

**EXPERIMENT #7(B) – POST-LAB REPORT GUIDELINES FOR THE  
INFRARED SPECTROSCOPY WORKSHOP  
THIS IS A GROUP REPORT.**

**NOTE: THERE IS NO PRE-LAB REPORT FOR THIS "EXPERIMENT"**

**MAKE SURE THAT YOUR GROUP COMPLETES ALL THE FOLLOWING ITEMS BEFORE TURNING IN THE GROUP REPORT. REFER TO THE LAB SCHEDULE FOR DUE DATE. FOR THIS REPORT, YOU MAY ANSWER ALL THE QUESTIONS ON THE IR WORKSHEETS.**

**(I)** Completed IR worksheets for the five molecules.

**The five molecules are: TWO "different" carbon dioxide; acetic acid; propionamide and allyl benzoate.**

**(II)** Compare the IR frequencies for carbon dioxide calculated by the **TWO** different quantum theoretical methods (*the ones you did on Spartan in the lab*) with the experimental IR frequencies for carbon dioxide listed on page 84 in the manual. What can you conclude? Explain.

**(III)** Label **ALL** the bond angles, distances and **strain energy** for the molecule of **caffeine**.

**(IV)** Analyze the **LITERATURE** caffeine IR spectrum by identifying as many vibrational motions for various functional groups as you can on the spectrum.

The literature caffeine IR spectrum is attached on the last page of your IR worksheets. If for some reason, you don't have the literature IR spectrum for caffeine, you can go to the following web site to download the IR spectrum of pure caffeine:

<http://chemfinder.cambridgesoft.com/>

In the search engine, type "**caffeine**". Scroll down the screen and there should be an item called "**NIST Chemistry WebBook**". Click on "**Information for this particular compound**" under the NIST link. You should be able to find the gas phase IR spectrum of pure caffeine.