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Detecting Hydrogen-Bound Complexes at Room Temperature - A Joined Experimental and Theoretical Approach

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Hydrogen bonds are the dominating intermolecular interaction in small neutral molecular clusters. In the atmosphere, the hydrogen bonds promote clustering of water molecules, alcohols and hydroperoxides to form what becomes aerosols and cloud condensation nuclei.

Throughout my master's, PhD and Post. Doc. at the Kjaergaard Group, UCPH, I have worked with detecting, characterizing and quantifying small molecular clusters of alcohols and hydroperoxides with vibrational spectroscopic methods. We take advantage of the redshift and intensity enhancement of the bound OH-stretch and accurately determine the cluster partial pressure by scaling the observed OH-stretching intensity by a calculated oscillator strength. Spectral subtraction of monomer signals leaves only signals from the clusters. We employ high level anharmonic calculations to accurately determine the OH-stretching oscillator strength. Recently we have presented an easy protocol for achieving similarly accurate results using a reduced dimensional VPT2 model implemented in the Gaussian16 package. We have made it possible to determine partial pressures and equilibrium constants at room temperature of a range of atmospherically important cluster species.

The room temperature spectrum of the strongly bound water-trimethylamine is unexpectedly structured. In a collaboration with the Suhm Group, GAUG, we were able to measure the complex in three different media and temperatures and we determined that the structure arises as a consequence of coupling between the bright OHb-stretching mode and two other dark combination states of intra- and intermolecular modes. Using room temperature static-, He-jet-expansion- and Ar-cryo-matrix techniques, we were able to tune the states in and out of resonance with each other.

Keywords

Hydrogen bond: weak, medium; State of system: Gas

This abstract is submitted for....

Early-career researchers´ workshop

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