

## INFLUENCE OF AROMATIC MOLECULES ON THE STRUCTURE AND SPECTROSCOPY OF WATER CLUSTERS

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Isomer-specific resonant ion-dip infrared spectra are presented for benzene-(water)<sub>n</sub>, 1-2-diphenoxyethane-(water)<sub>n</sub>, and tricyclophane-(water)<sub>n</sub> clusters. The IR spectra are modeled with a local mode Hamiltonian that was originally formulated for the analysis of benzene-(water)<sub>n</sub> clusters with up to seven waters. The model accounts for stretch-bend Fermi coupling, which can complicate the IR spectra in the 3150-3300 cm<sup>-1</sup> region. When the water clusters interact with each of the solutes, the hydrogen bond lengths between the water molecules change in a characteristic way, reflecting the strength of the solute-water interaction. These structural effects are also reflected spectroscopically in the shifts of the local mode OH stretch frequencies. When diphenoxyethane is the solute, the water clusters distort more significantly than when bound to benzene. Tricyclophane's structure provides an aromatic-rich binding pocket for the water clusters. The local mode model is used to extract Hamiltonians for individual water molecules. These monomer Hamiltonians divide into groups based on their local H-bonding architecture, allowing for further classification of the wide variety of water environments encountered in this study.