STRUCTURES OF THE LOWEST ENERGY NONAMER AND DECAMER WATER CLUSTERS FROM CHIRPED-PULSE ROTATIONAL SPECTROSCOPY

CRISTOBAL PEREZ, BROOKS H. PATE, *Department of Chemistry, University of Virginia, McCormick Rd., Charlottesville, VA 22904-4319*; ZBIGNIEW KISIEL, *Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warszawa, Poland*; BERHANE TEMELSO, GEORGE C. SHIELDS, *Dean's Office, College of Arts and Sciences, and Department of Chemistry, Bucknell University, Lewisburg, PA 17837*.

In the breakthrough paper reporting observation and analysis of pure rotational spectra of the hexamer, heptamer and nonamer water clusters only one nonamer species was identified.[a] The advances in this experiment, as described in the previous talk, allowed identification, among others, of five different nonamer, $(H_2O)_9$, conformers and of four different decamer, $(H_2O)_{10}$, conformers. Analysis of ^{18}O enriched spectra resulted in determination of oxygen framework geometries for three of the water nonamers and two of the water decamers. Determination of experimental geometries proved considerably more challenging than for the lighter clusters since isotopic changes to moments of inertia are proportionally smaller, and there are multiple instances of near-zero principal coordinates. There are also more indications of the effect of internal motions. These problems have been overcome by careful application of r_s and least-squares r_m techniques in concert with $ab\,initio$ calculations so that it was possible to match the experimental and theoretical geometries unambiguously. The precise oxygen framework geometries obtained from chirped-pulse spectroscopy for water clusters ranging in size from the hexamer to the decamer allow, for the first time, to identify some common features of the underlying hydrogen bonding from direct experimental evidence.

[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).