

THE COMPETITION AND COOPERATIVITY OF NON-COVALENT BONDS IN BENZOPHENONE-(H₂O)_{1,2,3} CLUSTERS REVEALED BY BROADBAND MICROWAVE SPECTROSCOPY

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Herein, the pure rotational spectra of benzophenone complexed with up to three water molecules were observed by using chirped-pulse Fourier transform microwave (CP-FTMW) spectroscopy. Benzophenone offers dispersion interaction sites through the phenyl rings and a hydrogen bond acceptor through the carbonyl oxygen, allowing us to study the competing binding sites for water molecules. The theoretical calculation combined with the isotopic substitution measurement provides the unambiguous structural information of the complexes. In benzophenone-(H₂O)_{1,2} clusters, the water molecules are located at one side of a phenyl group, where benzophenone and water molecules form a ring. Water monomer or dimer links with the carbonyl group through an OH...O hydrogen bond and links with the phenyl group through a CH...O weak hydrogen bond. The benzophenone-(H₂O)₃ complex is of interest as the water trimer was found located at the top of one phenyl group with the cooperativity of the hydrogen bond net. The water trimer forming an open loop through two hydrogen bonds is locked by benzophenone through one OH...O, one OH...π, and one CH...O hydrogen bonds, respectively.