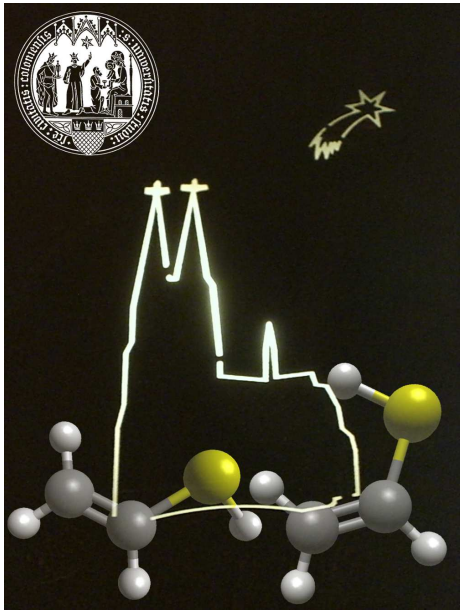


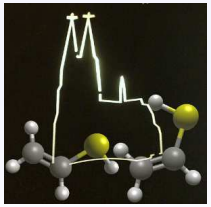
Pure rotational spectroscopy of Vinyl Mercaptan

Marie-Aline Martin-Drumel[1], Oliver Zingsheim, Sven Thorwirth, Holger S. P. Müller, Frank Lewen & Stephan Schlemmer

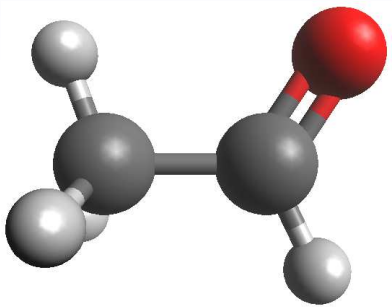
I. Physikalisches Institut, Universität zu Köln, Cologne, Germany

ISMS 69th meeting
June 16, 2014

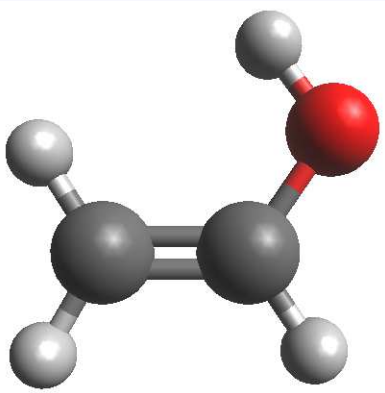
[1] *Present address:* Harvard-Smithsonian Center for Astrophysics, Cambridge, MA 02138, USA



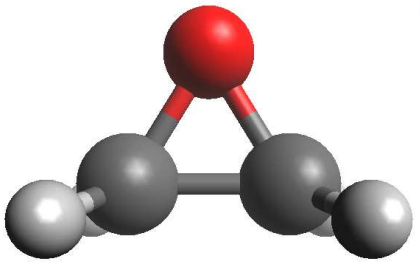
C_2H_4O vs. C_2H_4S



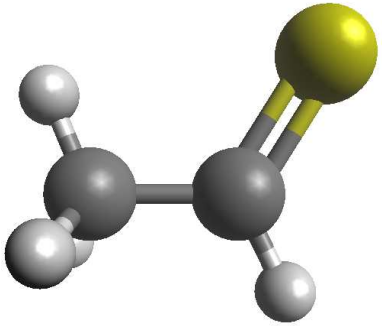
Acetaldehyde



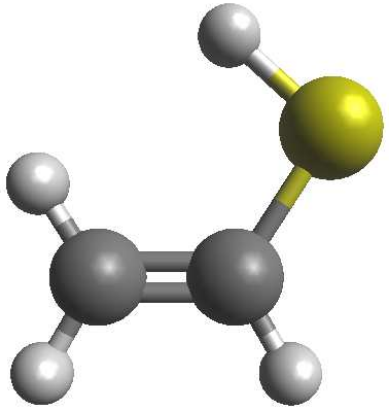
Vinyl Alcohol



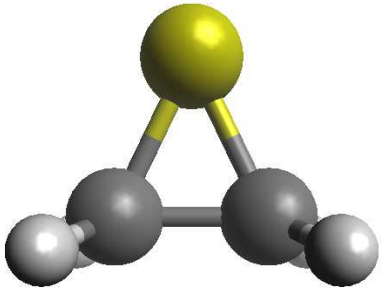
Oxirane



Thioacetaldehyde



Vinyl Mercaptan



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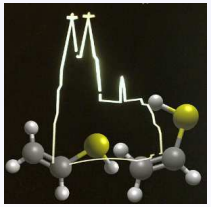

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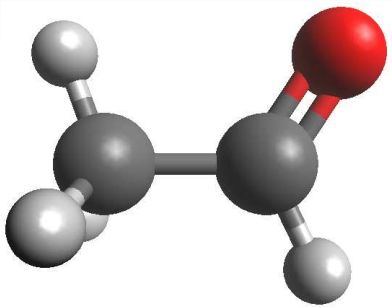

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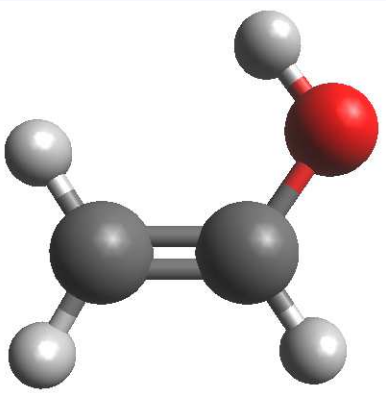

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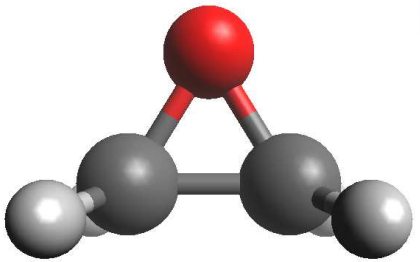

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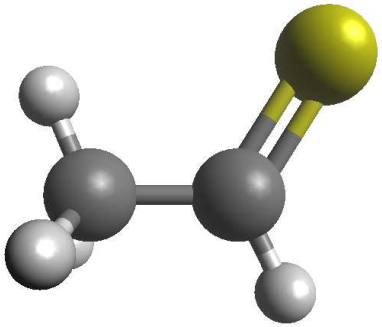
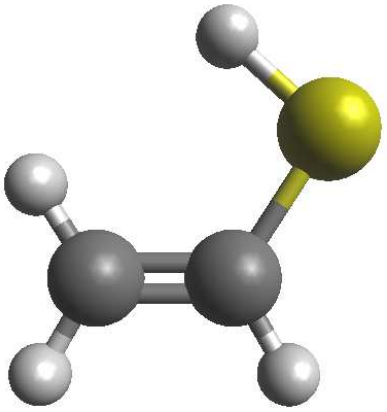
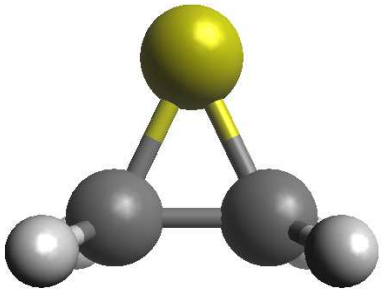


Thioacetaldehyde



Vinyl Mercaptan



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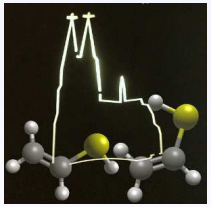

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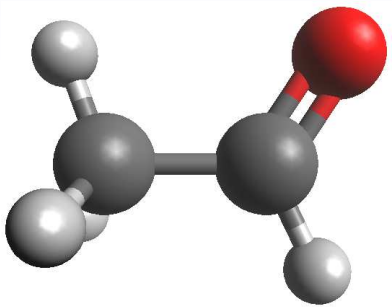

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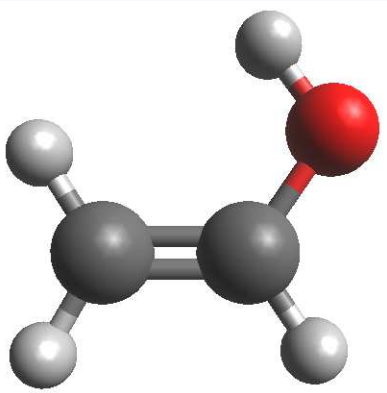

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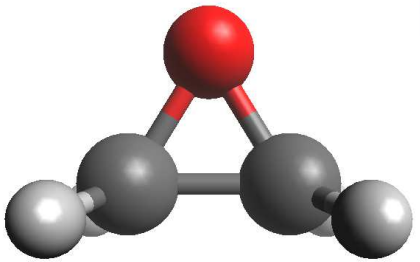

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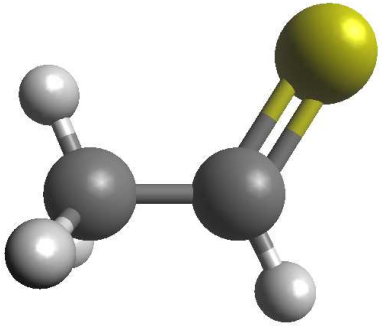

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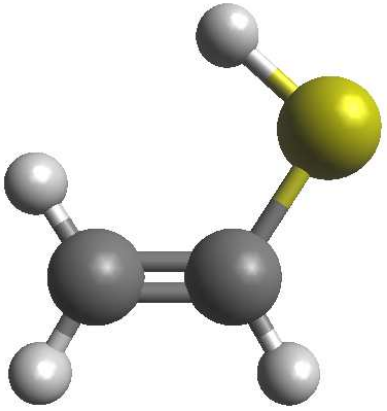
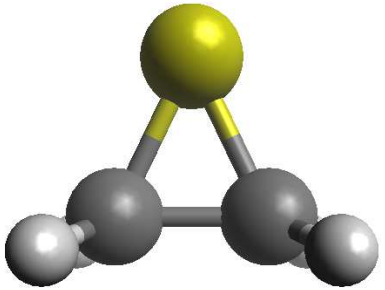


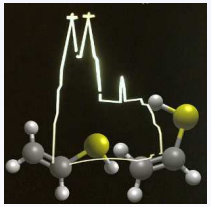
Vinyl Mercaptan



Thiirane

T. Hirao, J. Mol. Spectrosc. (2001)

M. K. Bane, J. Chem. Phys. (2012)



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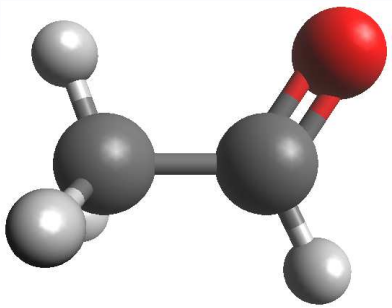

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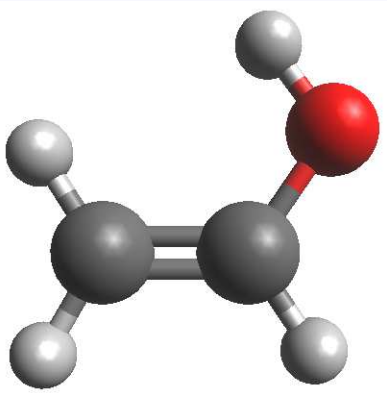

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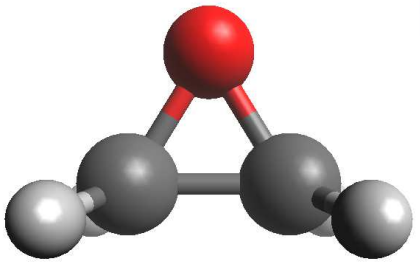

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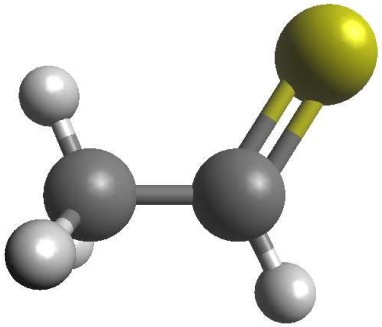

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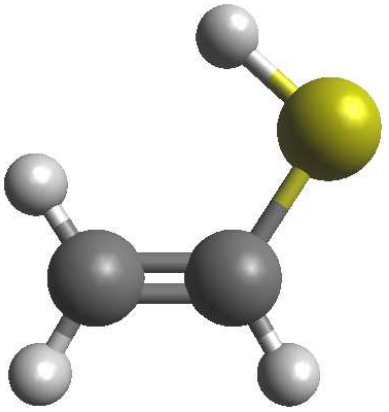
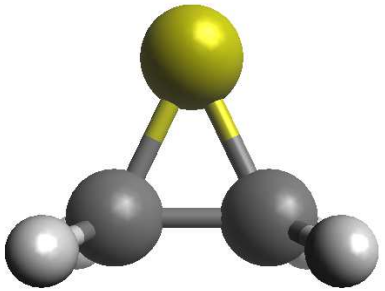


Vinyl Mercaptan



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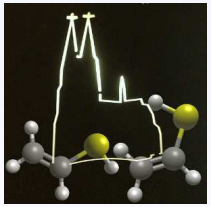
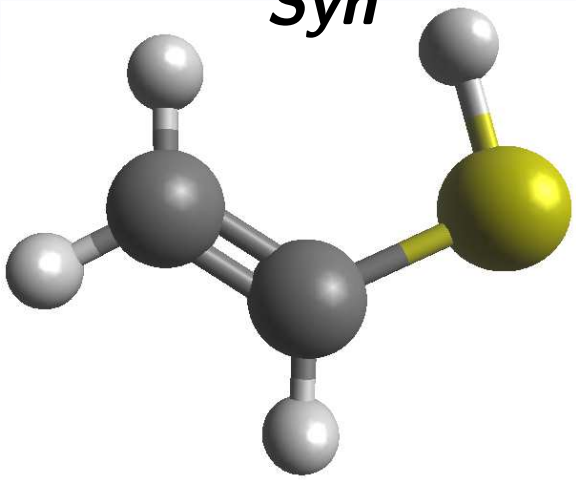
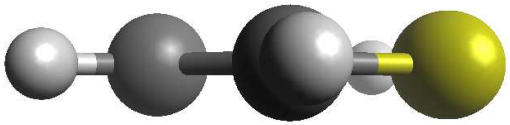


Vinyl Mercaptan conformers

Syn





$\mu_a = 0.813(1)$ D[1]

$\mu_b = 0.376(4)$ D

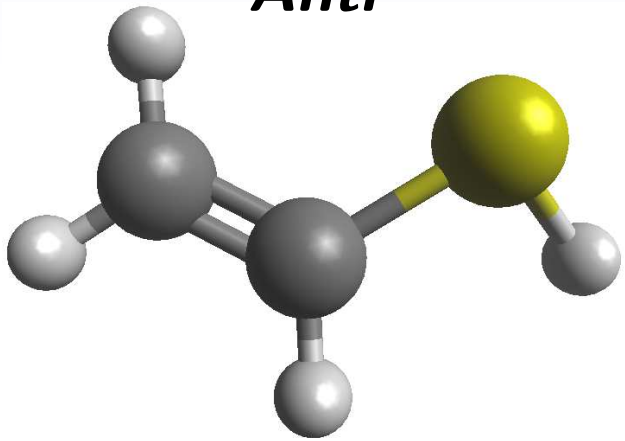
$\mu_{tot} = 0.896(3)$ D

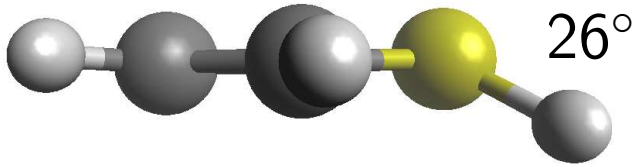
$\kappa = -0.97$[2]

near prolate

rotors

Anti





$\mu_a = 0.425(10)$ D[2]

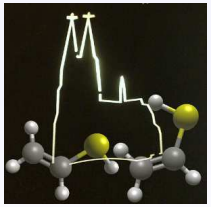
$\mu_b = 1.033(10)$ D

$\mu_{tot} = 1.117(14)$ D

μ_c

[1] M. Tanimoto *et al.*, *J. Mol. Spectrosc.* **78**, 95 (1979)

[2] M. Tanimoto & J. N. Mcdonald, *J. Mol. Spectrosc.* **78**, 106 (1979)



Vinyl Mercaptan conformers

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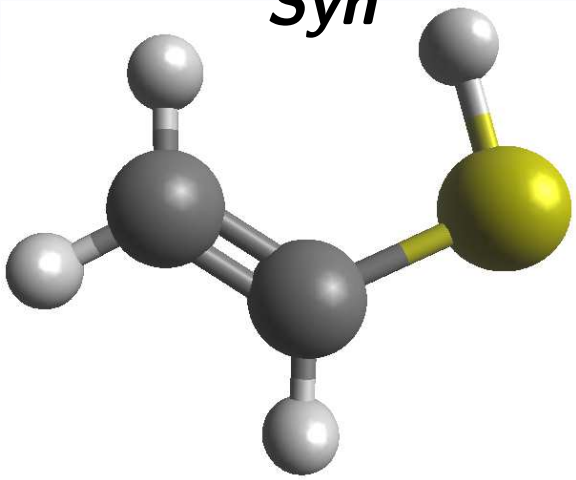

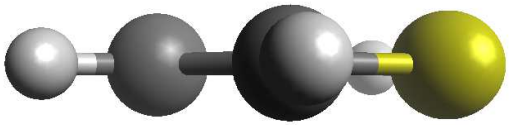

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$\mu_b = 0.376(4)$ D

$\mu_{tot} = 0.896(3)$ D

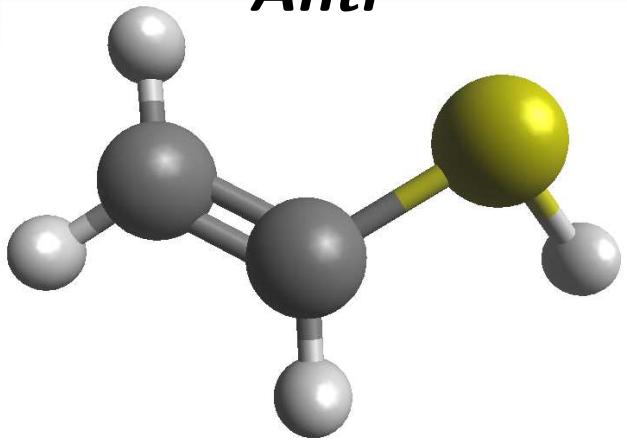
$\kappa = -0.97$[2]

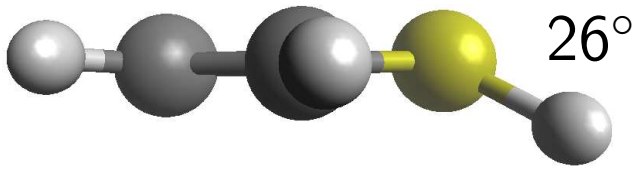
near prolate

rotors

a- and *b*-type transitions

Anti





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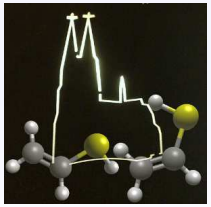
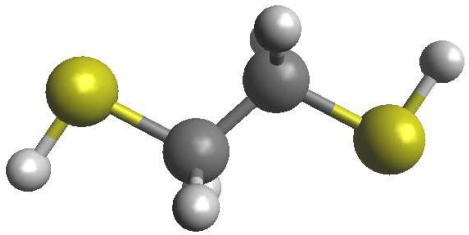


Experimental background

High resolution spectroscopy:
limited to MW studies (up to 40 GHz)[1,2,3]

- *syn* and *anti* rotamers
- Ground + excited states (SH torsion, CCS bending)
- D-isotopologues
- Produced by pyrolysis of 1,2-ethanedithiol



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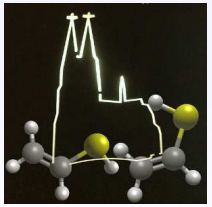
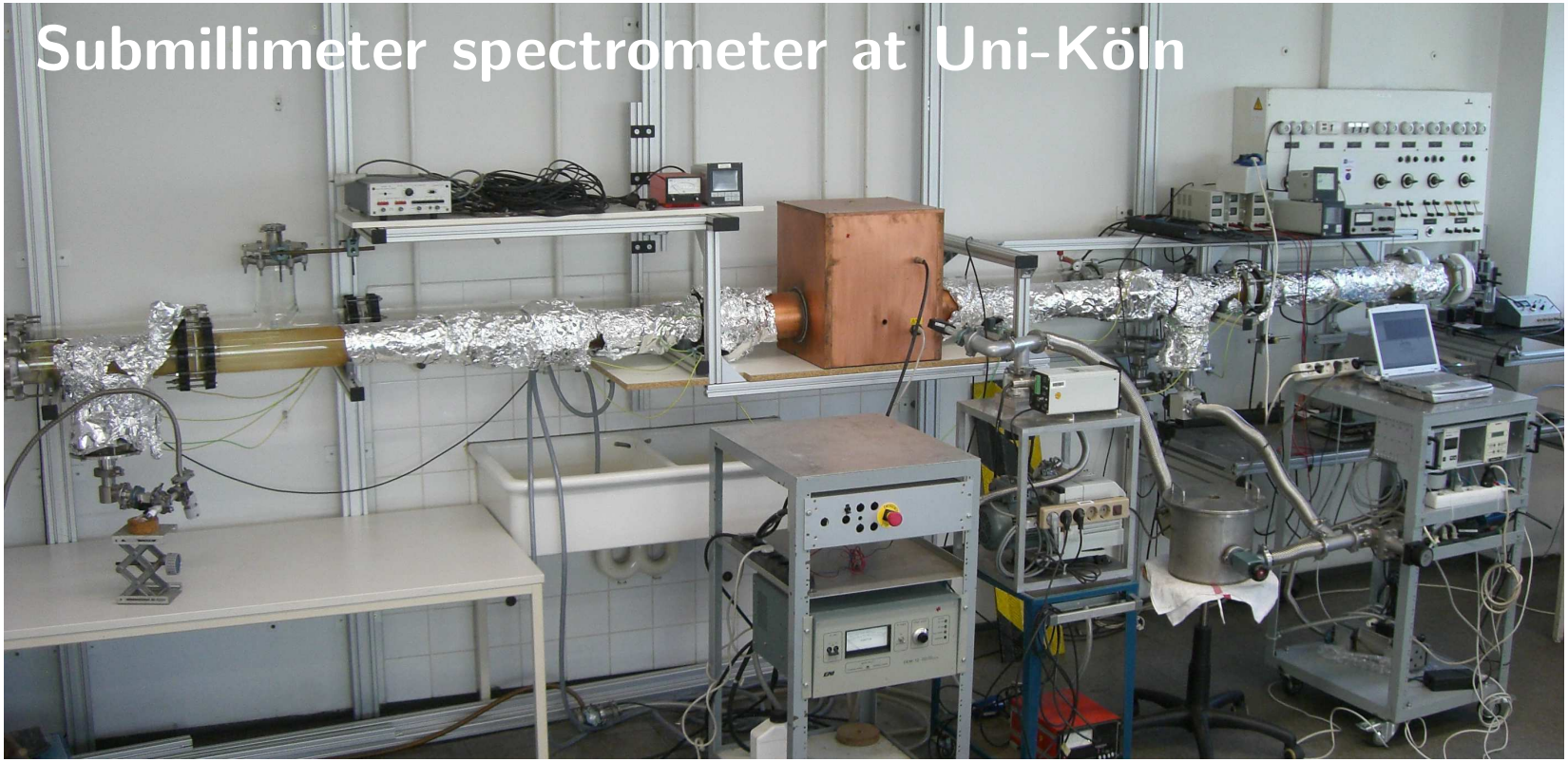
[2] M. Tanimoto & J. N. Mcdonald, *J. Mol. Spectrosc.* **78**, 106 (1979)

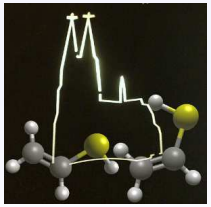
[3] V. Almond *et al.*, *J. Mol. Struct.* **128**, 337 (1985)



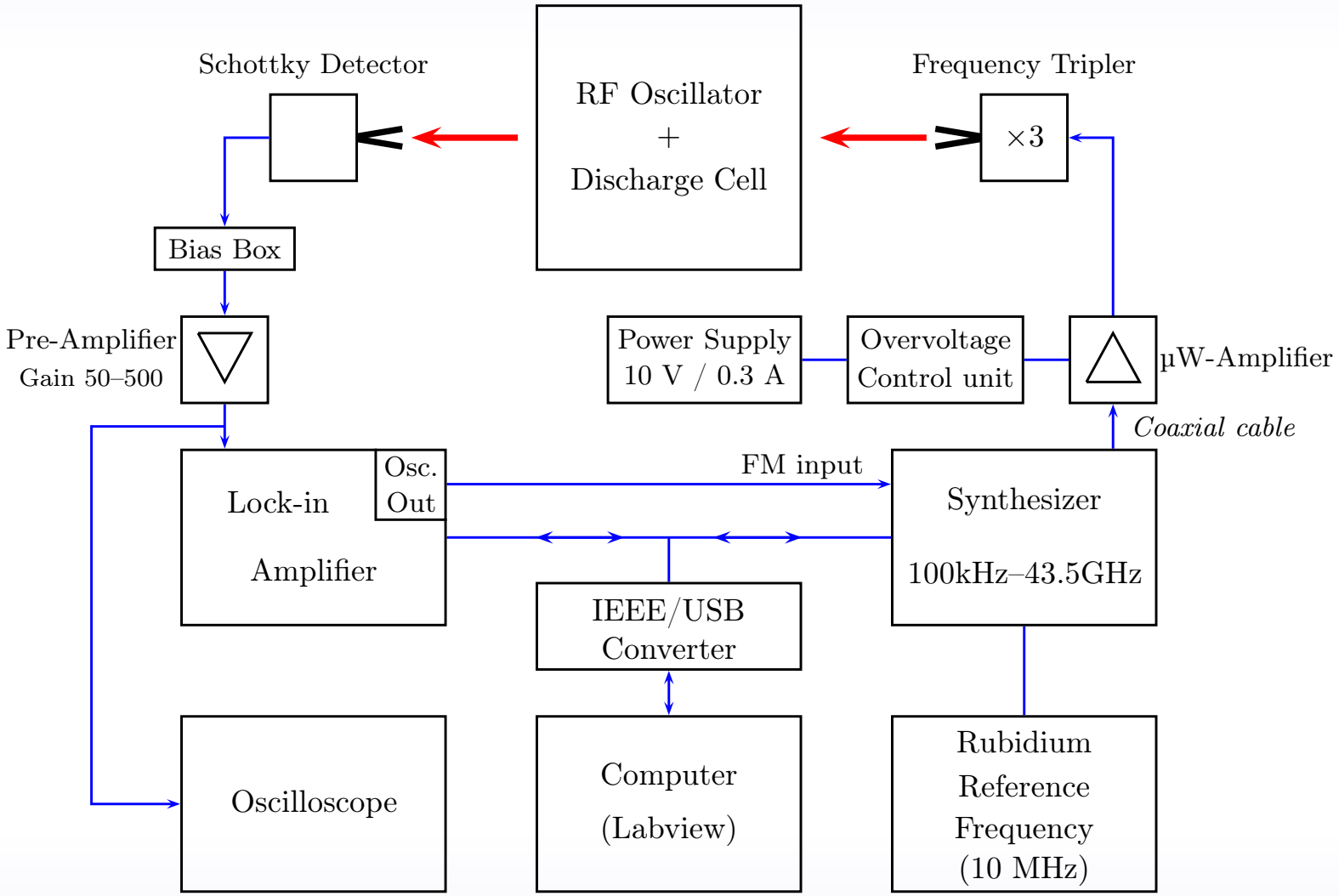
Experimental set-up

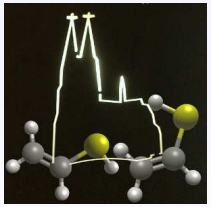


- Frequency multiplication chain (70 GHz – 1.1 THz)
- 5 m long absorption cell
- Radio-frequency (RF) discharge

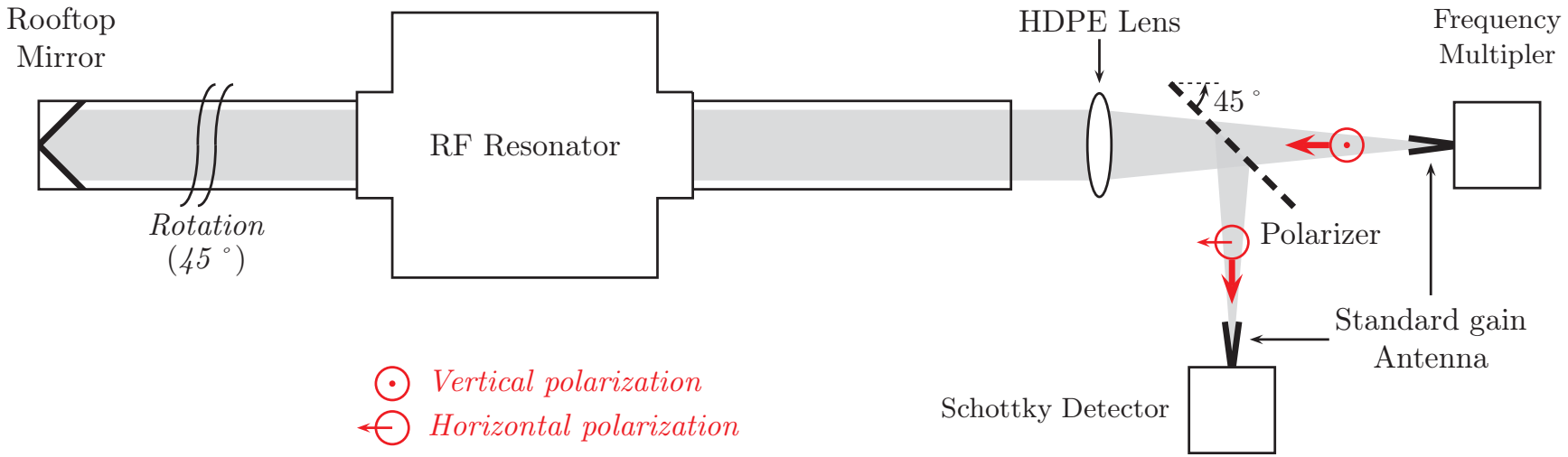


Electronic configuration

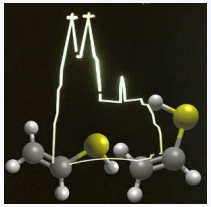




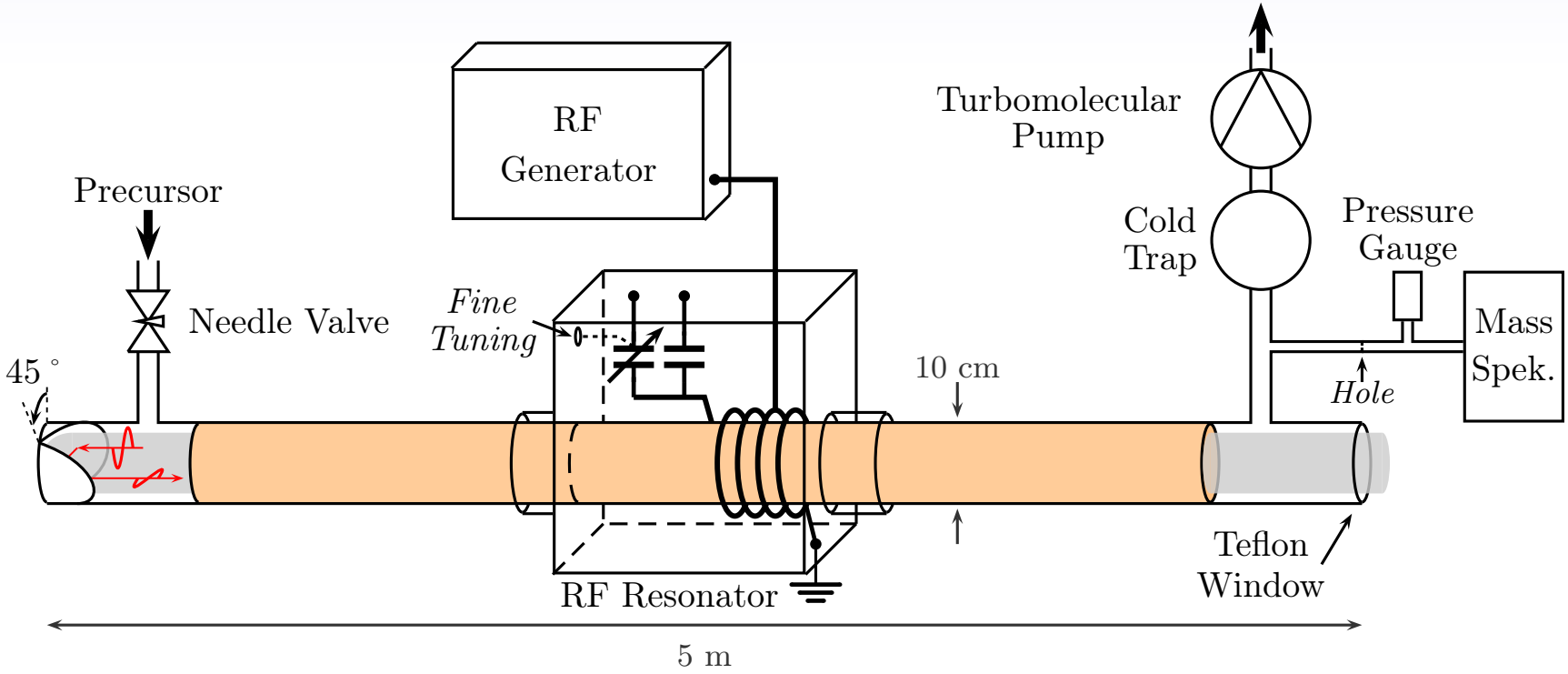
Optical arrangement



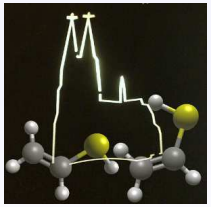
- 10 m absorption length



RF-discharge

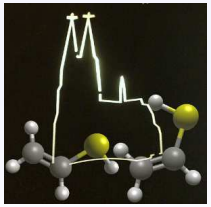


- Precursor: 1,2-ethanedithiol (*liquid*)
- Discharge power: $\leq$ 5W
- Pressure: 10 µbar (flow)

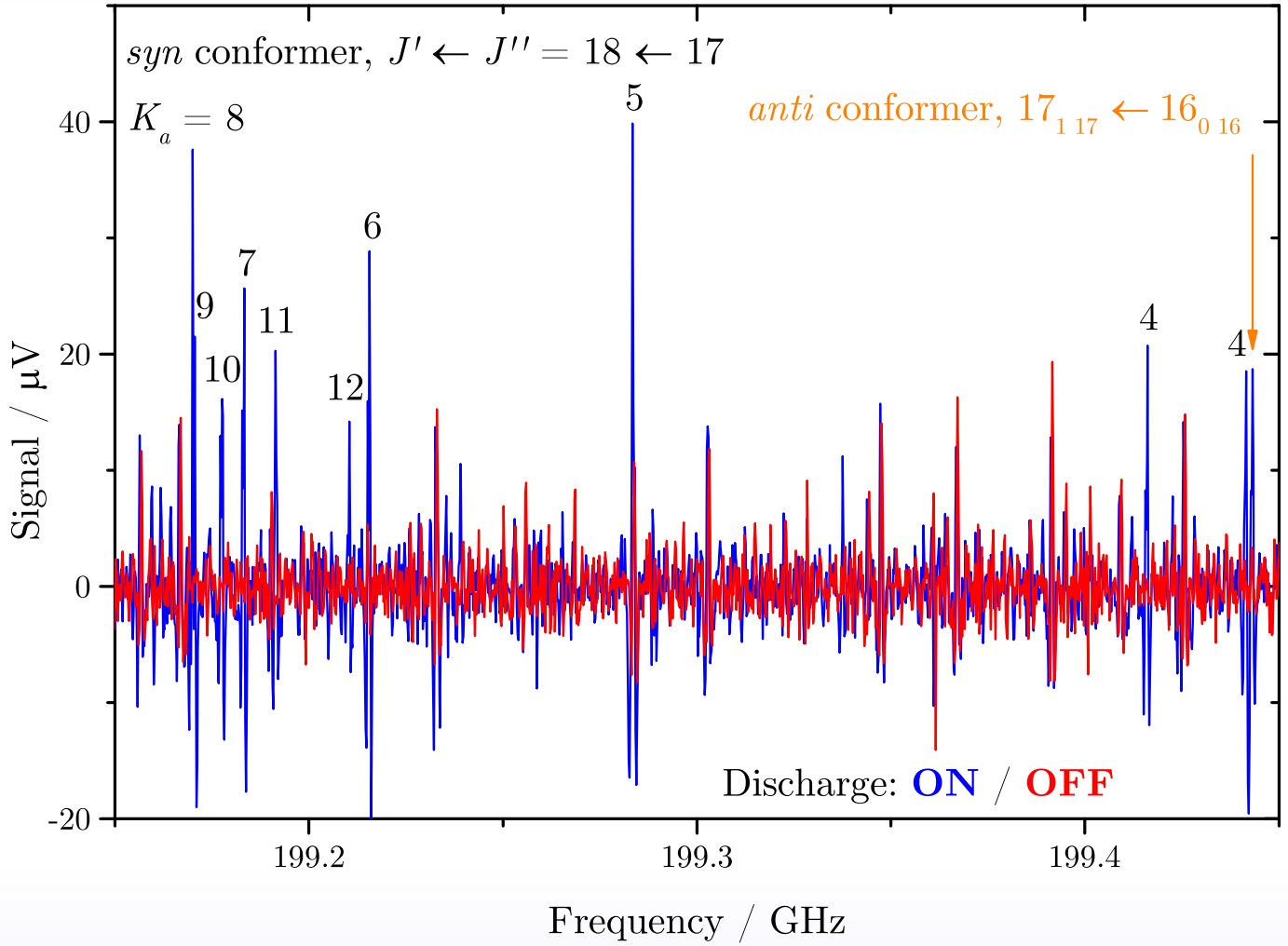


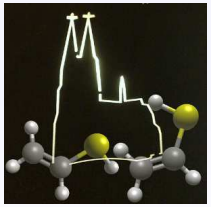
Experimental conditions

- Frequency range covered:
  - 70 – 120 GHz (steps 10 kHz)
  - 170 – 250 GHz (steps 20 kHz)
- 20 ms time constant
- Second harmonic detection

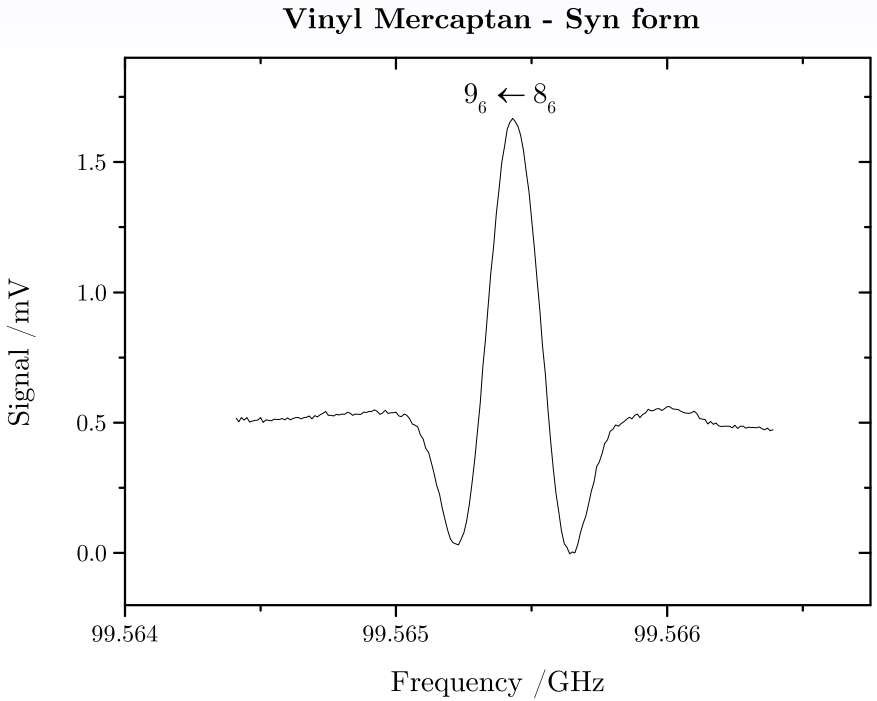


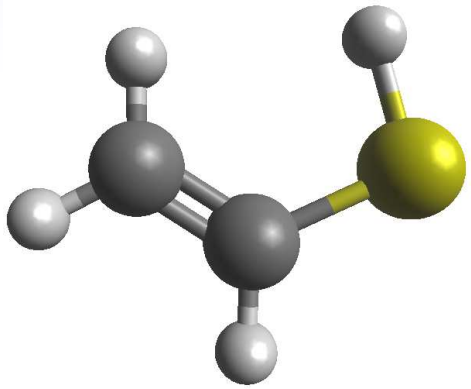
"broad" portion of the spectrum



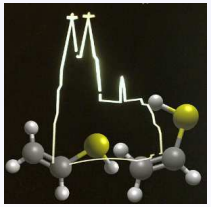


syn conformer

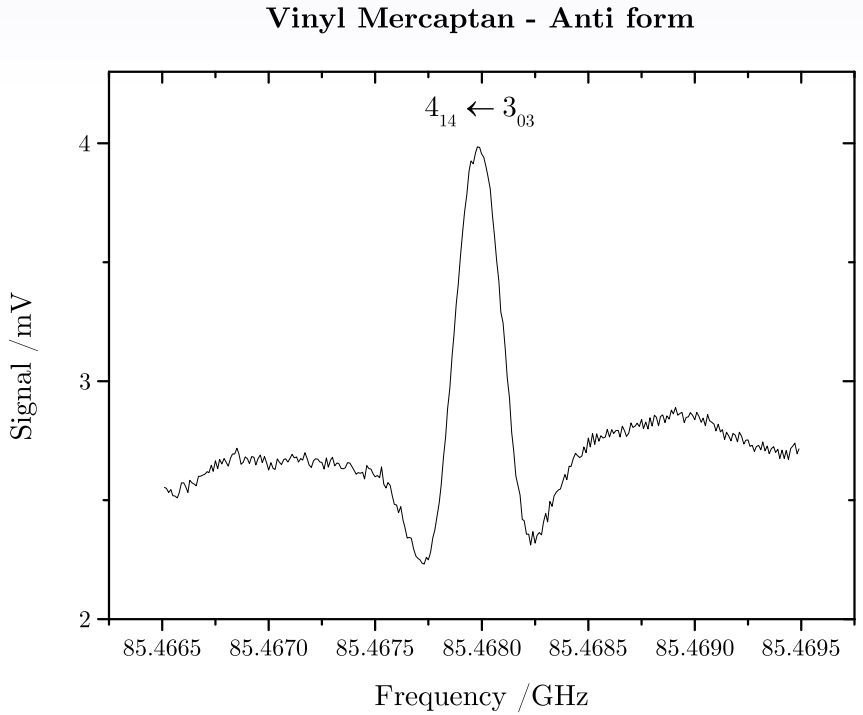


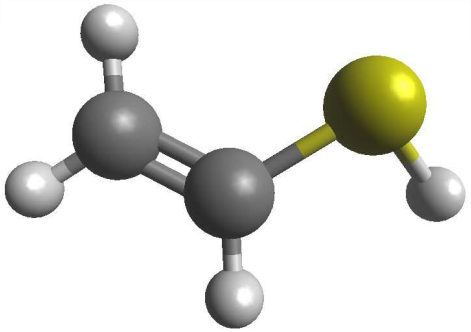


- 297 transitions (main isotopologue, GS)
- 263 *a*-type transitions ($J''_{max} = 23$, $K''_{a,\ max} = 17$)
- 34 *b*-type transitions ($J''_{max} = 24$, $K''_{a,\ max} = 3$)

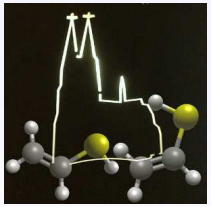


anti conformer





- 164 transitions (main isotopologue, GS)
- 150 *a*-type transitions ($J''_{max} = 20$, $K''_{a,\ max} = 14$)
- 14 *b*-type transitions ($J''_{max} = 18$, $K''_{a,\ max} = 3$)



Watson-*S* reduction (SPFIT/SPCAT[1])

- data from the literature[2,3] + new measurements

Parameter /MHz	*syn* This work		Previous study[2]		*anti* This work		Previous study[3]	
A	49816.0400	(40)	49815.28	(06)	49423.5651	(39)	49422.75	(5)
B	5835.708397	(70)	5835.716	(14)	5897.21141	(16)	5897.215	(9)
C	5222.075319	(66)	5222.081	(11)	5279.43977	(18)	5279.436	(9)
$D_J \times 10^3$	2.723864	(76)	2.85	(17)	3.09748	(16)	3.07	(17)
$D_{JK} \times 10^3$	−33.4946	(16)	−33.2	(21)	−37.6199	(32)	−38.5	(17)
D_K	0.79167	(32)			0.80927	(34)		
$d_1 \times 10^3$	0.424378	(54)	0.425	(35)	0.47277	(20)	0.498	(51)
$d_2 \times 10^3$	− 0.023615	(42)			−0.03114	(21)		
$H_{KJ} \times 10^6$	− 3.1334	(42)			−4.390	(28)		
$H_{JK} \times 10^9$	− 9.9	(20)						
*N*lines	329		37		196		32	
RMS /kHz	48				52			
σ	1.55				1.38			

[1] H. M. Pickett, *J. Mol. Spectrosc.* **148**, 371 (1991)

[2] M. Tanimoto *et al.*, *J. Mol. Spectrosc.* **78**, 95 (1979)

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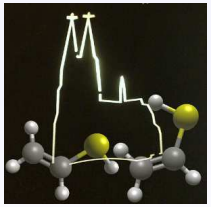

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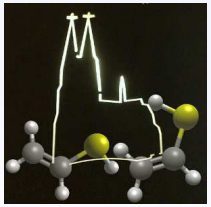

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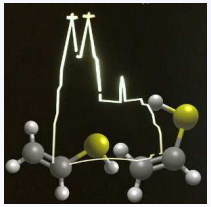
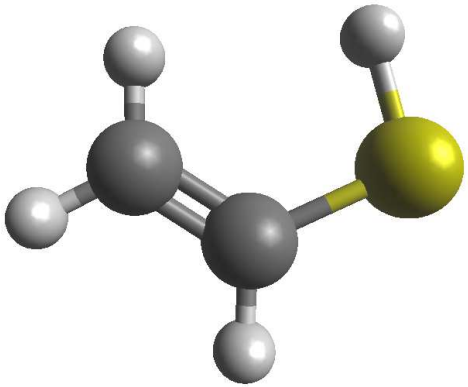
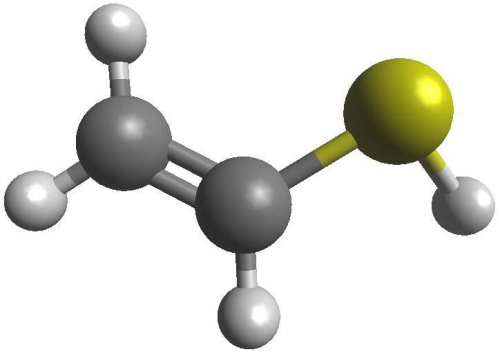
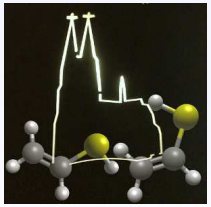


Prospects

- Geometry optimization
  $\rightarrow$ study of more isotopologues (FTMW)

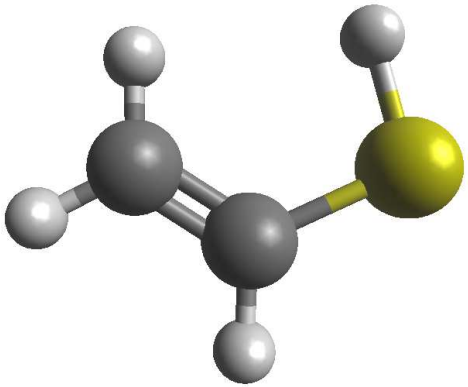


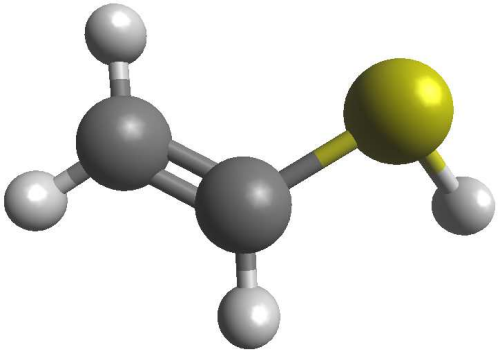


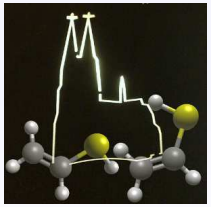


Prospects

- Geometry optimization
  $\rightarrow$ study of more isotopologues (FTMW)
- Astronomical searches in the millimeter-wave range

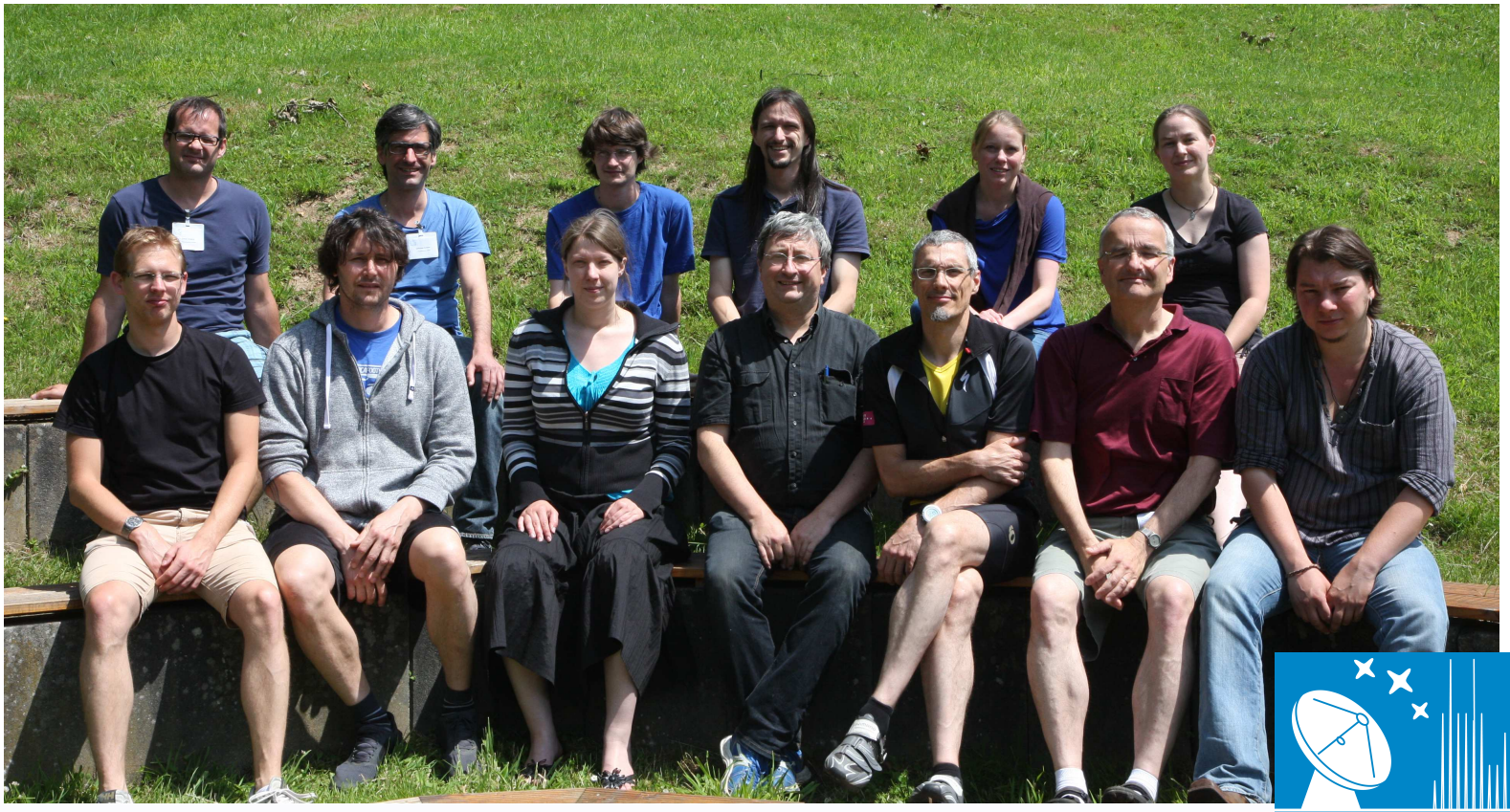


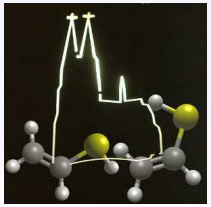




Acknowledgements

Cologne Laboratory Astrophysics Group





Acknowledgements