AB INITIO PREDICTION OF THE STRUCTURE AND ROTATIONAL CONSTANTS OF GROUND STATE METHYLAMINE, CH_3NH_2

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Accurate theoretical predictions can provide critical information for high resolution rotational spectroscopy, including both structural parameters and potential energy surfaces associated with hindered internal motions. With recent experimental data available [V. V. Ilyushin et al., J. Mol. Spectrosc. 229, 170 (2005)], methylamine is an ideal test case for benchmarking the computational demands for asymmetric top molecules with two internal motions. Several issues will be addressed: (1) What level of theory and basis set is required to accurately describe the equilibrium structure? (2) What procedure should be used to transform the equilibrium rotational constants to reflect zero-point motion? (3) What is required to obtain accurate potentials for the internal rotation and inversion of NH_2 with respect to the CH_3 group? Various levels of theory – B3LYP, MP2, and RCCSD(T) – were explored in conjunction with valence and core-valence correlation consistent basis sets.