Raman/IR Spectroscopy of CCl4 and CHCl3
Lab Report

This sheet should serve as a very general guide for this final lab report. You have spent a semester writing reports for J. Phys. Chem. G. and are familiar with the requirements. This guide lists some items I'd include in the results and discussion section of the report; there are likely some things on in this list that should be included as well.

Results:

1. IR and Raman spectra
2. Table including peak position (in cm^{-1} or rel. cm^{-1}), peak identification ($\upsilon_{\#}$), intensities, and literature values
3. Normal modes (assigned to the peaks) for both CCl_4 and $CHCl_3$ (Note: there are 4 modes for CCl_4 but 6 for $CHCl_3$). Draw out the modes (as in Table 1 of the handout) and assign them a $\upsilon_{\#}$.

Discussion:

1. Use the valence force model to find k and k_δ/ℓ^2 and determine if the stretch-stretch, stretch-bend and bend-bend interactions are important terms in potential energy of CCl_4 and $CHCl_3$.
2. Compare and contrast the IR and Raman spectra for both CCl_4 and $CHCl_3$
3. Compare and contrast the two Raman spectra (i.e., compare CCl_4 and $CHCl_3$)
4. Error sources and any differences between the literature values and experimental (remember we only looked at the Stokes lines)
5. Discussion on overlap of υ_3 and $\upsilon_1 + \upsilon_4$

Some good literature sources/resources:

1. NIST webbook (type in compound name/formula & find vibrational energy link)
2. SDBS (spectral database)… easiest way to access is to google SDBS
3. Gundogdu, K., et al., *J. Chem. Phys*. 2006, **125**, pg. 174503. (This doesn't have values for $CHCl_3$ or CCl_4, but does identify the normal modes of $CDCl_3$ which may be helpful as you assign the normal modes of $CHCl_3$.)
4. I've run a calculation for $CHCl_3$ on WebMO. To see the results, log-in to WebMO using the username: pchem and password: compute. Look for the job with $CHCl_3$ in the title. You can use this to aid you in assigning the normal modes to your spectra.