MICROSOLVATION COMPLEXES OF α-METHOXY PHENYLACETIC ACID STUDIED BY MICROWAVE SPECTROSCOPY

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Mandelic acid and its derivatives are useful as chiral synthons in the chemical and pharmaceutical industry because of their versatility. Their wide use in organic reactions makes them an important case to study their solute-solvent interactions. α-methoxy phenylacetic acid (AMPA), a methoxy-derived mandelic acid, can serve as a model to characterize the non-covalent interactions of such chiral solute with different solvents. The different functional groups in this chiral acid provide flexibility to the molecule, that conformational flexibility has been presented previously. Furthermore, the presence of a carboxylic acid and a methoxy group in AMPA provides good binding sites for solute-solvent interactions and thus serves as a good model system.

In this work, we investigate the microsolvation of AMPA in three different solvents using chirped-pulse Fourier transform microwave (CP-FTMW) spectroscopy. This technique coupled with the supersonic expansion reveals accurate structures of weakly bound complexes isolated in the gas phase. We chose three solvents that offer different functional groups and thus model more types of solute-solvent interactions. The three solvents were water, a small hydrogen bond donor partner, DMSO with a sulfoxide group, and phenol with a phenyl ring and a hydroxyl group. The preferred intermolecular interactions and the structural changes in complexes with three different solvents will be discussed.