

## STRUCTURE OF HIGH-ORDER WATER CLUSTERS OF $\beta$ -PROPIOLACTONE BY BROADBAND MICROWAVE SPECTROSCOPY

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The rotational spectra of  $\beta$ -propiolactone-(H<sub>2</sub>O)<sub>n</sub> (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<sub>2</sub><sup>18</sup>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<sub>2</sub>O)<sub>n</sub> (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.