SIZE- AND CONFORMATION-SELECTIVE SPECTROSCOPY OF HYDROGEN-BONDED CLUSTERS

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Gas phase clusters containing water are currently being used as an important testing ground for existing intermolecular potentials for water, both in the presence and absence of solutes. One of the particular experimental challenges to be overcome in such studies is the exponentiating number of conformational isomers which can be present in such H-bonded aggregates. When one or more molecules in the cluster can be resonantly ionized, a combination of resonant multiphoton ionization and hole-burning methods can often be used to sort out the ultraviolet spectrum of each size and conformation of cluster. The double-resonance method of resonant ion-dip infrared spectroscopy (RIDIRS) can then be used to record each cluster's hydride stretch infrared spectrum free from interference from others present in the expansion. The sensitivity of the hydride stretch region to the number, type, and strength of hydrogen bonds present make it a particularly powerful probe of the H-bonding topologies of the clusters. When benzene is used as aromatic chromophore, it serves as a surface-attached probe molecule for the (water)$_n$ cluster. Other aromatics, such as indole, N-methyl-indole, tropolone, and pyridone, have H-bonding sites which can serve as attachment points for water molecules. Examples will be taken from each to demonstrate the rich diversity of structural types taken up by water clusters in these contexts, emphasizing the spectroscopic signatures which each structure produces. The crucial role played by DFT calculations in assigning spectra to unique H-bonding topologies will also be stressed.