Equilibrium constants of hydrated complexes at room temperature

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Hydrated complexes are important for the understanding of formation and growth of particles and affects Earth's radiative balance. At the core of this is the accurate determination of the Gibbs energy of complex formation. A hybrid method, using FTIR spectroscopy and theoretically calculated oscillator strengths of the complex signals, has been shown to provide accurate equilibrium constants of hydrogen bound complexes at room temperature[1]. However, hydrated complexes pose an added challenge due to the difficulty in subtracting water monomer spectra. A solution to this is to simulate the water spectrum used for spectral subtraction based on reference data from the HITRAN database[2]. This method has previously been used for water-amine systems, where amine acceptors are known to form strong hydrogen bonds with intense IR signals, easing spectroscopic detection[3]. Here, we study the weakly bound water-dimethyl ether (H_2O-DME) complex (Figure 1, left), which serves as a model system for OH···O hydrated complexes. We present the gas phase detection of the H_2O-DME complex (Figure 1, right). With the previously described hybrid method, a room temperature equilibrium constant is reported.

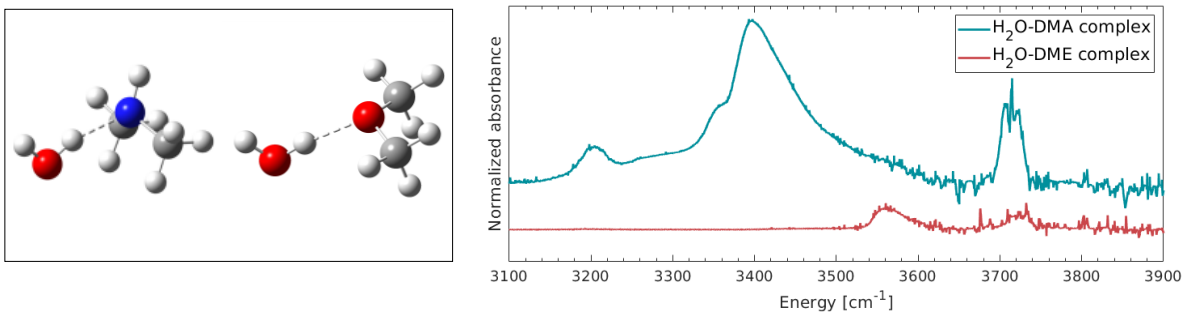

Figure 1 Left: Structures of the H_2O-DMA and H_2O-DME complexes. Right: Spectra of the H_2O-DMA and the H_2O-DME complexes. The absorbance is normalized to the product of the monomer pressures.

REFERENCES.

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