

## Spectroscopy of binary complexes

Henrik G. Kjaergaard

Department of Chemistry, Copenhagen University, Universitetsparken 5, DH-2100  
Copenhagen Ø, Denmark, Tel.: +4535320334, E-mail: hgk@chem.ku.dk

Vibrational spectroscopy is extensively applied to the study of hydrogen bonded complexes, however, measurements in solution and in matrices are effected by solvent effects and often difficult to interpret. Gas phase spectroscopy can avoid these problems and can possibly be used to quantify the complexes. We have measured OH-stretching and NH-stretching FTIR spectra of binary molecular hydrogen bonded complexes in the gas phase, with methanol (MeOH) and dimethylamine (DMA) as the hydrogen donor molecules.[1,2] The infrared spectra of the complexes in the gas phase are obtained by spectral subtraction of the monomer spectra from the corresponding mixture spectrum. The NH-stretching fundamental of DMA and the DMA dimer are shown at different pressures in the Figure.

We have determined the frequencies shift and intensity enhancements upon complexation and via temperature experiments also the interaction enthalpy. The measured spectra are compared with coupled cluster ab initio calculations within an anharmonic oscillator local mode model. The ratio of calculated to measured intensity provides the room temperature equilibrium constant for formation of the binary complex. These are good examples for benchmark calculations on challenging systems governed by weak intermolecular molecular interactions.[1-4] We observe a weak first overtone transition for some of the complexes. The results for these complexes will be put in context of our latest results for water dimer.

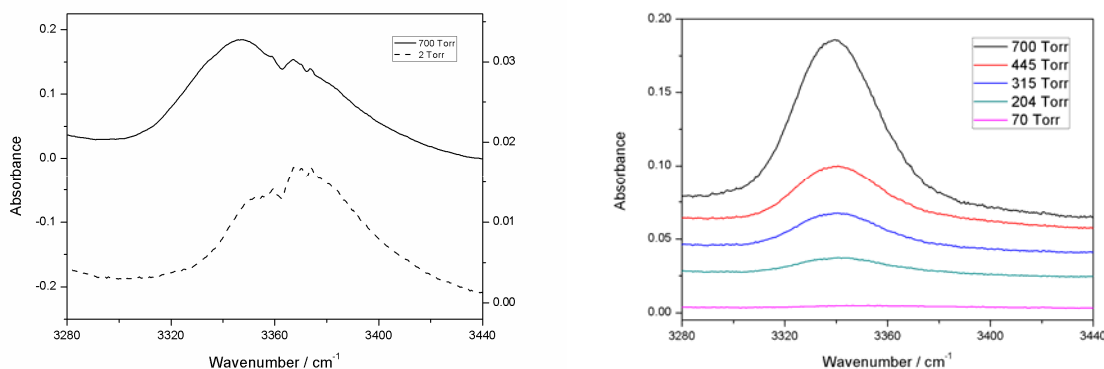


Figure. IR spectrum of DMA (left) at two different pressures and IR spectra of the DMA dimer (right) at different DMA pressures after spectral subtraction.

### References:

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- [3] D. L. Howard, H. G. Kjaergaard, *J. Phys. Chem. A* **2006**, *110*, 9597-9601.
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