WATER CLUSTERS OBSERVED BY CHIRPED-PULSE ROTATIONAL SPECTROSCOPY: STRUCTURES AND HYDROGEN BONDING

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The chirped-pulse rotational spectra of the hexamer, heptamer, and nonamer water clusters have been assigned and analysed as described in the preceding talk. The observation of all singly substituted ^{18}O isotopologues for several clusters allowed direct determination of the r_s geometries of their oxygen atom frameworks. The r_s analysis was then complemented by least-squares determination of the r_0 geometries, which circumvented the problems with some imaginary substitution coordinates and allowed direct comparisons with computations. For the cage, prism and the book water hexamer clusters the agreement in O$\cdots$O distances between experiment and vibrationally averaged computed geometries is typically at the 0.01Å level. This is a previously unanticipated level of agreement between experiment and theory, which facilitates more confident discussion of the internal properties of these clusters. The hexamer and larger water clusters begin to display the diversity of hydrogen bonding that is characteristic of condensed water and various aspects of this behaviour are discussed.