

Abstract Submitted  
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**Electron Distribution in Solid  $\text{BF}_3$  and  $\text{BF}_3 - \text{NH}_3$  - Associated Nuclear Quadrupole Interactions** DIP N. MAHATO, R.H. PINK, M.B. HUANG, T.P. DAS<sup>1</sup>, SUNY Albany, ARCHANA DUBEY, LEE CHOW, UCF Orlando, MAHENDRA K. MAHANTI, NEHU Shillong, India, R.H. SCHEICHER, MTU Houghton — The electronic structures of  $\text{BF}_3$  and the complex  $\text{BF}_3 - \text{NH}_3$  in the solid state[1] have been studied by the Hartree-Fock Cluster Procedure and including many-body effects by perturbation theory. The motivation is to understand the nature of the bonding between the individual molecules in the solid and changes in the bonding within the molecules. We also have attempted to understand the differences in the nuclear quadrupole interactions of  $^{11}\text{B}$  and  $^{19}\text{F}^*$  nuclei in the free molecules and the solid state systems and have compared the results of theory with available experimental results[2] in solid state. Nuclear quadrupole interaction results for  $^{14}\text{N}$  and deuteron will also be presented in the complex.

[1] D. Mootz and M. Steffen, *Angew. Chem. Int. Ed. Engl.* 19, 483(1980).

[2] P.A. Casabella and T. Oja, *J. Chem. Phys.* 50, 4814(1969); K. Berthholdt et al, *J. Mol. Struct.* 192, 199(1989).

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