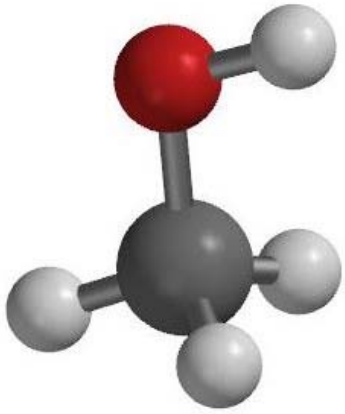
UNIVERSITY OF COPENHAGEN

Calculating Vibrational Spectra



Emil Vogt

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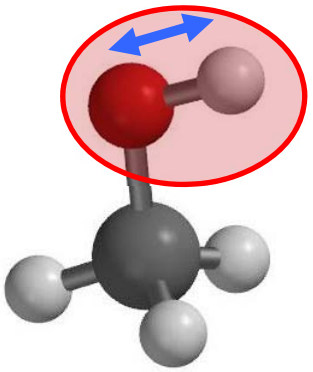
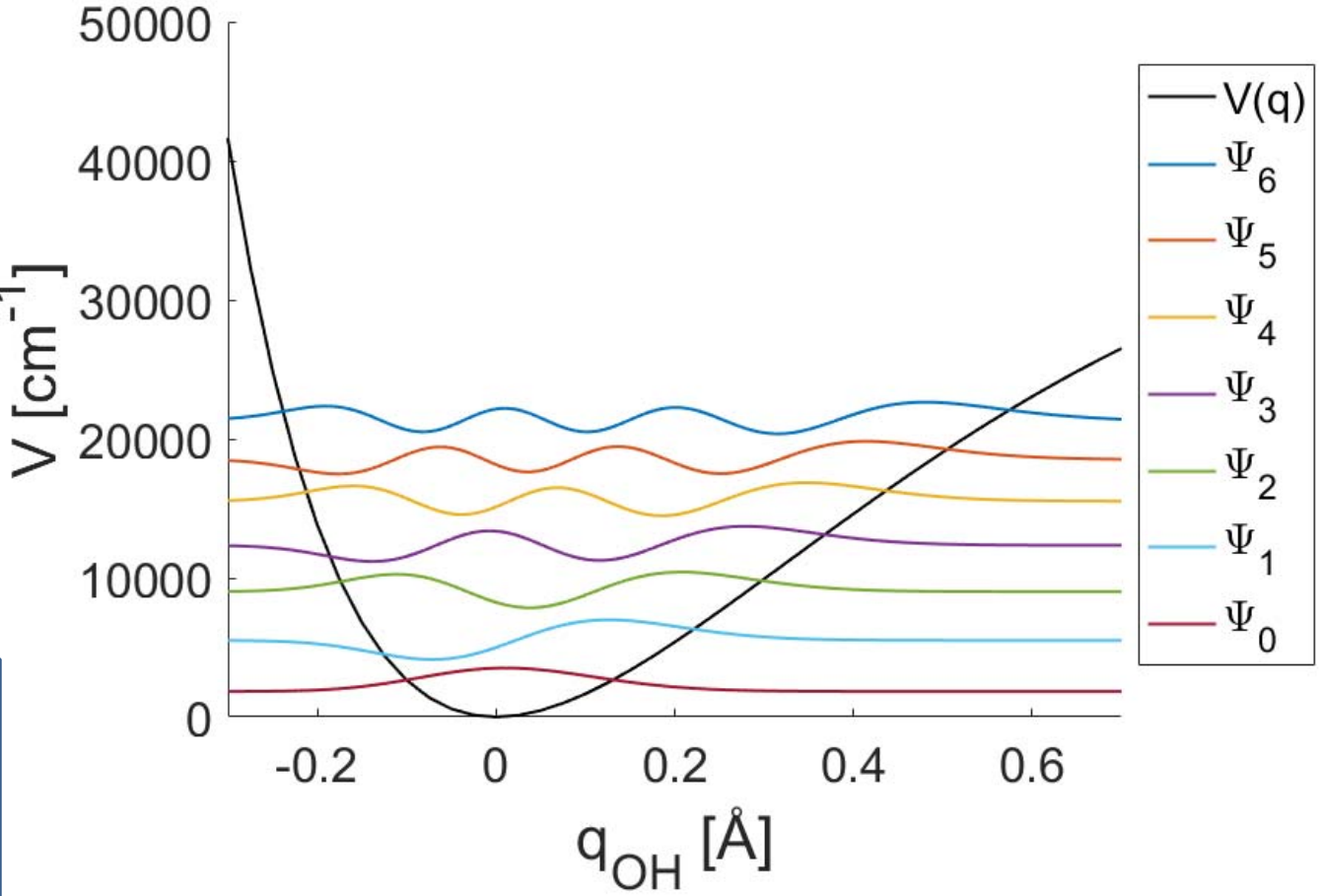
University of Copenhagen,
Copenhagen, Denmark.

Supervisor: Prof. Henrik G. Kjaergaard

The 1D Local Mode Model

q_{OH}





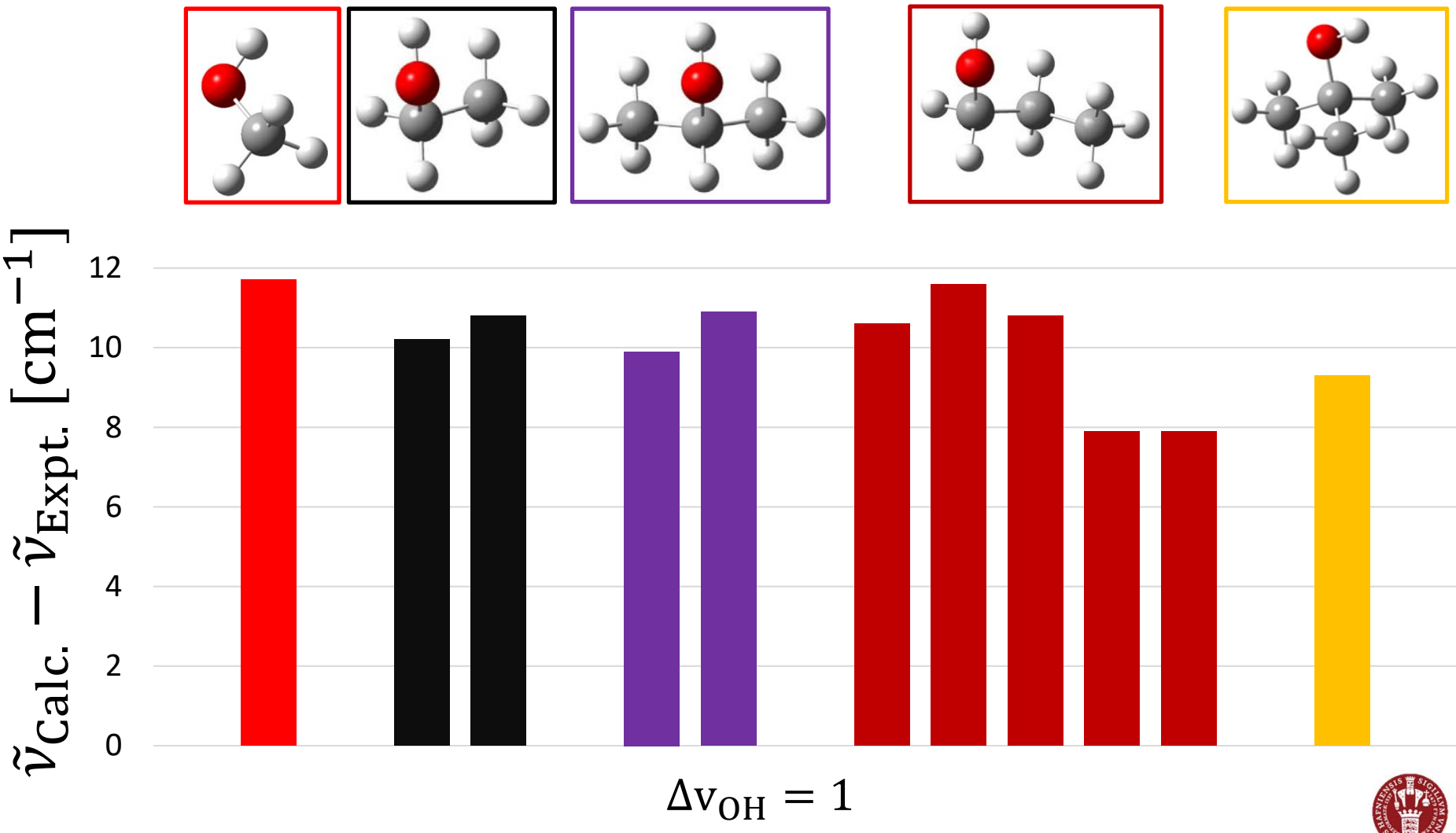
Solved Numerically

$$\hat{H} = \frac{\hat{p}_q^2}{2\mu} + V(q)$$

$$\hat{H}\psi_i = E_i\psi_i$$

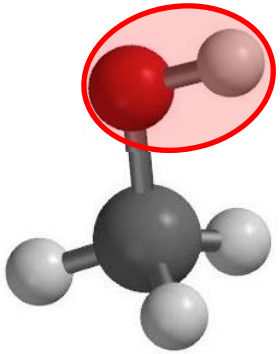
R. Meyer, J. Chem. Phys. 52, 2053, 1970

The 1D Local Mode Model



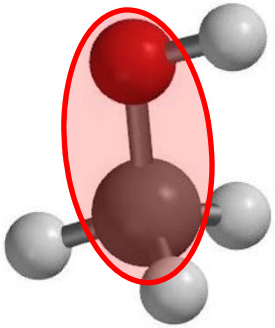
E. Vogt, P. B. Valls, and H.G. Kjaergaard, *J. Phys. Chem. A.*, 2020 | J. Wallberg and H. G. Kjaergaard. *Spectrochim. Acta. A.*, 2019

3D LM Model



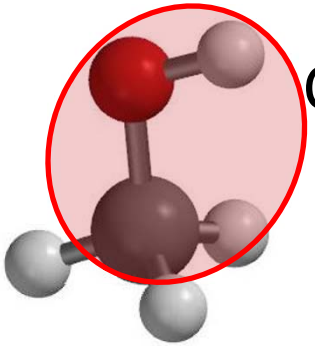
OH-stretch

q_{OH}



CO-stretch

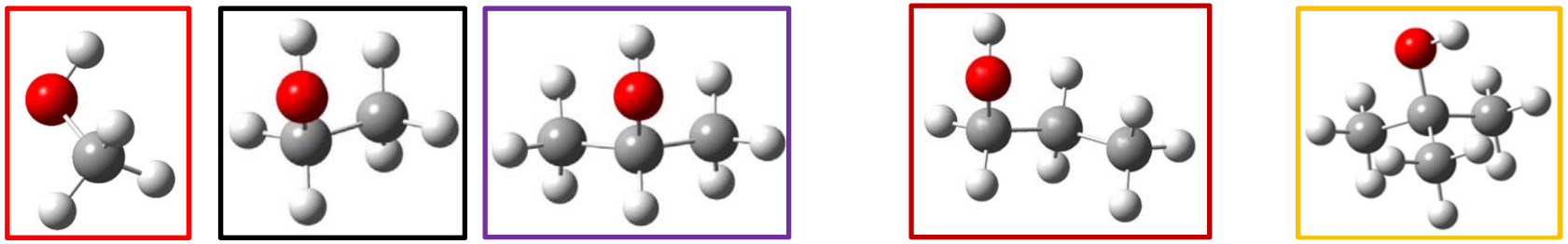
q_{CO}

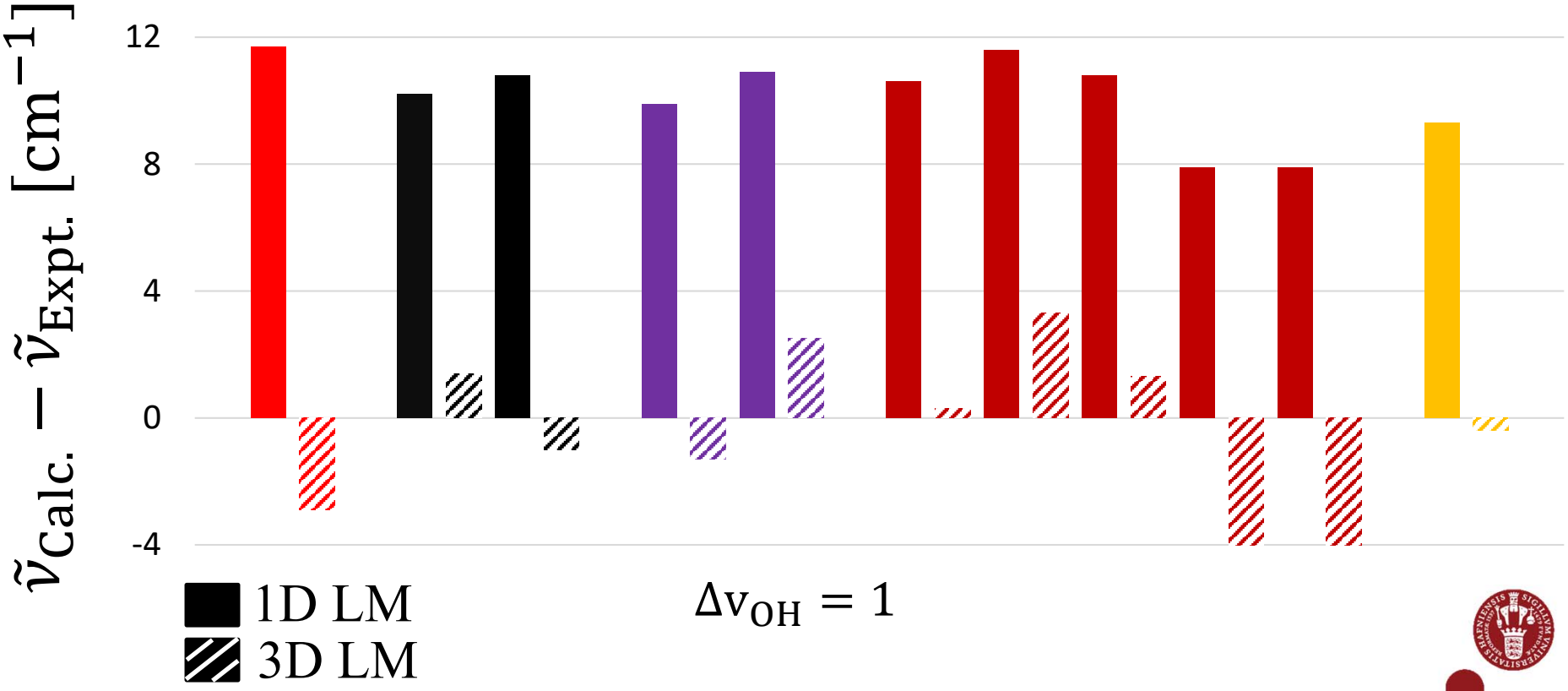


COH-bend

q_{COH}

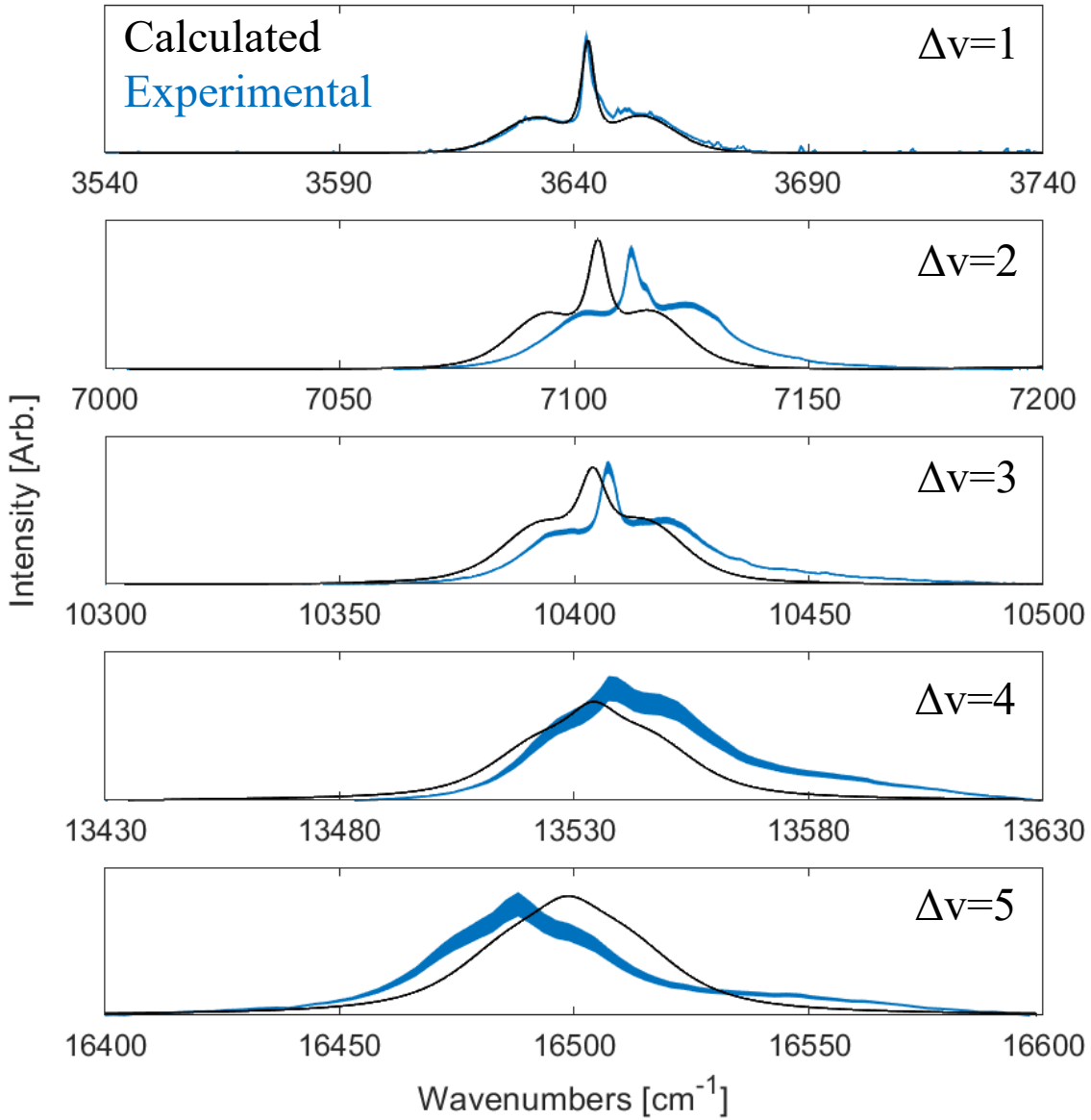
3D Local Mode Model

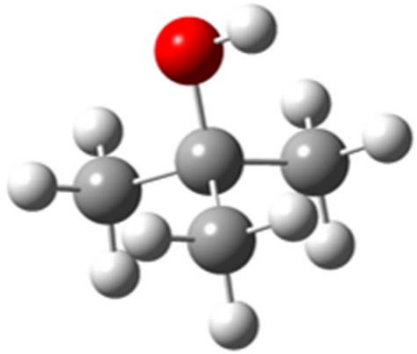




E. Vogt, P. B. Valls, and H.G. Kjaergaard, *J. Phys. Chem. A.*, 2020 | J. Wallberg and H. G. Kjaergaard. *Spectrochim. Acta. A.*, 2019

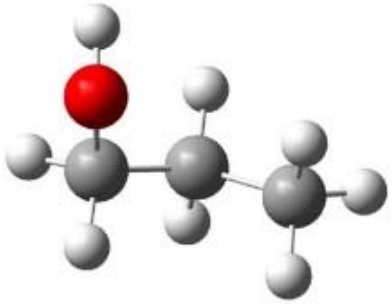
*t*BuOH OH-stretching Transitions

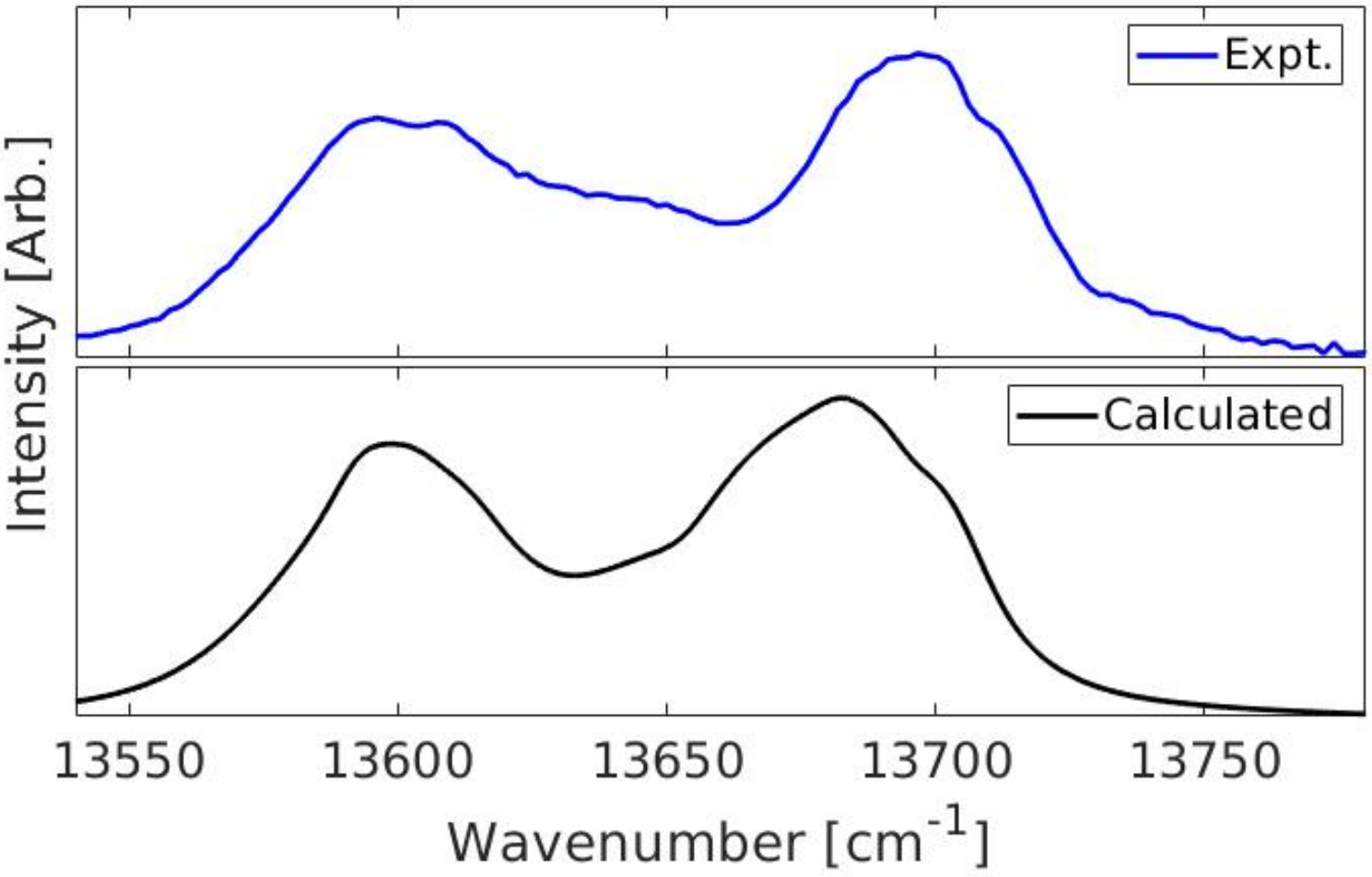




E. Vogt, P. B. Valls, and H.G. Kjaergaard, *J. Phys. Chem. A.*, 2020 | J. Wallberg and H. G. Kjaergaard. *Spectrochim. Acta. A.*, 2019

v=4, OH-stretch 1-Propanol

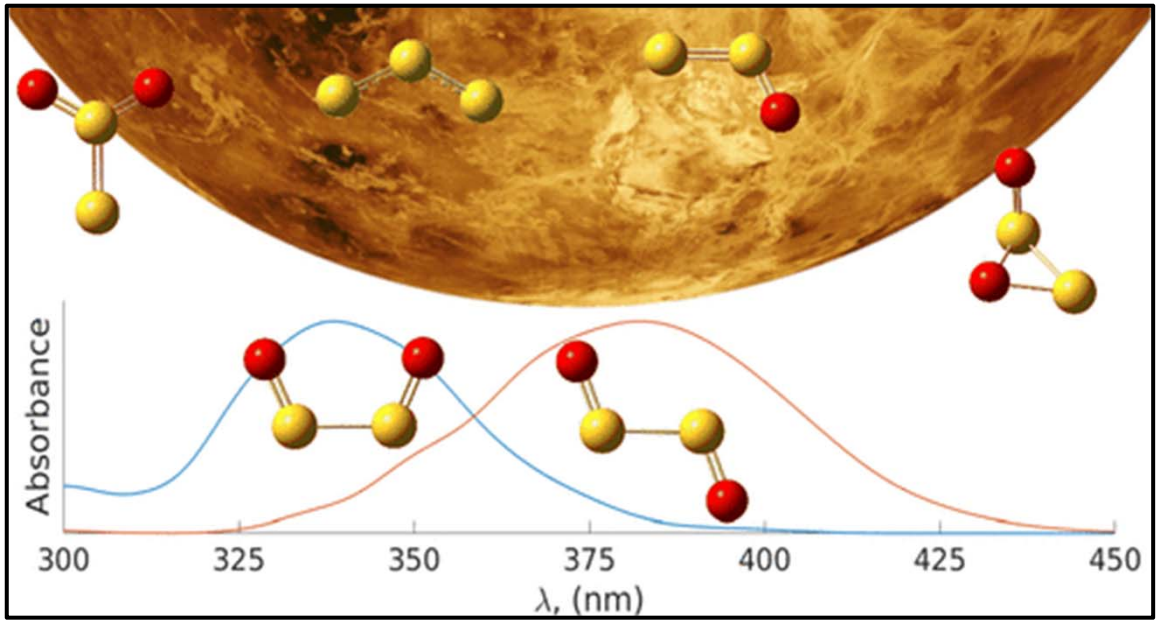


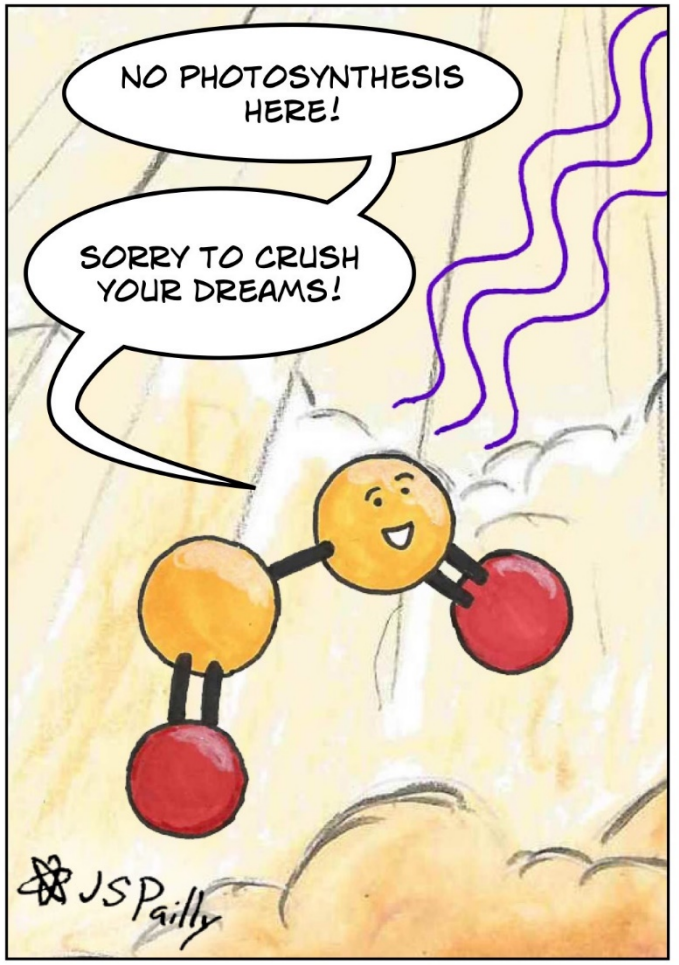


Vogt, Bertran Valls, and Kjaergaard, *JPCA 2020*

Wallberg, et al. SAA 2019

Is OSSO The Unknown UV-Absorber?

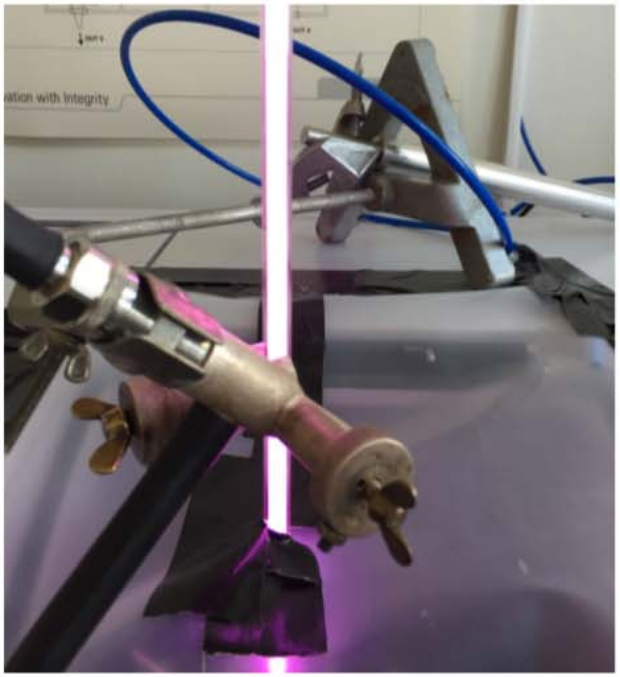




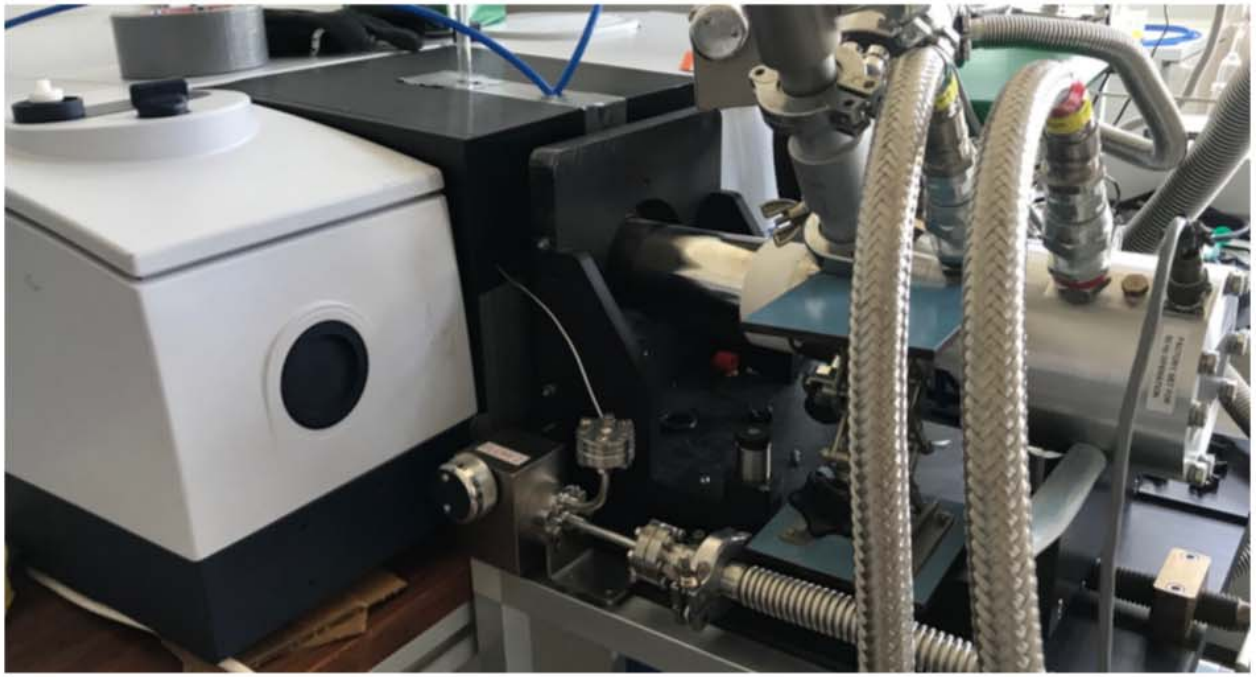
B. N. Frandsen, P. O. Wennberg, H. G. Kjaergaard, *Geophys. Res. Lett.* 2016

B. N. Frandsen, S. Farahani, E. Vogt, J. R. Lane, and H. G. Kjaergaard *J. Phys. Chem. A. 2020*

Matrix Isolation Spectroscopy



Microwave Discharge
On Ar + SO_2



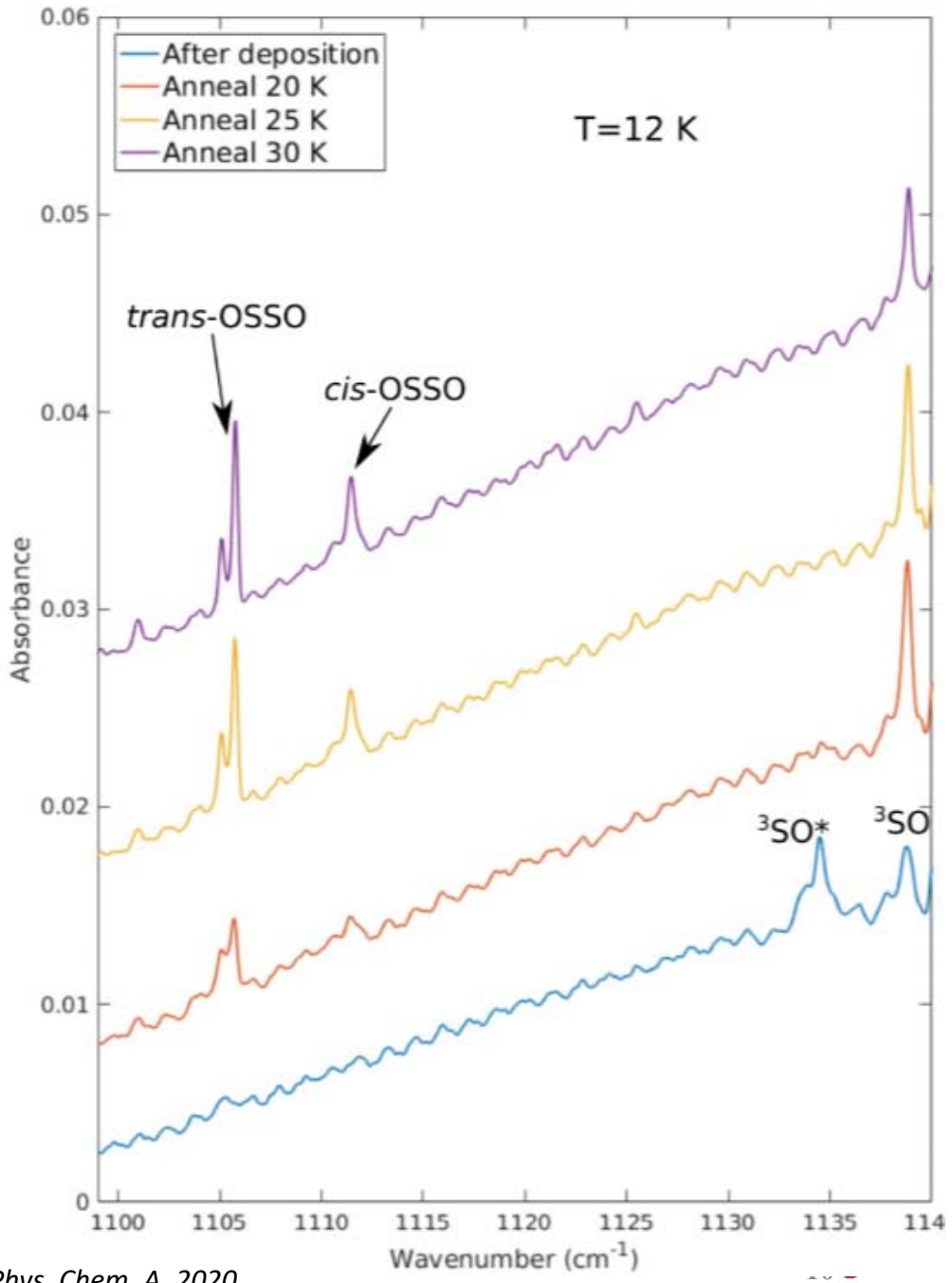
Matrix in the FTIR

Formation of OSSO?

B. J. Frandsen, PhD Thesis 2019

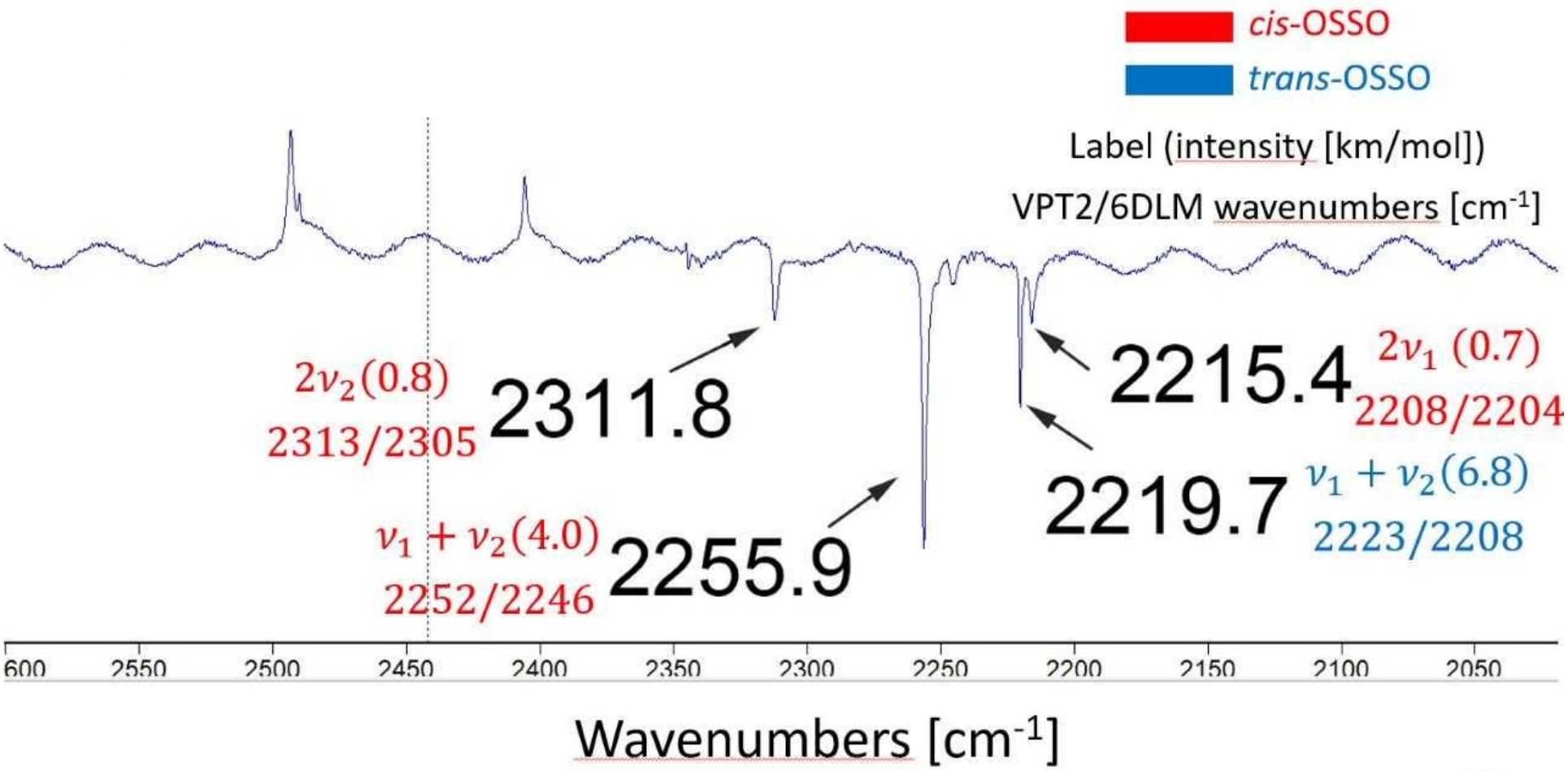
Frequencies (Intensities) [cm^{-1} (km/mol)]

	VPT2[a]	6-D LM[b]	
ν_1	1160 (51)	1154 (53)	cis-OSSO
ν_2	1107 (168)	1102.7 (160)	
ν_3	477 (0.1)	464 (0.2)	
ν_4	464 (15)	462 (15)	
ν_5	270 (0)	268 (0)	
ν_6	131 (4)	131 (4)	
$2\nu_1$	2313 (0.2)*	2305 (0.8)	
$\nu_1 + \nu_2$	2252 (0.2)*	2246 (4.0)	
$2\nu_2$	2208 (0.6)	2204 (0.7)	
ν_1	1135 (0)	1124.5 (0)	trans-OSSO
ν_2	1103 (289)	1097.2 (264)	
ν_3	556 (0)	544 (0)	
ν_4	336 (0)	330 (0)	
ν_5	183 (11)	180 (11)	
ν_6	176 (19)	172 (19)	
$2\nu_1$	2263 (0)*	2244 (0)	
$\nu_1 + \nu_2$	2223 (0.3)*	2208 (6.8)	
$2\nu_2$	2199 (0)	2187 (0)	



B. J. Frandsen, S. Farahani, E. Vogt, J. R. Lane, and H. G. Kjaergaard *J. Phys. Chem. A. 2020*

Overtones – Confirmation of OSSO!



Wu, Z. et al. *Chem. Commun.* 2018