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First Principles Study of Electronic Structure of BF3-NH3 Complex and Associated Properties ARCHANA DUBEY, LEE CHOW, Dept. of Physics, Univ. of Central Florida, Orlando, MAHENDRA K. MAHANTI, North Eastern Hill University, Shillong, India, ROGER PINK, M. B. HUANG, R. H. SCHEICHER (*) , T. P. DAS (**) , Dept. of Physics, SUNY at Albany, NY — BF_3 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 BF_3, we are studying from first-principles the electronic structures of BF_3 and its complexes with NH_3. The procedure used is the first principles Hartree-Fock-Roothaan procedure combined with many body perturbation theory. The results for BF_3-NH_3 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. (*) Present Address: Dept. of Physics, Uppsala University, Sweden (**) Also: Dept of Physics, University of Central Florida, Orlando, Florida

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