PROBING AZULENE-WATER INTERACTIONS AND AZULENE AGGREGATION BY BROADBAND ROTATIONAL SPECTROSCOPY

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Noncovalent interactions of aromatic complexes are highly significant in biological systems such as DNA, in materials science and in supramolecular chemistry. Gas phase studies of small aromatic complexes allow the determination of their preferred structural arrangements and of the relative contributions of various intermolecular forces to the interaction energy, laying the foundation for understanding the properties and interactions of larger systems. Azulene is one of the smallest aromatic hydrocarbons with a dipole moment. Here we present the investigation of azulene aggregation and its interactions with water using chirped-pulse Fourier transform microwave spectroscopy. We have observed one and two water molecules complexed with azulene, where water binds to azulene through an O-H$\cdots\pi$ hydrogen bond. Azulene dimer shows a stacked configuration where dispersion forces between the π electronic densities are predominant. Experimental observations are compared with predictions by various theoretical methods to evaluate their performance.