WATER BOUND TO REACTIVE SPECIES: THE INFLUENCE OF CLUSTERING ON MOLECULAR AND ELECTRONIC STRUCTURE

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While solute particles in aqueous solution interact with numerous water molecules, molecular clusters involving even as few as one or two waters can reveal striking signs of incipient solvation. Rotational spectroscopy provides a powerful means of investigating these changes, and several examples will be examined. The early stages of ionization of HNO_3 in small water clusters will be described, as will changes in the structure of H_2SO_4 upon solvation by a single water. The dipole moment of the H_2SO_4-H_2O complex, which may be important in atmospheric nucleation models, provides an interesting cautionary tale on the comparison between theory and experiment. Finally the effect of complexation on the electronic structure of the OH radical is probed through examination of angular momentum quenching and magnetic hyperfine structure in the OH-H_2O complex.[a]

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