STRUCTURE OF HIGH-ORDER WATER CLUSTERS OF β-PROPIOLACTONE BY BROADBAND MICROWAVE SPECTROSCOPY

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The rotational spectra of β-propiolactone-$(H_2O)_n$ (n=1-5) adducts have been extensively analyzed by broadband microwave spectroscopy (CP-FTMW). Unambiguous identification of their structures has been achieved from the spectra of the parent species and $H_2^{18}O$ single substitution clusters and Stark effect measurements. In addition to our previous work, the substitution structures for two n=4 and one n=5 complexes are presented. The three structures show a cyclic arrangement in the oxygen framework. For both n=4 structures, the water molecules form a quasiplanar ring that sits above the BPL unit. The structural differences between these two n=4 complexes are discussed in terms of the water oxygen atom positions and dipole moment orientations, enabling to distinguish between isomers with certainty by CP-FTMW spectroscopy. For n=5, a cyclic arrangement similar to n=4 was found with water molecules making a puckered five-water ring. Substitution coordinates for the oxygen framework support the assignment. Our results show that complexation with BPL induces measurable structural changes in the $(H_2O)_n$ (n = 3, 4, 5) pure water clusters. This fact is also discussed in terms of the variation in O-O distances within pure and complexed water clusters.