PH - 9 Poster

The CISS-1 Experiment: *ab initio* Study of Chiral Interactions

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We report results from the first Canadian Internetworked Scientific Supercomputer project, CISS-1. The chiral recognition surfaces of the two chiral molecules *cis*-1,2-propyleneimine and hydrogen peroxide were investigated by *ab initio* methods. The potential energy surfaces (PESs) for the chiral complexes between L-*cis*-1,2-propyleneimine and both enantiomeric forms of H_2O_2 were constructed by calculating the interaction energy at different separations and orientations.

The single-point calculations were performed with the MOLPRO suite of programs on the CCSD(T) level of theory. As a compromise between computational expense and accuracy, we employed Dunning's correlation-consistent polarized valence double-zeta (cc-pVDZ) basis sets. To eliminate the well-known problem of the basis-set superposition error, we adopted the counterpoise correction method of Boys and Bernardi [1].

Because of the complexity of the molecular system, some of its many degrees of freedom had to be confined. Altogether 27,000 points were calculated. It would not have been possible for us to perform this large-scale computation on our own Beowulf cluster where each point takes about 220 minutes on a single node.

The selected cuts of the PESs provide important information about the subtle differences in the interactions of homochiral and heterochiral complexes.

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[1] S. F. Boys and F. Bernadi, *Mol. Phys.* **10(4),** 553, (1970).