

The Infinite Basis Set Limit for the Dissociation Energy of Dimers Involving Hydrogen Sulfide¹

Gennadiy N. Berezutskiy,² Thomas Watson² and Glênisson de Oliveira

Rhode Island College, Physical Sciences Department
600 Mt. Pleasant Ave., Providence, RI 02908

Hydrogen sulfide (H_2S) is not ubiquitous in the atmosphere, but to the extent that it is present, it contributes to the formation of H_2SO_4 , which is a major cause for acid rain. The study of relative energies using computational chemistry may help to predict the onset of reaction between hydrogen sulfide and water in atmosphere. Weak interactions involving H_2S are dominated or greatly affected by dispersion forces, and potential energy surfaces are very shallow for H_2S dimers. Small errors may represent a large percentage of the total interaction, and obtaining accurate and reliable results for relative energies is extremely costly.

Using extrapolation formulas to estimate the basis set limit is a popular approach to study thermochemical properties. Traditionally, Dunning type bases are used, where with every increasing basis set, extra functions are added and the highest angular momentum is increased. For weakly bound systems, basis set demands are even greater and these extrapolations may not be practical.

Recently we developed new methodology to greatly decrease the cost of infinite basis set evaluations for hydrogen bonded systems, by making certain truncations for the increasing basis set, and using CP corrections. Here we examine whether the same methodology can be applied to systems where dispersion dominates or plays a significant role, and conclude that the basis set demands on dispersion-dominated systems are slightly different from systems where hydrogen bonding occurs.

¹ This work was partly supported by the Rhode Island College Faculty Research Funds.

² Undergraduate students.