INTERACTION ENERGY OF IODIDE ION WITH DECABORANE

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Our goal is to compute the ground-state interaction energy of the iodide ion with decaborane in the complex, $B_10H_14I^-$, and to compare with the interaction between the xenon atom and B_10H_14 in the isoelectronic compound B_10H_14Xe.Under certain experimental conditions $B_10H_14I^-$ 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 interpet the nature of this interaction and efficiently describe the electronic charge transfer from the iodide ion to B_10H_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.