HYDROGEN BOND NETWORK ISOMERS OF THE WATER NONAMER AND DECAMER OBSERVED BY BROADBAND ROTATIONAL SPECTROSCOPY

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After our previous study of the rotational spectrum of water clusters in the 6-18 GHz[a] region, in order to study clusters of larger size (>8 water molecules), a chirped-pulse Fourier transform microwave spectrometer in the 2-8 GHz frequency range has been used to obtain the broadband rotational spectra of five water nonamer isomers and four water decamer isomers in a pulsed molecular beam. The oxygen atom framework geometries for three nonamers and two decamers have also been unambiguously identified from isotopic labeling measurements using an $H_2{}^{18}O$ enriched sample. Three of the four observed water decamer show tunneling effect associated with the internal dynamics of hydrogen-bond network in a similar fashion as the prism water hexamer. These tunneling paths are quenched upon a single incorporation of a $H_2{}^{18}O$ molecule in the cluster. Due the large amount of closely-spaced rotational transitions in the $H_2{}^{18}O$ spectrum, automated fitting tools were employed to extract the corresponding rotational spectra, which will be also briefly described.

[a] C. Perez, M. T. Muckle, D. P. Zaleski, N. A. Seifert, B. Temelso, G. C. Shields, Z. Kisiel, and B. H. Pate, Science 336, 897 (2012).