NON-CYCLIC ISOMERS OF $(H_2O)_4$ IN HELIUM NANODROPLETS: INFRARED SPECTROSCOPY AND AB INITIO CALCULATIONS

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Water clusters are assembled via the sequential pick-up of water molecules by helium nanodroplets. Unlike previous infrared spectroscopy experiments of water clusters in helium droplets,[a] one or two Neon atoms are added to the droplets prior to water pick-up. The upstream pick-up of a Neon atom results in several new bands in the infrared spectrum in addition to the bands that correspond to the water monomer, dimer and larger *cyclic* water complexes. The new spectral features are determined to be signatures of a $(H_2O)_4$ cluster on the basis of the pick-up cell pressure dependence of the band intensities. A dc electric field is applied to the laser droplet beam interaction region, and these clusters are determined to be polar with permanent dipole moments between 2 and 3 Debye. On the basis of comparisons to CCSD(T) anharmonic frequency calculations, the new bands are assigned to OH stretch vibrations of a non-cyclic 3+1 cluster, which corresponds to a water molecule hydrogen bonded to a trimer ring. The presence of the Neon atom substantially affects the barrier to ring insertion of the fourth water molecule into a preformed cyclic trimer complex. In contrast, no new bands corresponding to open (non-cyclic) trimers or pentamers are observed.

[a] K. Nauta and R. E. Miller, *Science* **287, 293 (2000).**