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Theory of Nuclear Quadrupole Interaction in Trifluoro-Aminoboranes [$\mathbf{BF_3}$-$\mathbf{NH_{3-X}(CH_3)_X}$] MAHENDRA K. MAHANTI, NEHU Shillong, India, ARCHANA DUBEY, H.P. SAHA, LEE CHOW, UCF Orlando, R.H. SCHEICHER, MTU Houghton, R.H. PINK, DIP N. MAHATO, M.B. HUANG, T.P. DAS[1], SUNY Albany — The understanding of the catalytic properties of BF_3 of great current interest require information about the electronic structures of the associated complexes of BF_3 with the molecules involved in the process. In this work we have studied the corresponding complexes for methylamines using the Hartree-Fock procedure combined with many-body perturbation theory. Results will be presented for the natures of the three complexes and the ^{19}F* quadrupole coupling constants and asymmetry parameters for which experimental data [1] are available. Comparisons will be made with the corresponding properties for BF_3-NH_3, allowing valuable insights into the trends in the electron distributions in this family of complexes.

[1] K. Bertholdt et al., J. Mol. Struct. 192, 199 (1989)

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