Systematic Classification and Analysis of Hydrogen Bonded Systems

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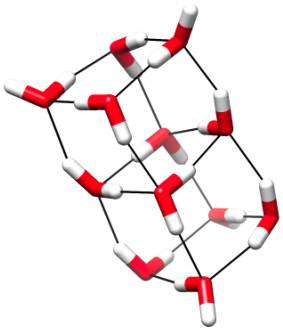
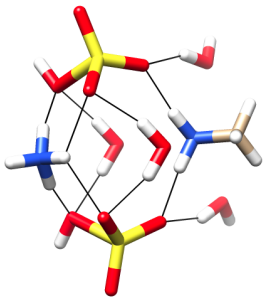
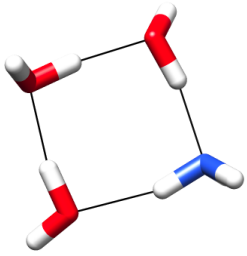
In hydrogen bonded systems, as the size of the system increases the number of local minima on the potential energy surface also increase exponentially. To ensure that we have found the putative global minimum and other low-lying local minima, a systematic sampling scheme need to be applied. And to minimize the number of structures analyzed, an efficient classification approach must be used. To start with, many initial structures are generated, reflecting the diverse range of structure possibilities. Then, a genetic algorithm heuristic is used to minimize the energies of the initial set. The natural-selection-like process combines structures over many iterations, finding new structures that are lower in energy than their predecessors. The final set of structures has significantly lower energy than the original but many of these are duplicates of each other. Classification is needed to narrow down this final set to a leaner, more workable one. Rotational constants and energies are found for each structure and compared; cutoffs are employed to determine how different two structures' energies and rotational constants must be for them to be unique. This new, unique final set is minimized using *ab initio* methods. The properties of these minimized structures are once again compared against cutoffs to determine which ones are unique. The structures shapes are then taken into account, being grouped based on similarity of shape. The end result of this process is a set of unique low energy structures, grouped based on similarity of properties. This process was applied to $(H_2SO_4)_2(CH_3NH_2)(NH_3)(H_2O)_n$ and $(NH_3)(H_2O)_n$ systems for $1 \leq n \leq 6$.



$(H_2O)_{12}$



$(H_2SO_4)_2(CH_3NH_2)(NH_3)(H_2O)_5$



$(NH_3)(H_2O)_3$