COMPUTATIONAL STUDIES OF THREE CHEMICAL SYSTEMS

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ABSTRACT

The subject of this dissertation is the use of electronic structure calculations to examine and supplement the experimental observations of three different chemical systems. Both *ab initio* and DFT methods have been employed. The first topic is the study of pyrogallol[4]arene with R-groups R=H and R=phenyl. This macrocycle self-assembles into dimeric and hexameric nanocapsules. Several different structures for the macrocycle and its subunits, their relative energies, and their solvent interactions are examined to better understand the process by which self-assembly of the nanocapsule occurs. The second topic is the study of the addition of H_2O and O_2 to vanadyl complexes of the form $[VOX(NCCH_3)]^+$ where X = F^-, Cl^-, Br^-, I^-, and OH^-. Changing the identity of X allows the observation of how the electron density on the metal center influences the addition of H_2O or O_2. The final chapters discuss the high-level quantum chemical calculations performed to study the structure and energetics of isomers of CH_2BF on both the singlet and triplet PES. MP2 optimizations were used to identify minima and transition states. A series of CCSD(T) single-point calculations were used to extrapolate to the complete basis set limit.