

BROADBAND MICROWAVE SPECTROSCOPY AS A TOOL TO STUDY INTERMOLECULAR INTERACTIONS IN THE DIPHENYL ETHER - WATER SYSTEM

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Many biological processes, such as chemical recognition and protein folding, are mainly controlled by the interplay of hydrogen bonds and dispersive forces. This interplay also occurs between organic molecules and solvent water molecules. Broadband rotational spectroscopy studies of weakly bound complexes are able to accurately reveal the structures and internal dynamics of molecular clusters isolated in the gas phase. Amongst them, water clusters with organic molecules are of particular interest. In this work, we investigate the interplay between different types of weak intermolecular interactions and how it controls the preferred interaction sites of aromatic ethers, where dispersive interactions may play a significant role. We present our results on diphenyl ether ($C_{12}H_{10}O$, 1,1'-Oxydibenzene) complexed with up to three molecules of water. Diphenyl ether is a flexible molecule, and it offers two competing binding sites for water: the ether oxygen and the aromatic π system. In order to determine the structure of the diphenyl ether-water complexes, we targeted transitions in the 2-8 GHz range using broadband rotational spectroscopy. We identify two isomers with one water, one with two water, and one with three water molecules. Further analysis from isotopic substitution measurements provided accurate structural information. The preferred interactions, as well as the observed structural changes induced upon complexation, will be presented and discussed.