SUPPLEMENTARY INFORMATION

Effects of Halogen, Chalcogen, Pnicogen, and Tetrel Bonds on IR and NMR Spectra

Jia Lu and Steve Scheiner*



Fig S1. Optimized geometry of complexes with NH₃. The geometry that includes FSH is not a pure minimum as it includes one negative frequency which corresponds to torsional rotation of the NH₃ group.



Fig S2. Electron density shifts caused by complexation between Lewis acid and NH₃. Purple areas indicate gains and losses are shown in green. Contours shown represent 0.001 au.