

INTERACTION ENERGY OF IODIDE ION WITH DECABORANE

ILIAS SIOUTIS, RUSSELL M. PITZER, *Department of Chemistry, The Ohio State University, 100 W.18th Avenue, Columbus, OH, 43210.*

Our goal is to compute the ground-state interaction energy of the iodide ion with decaborane in the complex, $B_{10}H_{14}I^-$, and to compare with the interaction between the xenon atom and $B_{10}H_{14}$ in the isoelectronic compound $B_{10}H_{14}Xe$. Under certain experimental conditions $B_{10}H_{14}I^-$ is found to be stable both in the solid state and in solution. Experimental investigation of this system reveals a C_{2v} point symmetry which is consistent with the symmetry of the B_{10} cage. The formation of this complex, though, results in some perturbation of the B_{10} framework; the unique iodine is situated at the open end of the decaborane, effectively resting on the four bridging hydrogens. The interaction involves distances which are consistent with van der Waals interactions. On the other hand, the dipole nature of decaborane and the charge of iodide ion are expected to have some contribution in the interaction energy of this system. Our hope is to sufficiently interpret the nature of this interaction and efficiently describe the electronic charge transfer from the iodide ion to $B_{10}H_{14}$, a consequence of the ion-dipole interaction between the fragments. Prediction of an accurate molecular binding energy involves use of an accurate correlation treatment and adequate basis sets. The ab initio methods that we apply are restricted Hartree-Fock self-consistent field of theory and single-reference single and double excitation configuration interaction (CISD). We use relativistic core and spin-orbit potentials and also correlation consistent polarized valence basis sets.