Getting Down to the Fundamentals of Hydrogen Bonding with Convergent Quantum Chemistry

Gregory S. Tschumper
Department of Chemistry and Biochemistry, University of Mississippi

Non-covalent interactions, such as hydrogen bonding and London dispersion forces, play vital roles in a wide range of chemical, physical and biological phenomena. Examples include, but are certainly not limited to, molecular recognition, crystal engineering and self-assembly processes as well as the structure and function of biological macromolecules. Reliable *ab initio* electronic structure calculations have provided much insight into the strength, anisotropy and nature of these relatively weak interactions [1]. The first part of this talk will provide a very basic introduction to fundamental principles and concepts associated with quantum mechanical (QM) electronic structure computations. It will focus on computaional strategies that systematically converge toward exact numercial solutions of the electronic Schrödinger equation via methodical application of correlated wave function methods and Gaussian atomic orbital basis sets. This "crash course" in convergent computational quantum chemistry will use simple H_2O clusters to provide concrete examples, and it will also set the stage for the remainder of the lecture. As time permits, some recent applications of these strategies to hydrogen bonding and other non-covalent interactions will be highlighted [2,3].

References

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