GAS-PHASE WATER AMINE COMPLEXES

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A hydrogen bound bimolecular complex consists of a hydrogen bond donor and acceptor unit. The OH-stretching fundamental transition of the hydrogen bond donor is typically redshifted and its infrared intensity enhanced upon complexation.[1] This facilitates detection of weak complexes even though the equilibrium is strongly shifted towards the monomers at room temperature. The ratio of a measured and calculated intensity of a vibrational band is proportional to the complex abundance, which with known monomer pressures gives the equilibrium constant.[2] We calculate absolute transition intensities with a reduced dimensionality variational local mode model that also includes low-frequency vibrations. Calculated and experimental intensities of multiple bands are combined to give the equilibrium constant of complex formation for the water·dimethylamine and water·trimethylamine complex.[3] The equilibrium constant obtained from different bands should be equivalent, and the detection of multiple bands therefore allows us to validate the accuracy of our combined experimental and theoretical approach.

[1] Arunan, Elangannan, et al. Pure Appl. Chem. **83**, 1619 (2011).
[2] A. S. Hansen, E. Vogt, and H. G. Kjaergaard, Int. Rev. Phys. Chem., 2019, **38**, 115.
[3] E. Vogt, A. Kjaersgaard, and H. G. Kjaergaard, Unpublished

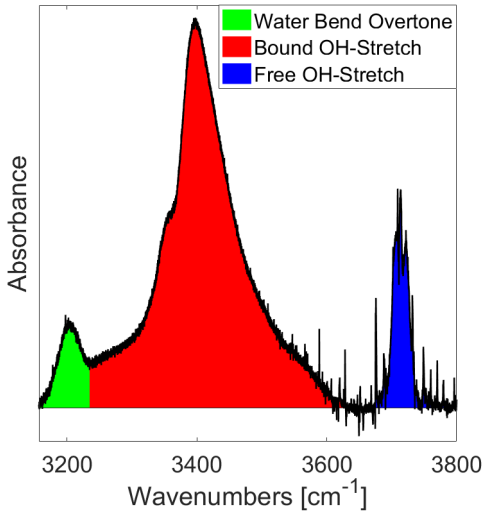

Figure 1: Room temperature gas-phase infrared spectrum of the water·dimethylamine complex.