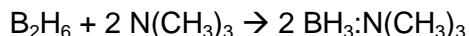


Chem531

Prelab 5 – Borane Amine Complex

1. Label the Lewis acid and Lewis base in this reaction. (2 pts)



2. Consider the compound $\text{BH}_3:\text{NH}_2\text{C}(\text{CH}_3)_3$. How many peaks do you expect to see by IR and why? (3 pts)

3. (a) Draw the Lewis structure of $\text{BH}_3\text{-NH}_3$ (include formal charges) (1 pt).

(b) (i) Using Spartan, build the $\text{BH}_3\text{-NH}_3$ adduct. Calculate the ground state equilibrium geometry (vacuum) using the Hartree-Fock 3-21G basis set. (ii) Determine the "Mulliken charge" on both boron and nitrogen (Click "Display" → "Properties" then click on the atom of interest – you will see a table of properties, one of which will be the Mulliken charge on that atom). (iii) Comment on the differences between the calculated atomic charges and the formal charges in the Lewis structure. Discuss which is more realistic and why. (4 pts)