

## **Thermodynamic Properties of Hydrogen Bonding Complexes**

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Study of hydrogen bonding interactions is important in understanding many fundamental aspects of the working mechanisms in biological systems. For example, the genetic information originates from hydrogen bonding interactions in DNA. Molecular level investigation of different hydrogen bonding interaction patterns has been the focus of both experimental and theoretical research. We present an investigation on the interactions of DNA base pair GC and many other bimolecular complexes of biological interest. We systematically studied the structures of all the compounds involved in this work by a variety of molecular orbital and density functional theory methods. Solvent effects were included with the use of SMD model of Cramer and Truhlar. We will present our latest results on accurate evaluations of thermodynamic parameters such as interaction enthalpies and Gibbs free energies in solution that govern the stabilities of real biological and chemical systems at certain temperatures.

### **Acknowledgement:**

This research is supported by a grant from NSF awarded to Dr. Daqing Gao, Central State University, Wilberforce, Ohio.

This research is also supported by Ohio Supercomputer Center.