

CHEM422 Problem Set

Molecular Vibration Calculations for Metal Carbonyls

1. Using Spartan, determine the frequency and type of vibration (E' , A_1' , A_2' , etc.) for $\text{Ni}(\text{CO})_4$.
2. Using Spartan, determine the frequency and type of vibration (E' , A_1' , A_2' , etc.) for $\text{Fe}(\text{CO})_5$.
3. Using Spartan, determine the frequency and type of vibration (E' , A_1' , A_2' , etc.) for $\text{Cr}(\text{CO})_6$.
4. Using Spartan, build a model of $\text{Mn}_2(\text{CO})_{10}$.

Spartan Molecular Vibration Calculations

Start Spartan. If already running, go to **File, New**. Then select the **Exp.** tab, select the metal from the periodic table by clicking the Left Mouse Button (LMB) on its chemical symbol. Now select the geometry about that metal atom by clicking the LMB on its symbol. Finally click the LMB in the work area of the screen. If more than one metal center is involved, complete the metal centers.

Next, select the **Ent.** tab, the triple bonded C, and click the LMB at each bond to the metal.

There is not a triple bonded oxygen in the options. Therefore, select the triple bonded nitrogen and add one to each carbon.

Now to convert N to O, select the **Exp.** tab, select O from the periodic table, and double click the LMB on each nitrogen.

Now go to **Setup, Calculations**. Change **Semi Empirical** to **Hartree-Fock**. Click the LMB on the box in front of **Freq.** and then click the LMB on the **Submit** button to submit the job for calculations.

Give the file a name, click **OK** to start the calculations and wait for them to finish. This step may take several minutes to complete, more time for larger molecules.