Global Optimization of $(H_2O)_{16}$ Clusters

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When searching for the global minimum of a molecular cluster, many steps have to be taken to ensure that one has an accurate potential energy surface and that it is searched thoroughly and efficiently. Our work focused finding the minima of $(H_2O)_{16}$ and classifying them to physically meaningful groups. We chose $(H_2O)_{16}$ because it is in the size regime where clusters transition from surface-only to internally-solvated forms, thereby mimicking bulk water. Also, this cluster has many nearly degenerate local minima which makes assigning a global minimum very difficult.

To sample the possible configurations, we used genetic algorithm (GA) with the TTM3-F water potential on an initial pool of 1000 structures ran for 1,000,000 mating or global optimization steps. After removing duplicates from the final pool of structures, the unique ones were minimized using the MP2/6-31G* *ab initio* method. These *ab initio* structures were classified on the basis of their water type (WT), hydrogen bond type (HB-type) and rotational constants (RC). Of the 377 structures that were within 10 kcal/mol of the global minimum, 18 and 113 were within 2 and 4 kcal/mol, respectively. The 18 structures were grouped into 8 classes and the 113 into 50 classes, each with a distinct shape. The TTM3-F water potential yielded a stacked tetramer with alternating homodromicity (direction of hydrogen bonding). Other model potentials, density functional methods and *ab initio* methods predict different global minima. The reasons for these differences are explored.

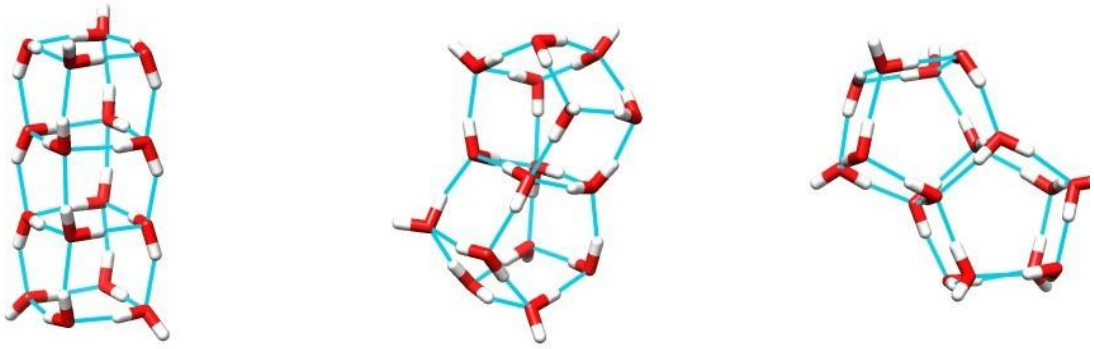

Figure 1. The three most common classes of $(H_2O)_{16}$ clusters; stacked tetramers, fused pentamers, stacked pentamer (left to right)