Electronic and Vibrational Properties of Small Molecules – NH_3 versus NF_3

Basic problem: Obtain the bond length, bond angles, dipole moment, and charge distributions for NH_3 and NF_3 at two levels of theory. Compare the dipole moment at each level of theory to experiment, to evaluate the effects of increasing the level of ab initio theory upon accuracy in predicting this dipole moment and the bond length.

Method: AM1 and 6-31G* are oft-used levels of theory. In your Results table, record the optimized bond lengths, H-N-H and F-N-F angles, charge distribution, and dipole moment for each calculation, and compare to the experimental values from the literature. How sensitive are the values of these molecular properties for this simple molecule to changes in the computational method? How well do the computations compare to the experiment.

Literature: Use Beilstein Online, Chemical Abstracts, or TheoChem database for literature information on NF_3.

METHOD	N-F Bond Length	Nitrogen Charge	Fluorine Charge	Dipole Moment
Exptl Values		----------	----------	
AM1				
RHF/6-31G*				