

INFRARED SPECTROSCOPY OF LARGER BENZENE-(H₂O)_n HYDROGEN-BONDED CLUSTERS: EVIDENCE OF CUBIC STRUCTURES

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One color R2PI-TOFMS, ultraviolet hole-burning, and RIDIRS have been used to assign and characterize the hydrogen-bonding topology of size-selected benzene-(H₂O)_n clusters formed in a supersonic molecular beam. Hole-burning spectroscopy confirms the presence of conformers in the increasingly congested R2PI spectra of these larger clusters. Two transitions in the benzene-(H₂O)₆⁺ R2PI-TOFMS are assigned to the benzene-(H₂O)₈ cluster. Comparison of the experimental RIDIR spectra to density functional theory calculations results in the assignment of these conformers to cubic octamers of S₄ and D_{2d} symmetry. The presence of benzene weakly distorts the cubic structures, breaking the degeneracy of several OH stretch vibrations and inducing intensity in otherwise forbidden infrared transitions. Four transitions in the benzene-(H₂O)₇⁺ R2PI-TOFMS are tentatively assigned as two conformers each of the (benzene)₂-(H₂O)₈ and the benzene-(H₂O)₉ clusters. The RIDIRS of these species share common features with those of the cubic benzene-(H₂O)₈ octamers; thus, a structure for the benzene-water nonamer built by adding one water molecule to a cubic octamer is tested against calculations.