CHARACTERIZATION OF LARGE WATER CLUSTERS BY BROADBAND ROTATIONAL SPECTROSCOPY

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Most theoretical water models match with experimental result reasonably well up to n=10. For clusters larger than the decamer there is no clear consensus in the global minimum geometries, as the low-energy landscape for a given cluster size changes considerably depending on the model applied. However, there is agreement in considering the undecamer regime as one of the richer pure water cluster regimes, with a large number (>50) of isomers within 1 kcal/mol of the global minimum. Using broadband chirped-pulse Fourier transform microwave (CP-FTMW) spectroscopy operating in the 2-8 GHz frequency range, seven low-energy isomers of the water undecamer have been identified in a pulsed molecular beam. The observed water cluster structures have been identified as belonging to four families on basis to their rotational constants according to their different oxygen atom frameworks. These families can be explained by building up the structures from smaller water cluster subunits. Rotational spectra consistent with theoretical predictions for two isomers of $(H_2O)_{13}$ and one of $(H_2O)_{15}$ have also been identified. Due to the high density of lines observed in the broadband spectrum, the traditional method of pattern recognition using ab-initio calculations was replaced with a new approach combining high-level ab-initio calculations with automatic fitting tools. These autofitting routines were tested on these systems and are also briefly described.