Accurate Predictions of the Structure and Energetics of Water Decamers

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As yet, the structure of small water clusters is not fully understood. We focused on the less studied $(H_2O)_7$, $(H_2O)_9$ and $(H_2O)_{10}$[‡], in an attempt to gain a better understanding of trends in growing water clusters. Candidate structures were generated by running molecular dynamics simulations and extracting coordinates at regular intervals. The low energy structures were optimized using MP2/6-31G*. MP2/aug-cc-pVDZ// MP2/6-31G* electronic and free energies were used to order the optimized structures. We found 30 unique structures within 2 kcal/mol of the free energy of the global minimum structure. These varied from symmetric container-like shapes to more disordered structures; G_{rel} and E_{rel} ordering generated the same global minimum structure.

	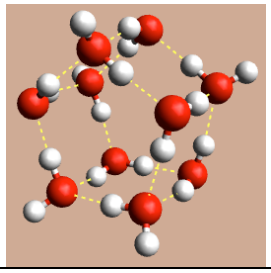	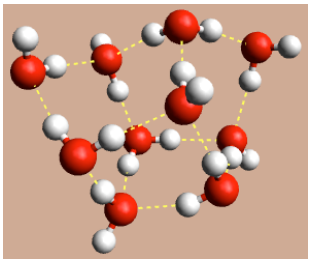	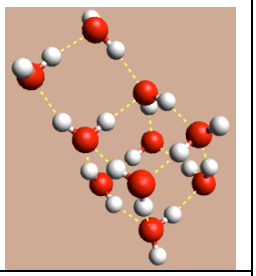
Conformer #	1	3	16
G_{rel} (kcal/mol)	0.00	0.33	1.23
G_{rel}^{BSSE} (kcal/mol)	0.00	0.18	1.22
E_{rel} (kcal/mol)	0.00	2.74	2.19
E_{rel}^{BSSE} (kcal/mol)	0.00	2.58	2.18

Fig 1. Most frequently occurring Conformer Shapes

[‡]This presentation will focus on water decamers only.