Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Theory of Electronic Structure and Nuclear Quadrupole Interactions in the BF3-NH3 Complex R.H. PINK, DIP N. MAHATO, M.B. HUANG, T.P. DAS[1], SUNY Albany, ARCHANA DUBEY, LEE CHOW, UCF Orlando, MAHENDRA K. MAHANTI, NEHU Shillong, India, R.H. SCHEICHER, MTU Houghton — Boron Trifluoride is widely used as a catalyst in chemical research and industry forming complexes in the process with other molecules like NH_3, H_2O, and CH_3OH. We have studied the BF_3-NH_3 molecular complex using Hartree-Fock procedure combined with many-body perturbation theory. The B-N bond is found to involve about 75% covalent and 25% van der Waals characters. The calculated geometry of the complex compares well with experimental results. The nuclear quadrupole interaction parameters for the $^{19}F^*$ nucleus [1] show good agreement with experiment for both solid BF_3 and the complex including the nuclear quadrupole coupling constants and the sizable asymmetry parameters. The ^{11}B quadrupole coupling constant is however found to be about 1.5 times the available experimental value [2] for solid BF_3, possibly due to the influence of intermolecular bonding.

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

[1]Also UCF Orlando

Tara P. Das
SUNY Albany

Date submitted: 21 Nov 2005 Electronic form version 1.4