IR SPECTRA OF BENZOIC ACID-WATER CLUSTERS IN A SUPERSONIC JET USING VUV IONIZATION DETEC-
TION

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Hydrogen bonding (H-bonding) of aromatic clusters in dilute aqueous solutions has been a subject of great interest in recent years. In the present work, we investigated the hydrogen-bonded structures of jet-cooled benzoic acid-water clusters, $(BA)_m$-$(H_2O)_n$ (m, n = 1 or 2), with IR spectroscopy and quantum-chemical calculations. We measured the IR spectra of mass selected $(BA)_m$-$(H_2O)_n$ in the C-H and O-H stretching regions by IR excitation -VUV ionization with a reflectron time-of-flight mass spectrometer (RF-TOF-MS). The IR spectrum of BA monomer was obtained by 1+1 IR-VUV photoionization technique, and those of the clusters were obtained by the depletion of the VUV-induced ion signal upon IR predissociation. The observed IR spectra were analyzed by comparison with spectra of possible structures predicted with anharmonic calculations at the B3LYP/6-311++G(d,p) level of theory. We discuss the structures of $(BA)_m$-$(H_2O)_n$ and how the H-bonding network developed in these clusters.