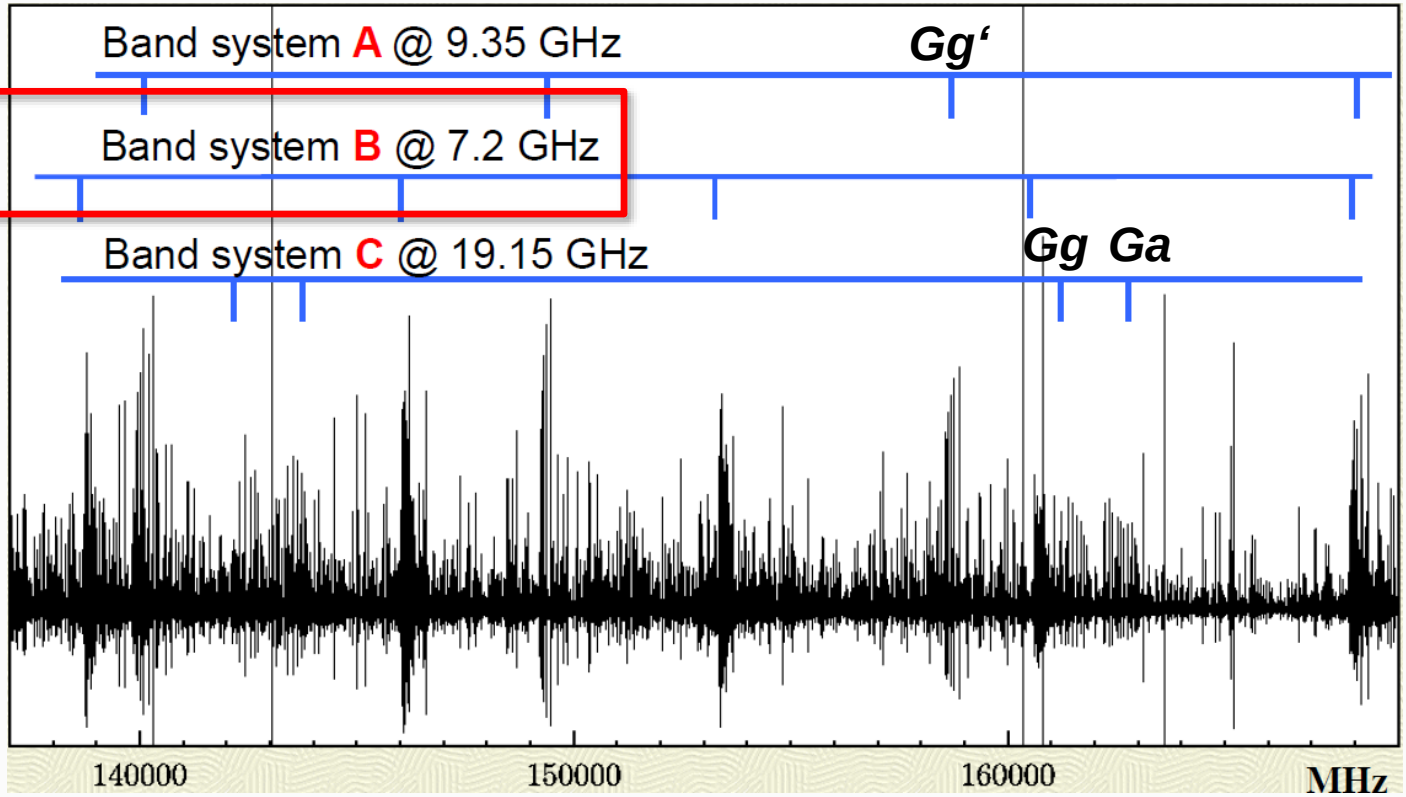
O. Zingsheim et al.,
Journal of Molecular Spectroscopy **384** (2022) 111565

➢ *Ag n*-propanol



$J_{Ka;Kc} = 3_{Ka;Kc} \leftarrow 2_{Ka;Kc-1}$

Band systems of *normal*-propanol



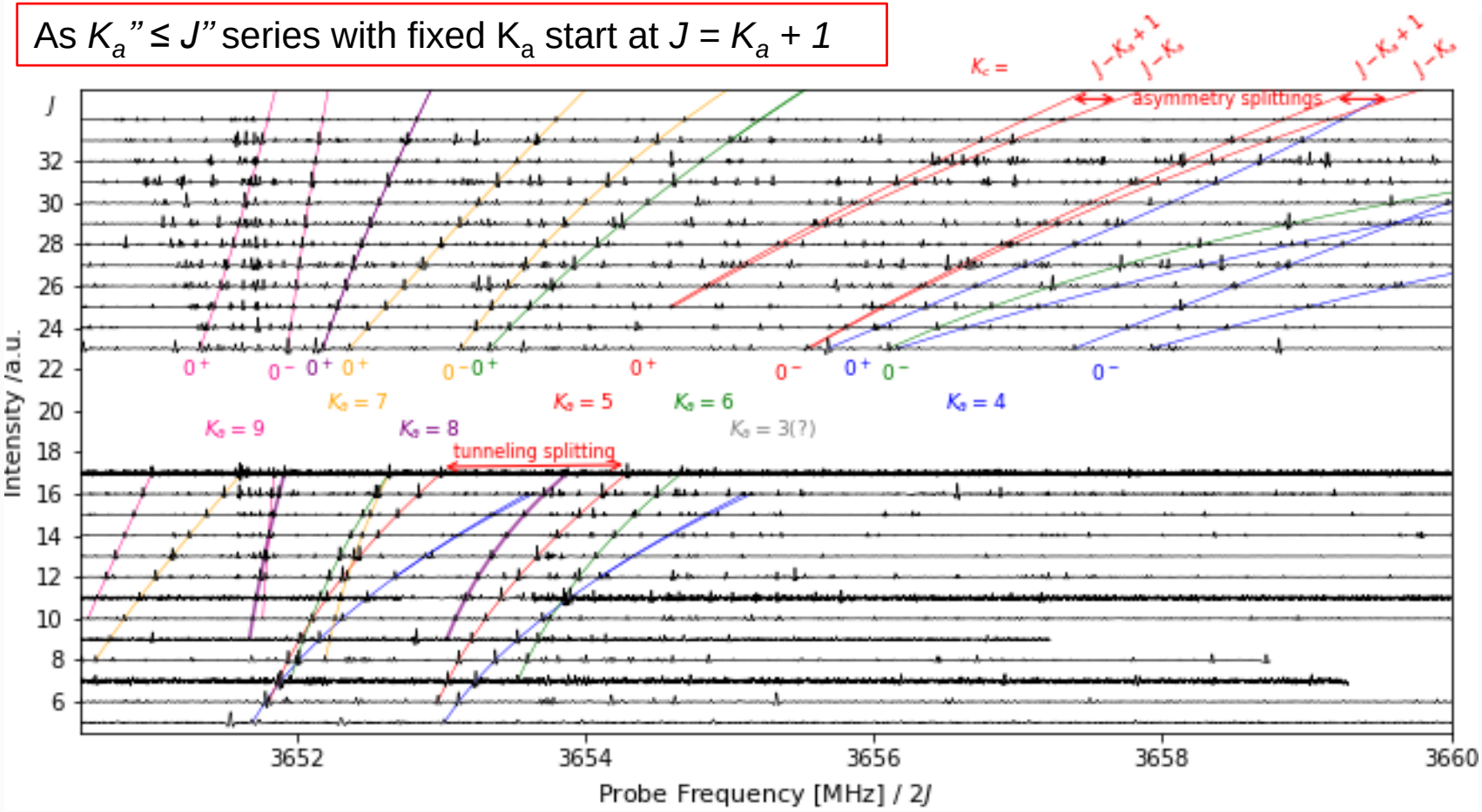
➢ Fortrat diagram with 2*B* = 7.2 GHz

Picture is taken from: Z. Kisiel et al., Talk RI14 @ 61st ISMS (2006)
More accurate results can be found in: Z. Kisiel et al., *Phys. Chem. Chem. Phys.* **12** (2010) 8329

Fortrat diagram: *Ag n*-propanol

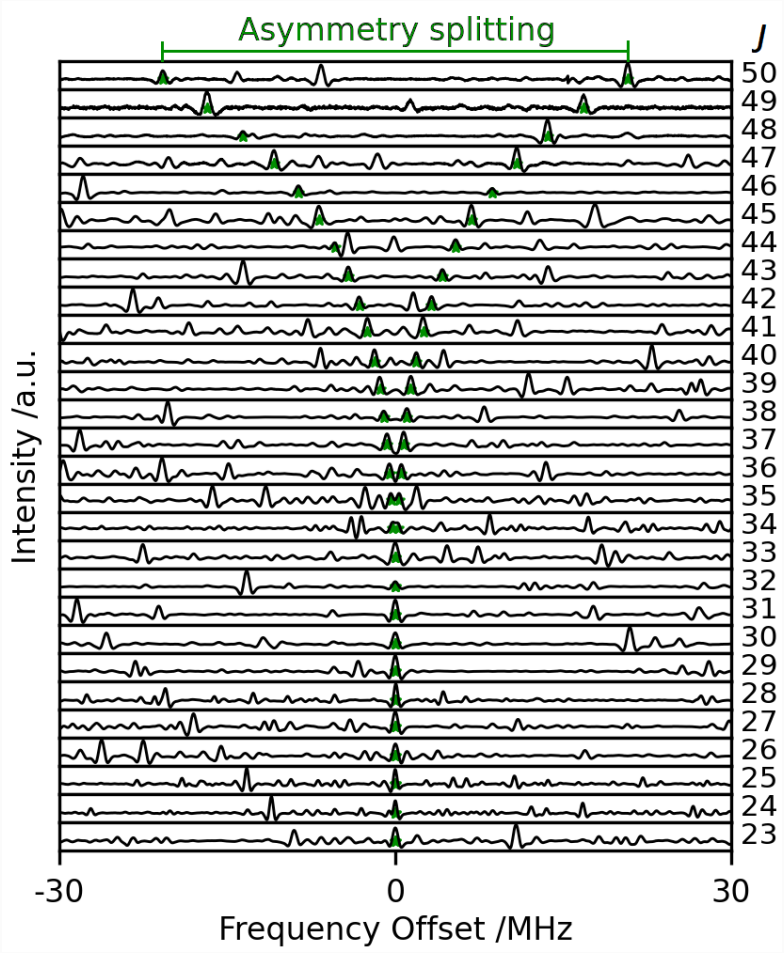
$J_{Ka;Kc} \leftarrow (J\text{-}1)_{Ka;Kc-1}$

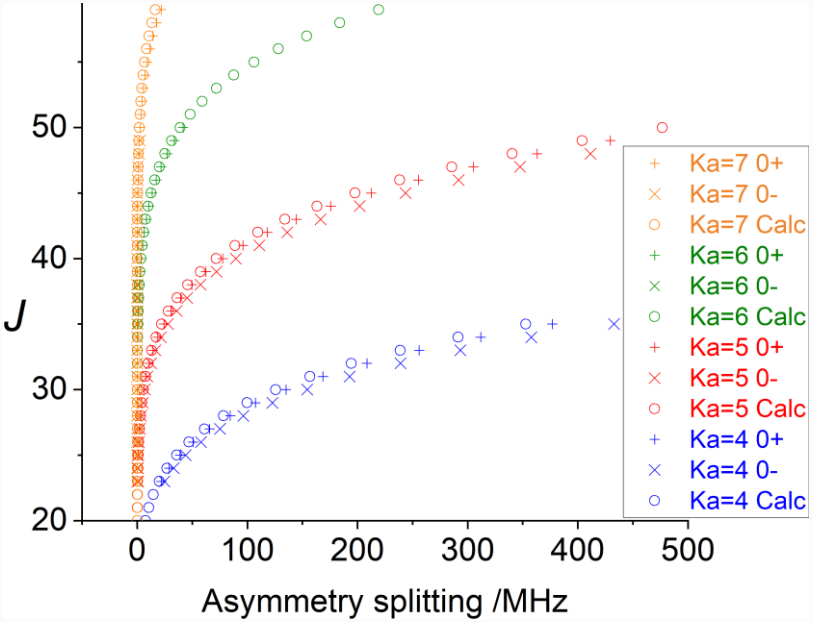
As $K_a'' \leq J''$ series with fixed K_a start at $J = K_a + 1$



- Linkages verified by DM-DR spectroscopy (W-band region)
- Perturbed system

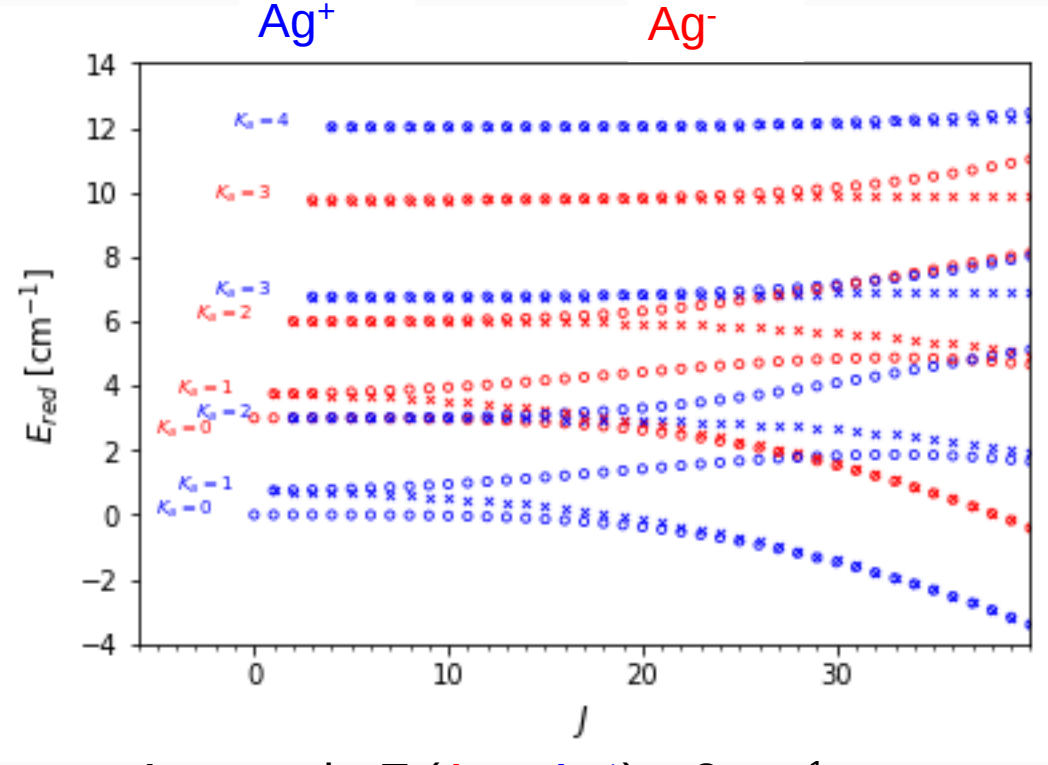
Asymmetry splitting: *Ag n*-propanol





Calc.: Z. Kisiel et al., *Phys. Chem. Chem. Phys.* **12** (2010) 8329

Reduced energy diagram: *Ag n*-propanol



Assumed Δ E (Ag$^-$ - Ag$^+$) = 3 cm^{-1}

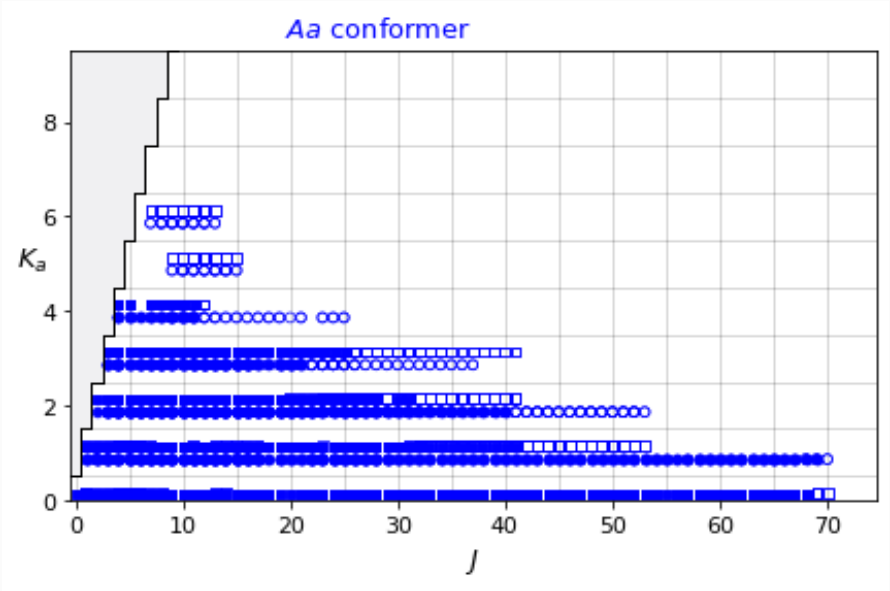
Δ E (Ag$^+$ - Aa)=

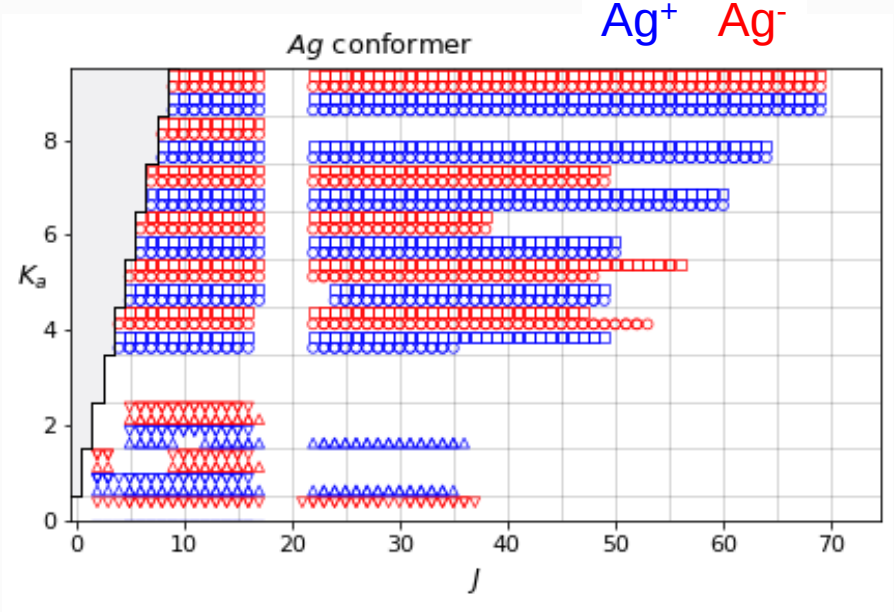
352043.(884)MHz
or
11.44(3)cm^{-1}

Ref: Z. Kisiel et al.,
61st ISMS (2006) RI14

➢ A coupled state fit of the *Aa* conformer and both tunneling states of *Ag* is needed

Quantum number overview: *Aa* and *Ag* *n*-propanol





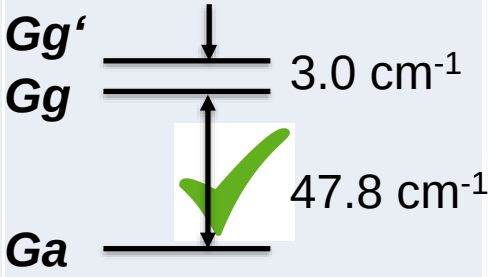
Assigned — *Assigned + Fit* : $K_a + K_c = J$

Assigned — *Assigned + Fit* : $K_a + K_c = J+1$

- Create *.cat files with *ab-initio* calculations, but use only assigned transition frequencies

Molecule of interest: *normal*-Propanol

- Coupled state fit for the *A* conformers is still desired
  → relative energies
- Predictions (*.cat files) are available now for all five conformers of *normal*-propanol
- Astronomical search of *normal*-propanol is possible

family	*.cat file	3-state analysis
A	✓	X
G	✓	

Ref. Z. Kisiel et al., *Phys. Chem. Chem. Phys.* **12** (2010) 8329

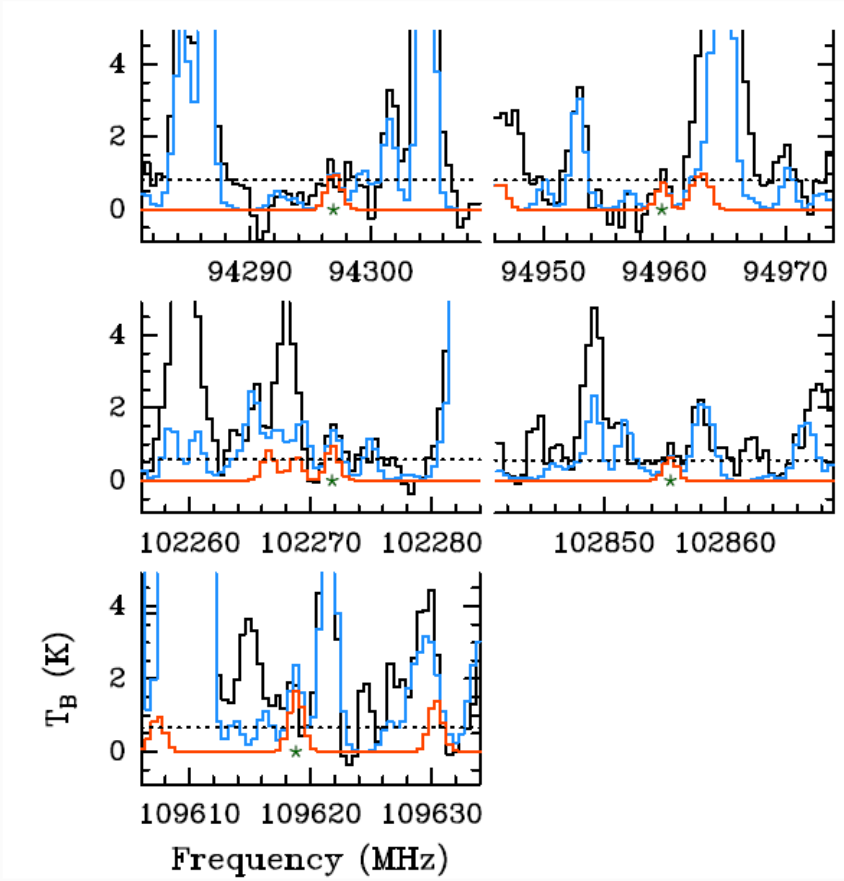
Astronomical detection

normal-propanol:
Gg‘ : 8 lines
Ag : 5 lines

- propanol (C_3H_8O):
[*iso*] / [*normal*] = 0.6

- propyl cyanide (C_3H_7CN):
[*iso*] / [*normal*] = 0.4

- [ethanol] / [*normal*-propanol] = 20



ReMoCA survey toward Sgr B2(N2b)

More details can be found in an acompanion article:
A. Belloche et al., *A&A (2022)* accepted:
https://doi.org/10.48550/arXiv.2204.09912

THANK YOU FOR YOUR ATTENTION!

Special thanks goes to:

- J. Maßen
- H.S.P. Müller
- B. Heyne
- M. Fatima
- L. Bonah
- S. Thorwirth
- A. Belloche
- S. Schlemmer
- …

COLOGNE CENTER FOR TERAHERTZ SPECTROSCOPY

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