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 $^{19}$F* (spin 5/2), $^{14}$N, $^{11}$B, and $^2$H will be presented and compared with available experimental data.

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