STRUCTURES OF THE CAGE, PRISM, AND BOOK HEXAMER WATER CLUSTERS FROM MULTIPLE ISOTOPIC SUBSTITUTION

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The rotational spectra of the three lowest energy conformers of the water hexamer have recently been observed and assigned using chirped-pulse Fourier-transform microwave spectroscopy.[a] In that study single ^{18}O isotopic substitution allowed determination of oxygen framework geometries for all three clusters. Further isotopic spectra have been recorded since then: of water samples with ^{18}O:^{16}O ratios of 3:1 and 1:3, and of weakly deuterated water. Each spectrum results from averaging of around 10M free-induction-decays and the achieved high S/N ratio allowed assignment for each cluster of isotopic species with practically all possible ^{16}O,^{18}O isotopic combinations, ranging from all ^{16}O to all ^{18}O species. In addition, all 12 single deuterium species of each conformer have been assigned. This unprecedented abundance of isotopic information, resulting in rotational constants for close to 228 different species, is combined in new determinations of the structures of these clusters, providing a deeper insight into the properties of the underlying hydrogen bonding.

[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).