

A BROADBAND MICROWAVE STUDY OF ISOLATED α -METHOXY PHENYLACETIC ACID: STRUCTURE, INTERNAL ROTATION, AND MICRO-SOLVATION

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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 solute-solvent interactions. In this work, we study the structure of α -methoxy phenylacetic acid (AMPA), a mandelic acid derivative, and its solute-solvent interaction in a weakly bound complex with the solvent dimethylsulfoxide (DMSO). This system can serve as a model to characterize the non-covalent interactions of such chiral solutes with different solvents. Rotational spectroscopy studies of weakly bound complexes are able to accurately reveal the structures and internal dynamics of molecules and complexes isolated in the gas phase.

We present a conformational study of AMPA and its 1:1 complex with dimethylsulfoxide (DMSO) using chirped-pulse Fourier transform microwave (CP-FTMW) spectroscopy in the 2-8 GHz range. Two conformers of AMPA were identified in the rotational spectrum. Splitting patterns arising from internal motions in the molecule are observed and will be analyzed. The computational structures of AMPA determined from its singly-substituted ^{13}C -isotopologues are in good agreement with the two lowest energy conformers observed in experiments. However, in the 1:1 lowest energy complex with DMSO, the structure of AMPA does not correspond to the lowest energy conformation of the monomer. This showed the influence of solvent over the conformational landscape of the solute. The preferred intra- and intermolecular interactions, as well as the observed structural changes upon complexation, will be discussed.