

280 **H₁₂O₆**

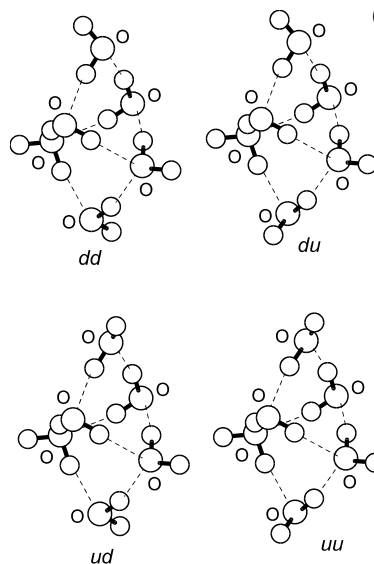
MW, tunable terahertz laser

Water hexamer

(weakly bound complex)

G₄(effective symmetry class)
(large-amplitude motion)(H₂O)₆

Striking similarities are found between the structure and the average interoxygen distance O...O (2.82 Å) of the hexamer cage and those of the basic unit of ice VI. The trends of two molecular properties – the contraction of the O...O distance and enhancement of the average individual monomer dipole with increasing cluster size up to the cyclic hexamer – are found to converge exponentially to the bulk phase values. In both cases, the cage properties deviate from the trends established by the dimer and cyclic clusters. Four nondegenerate cage hexamers, *dd*, *du*, *uu* and *ud*, produced by flipping the two doubly bonded monomers, are shown in the figure. The lines represent the hydrogen bond connectivity established between the monomers.



Liu, K., Brown, M.G., Saykally, R.J.: J. Phys. Chem. A **101** (1997) 8995.