Boron Trifluoride is widely used as a catalyst in chemical research and industry forming complexes in the process with other molecules like NH₃, H₂O, and CH₃OH. We have studied the BF₃-NH₃ 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 ¹⁹F* nucleus [1] show good agreement with experiment for both solid BF₃ and the complex including the nuclear quadrupole coupling constants and the sizable asymmetry parameters. The ¹¹B quadrupole coupling constant is however found to be about 1.5 times the available experimental value [2] for solid BF₃, possibly due to the influence of intermolecular bonding.


¹Also UCF Orlando

Tara P. Das
SUNY Albany

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