First Principles Study of Electronic Structure of BF3-NH3 Complex and Associated Properties

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BF3 is a planar molecule with three-fold symmetry which is widely used to promote various organic reactions such as Friedel-Crafts acylations and alkylations. To obtain a thorough understanding of the mechanisms for this role of BF3, we are studying from first-principles the electronic structures of BF3 and its complexes with NH3. The procedure used is the first principles Hartree-Fock-Roothaan procedure combined with many body perturbation theory. The results for BF3-NH3 system will be reported, such as the binding energy and equilibrium geometry of the complex, the nature of the B-N bond and the changes in the B-F and N-H bond strengths on complex formation. The Nuclear Quadrupole Interactions of the 19F* (spin 5/2), 14N, 11B, and 2H will be presented and compared with available experimental data. (*) Present Address: Dept. of Physics, Uppsala University, Sweden (**) Also: Dept of Physics, University of Central Florida, Orlando, Florida