Infrared Spectroscopy
Student Instructions for the IR Laboratory
October 2 – 8, 2012

- Your Instructor will describe principles of IR spectroscopy and how to interpret IR spectra to identify the presence or absence of functional groups.
- The Index of Hydrogen Deficiency (IHD) will also be described and defined; this index is useful for determining the number of rings and/or double bonds present in a compound with a given molecular formula. By using the Molecular Formula and IHD of a specific compound, one can propose a number of viable structures fitting this data. Used in conjunction with information obtained from the IR spectrum of a compound, one can quite often determine the actual structure of the compound.
- TAs will demonstrate how to run a liquid (Ethyl Benzoate) and a solid (4-Methylbenzyl alcohol) sample on the IR instruments.
  o Determine the IHDs of these two compounds.
  o Look at handouts of the IR spectra of these 2 compounds to see how pertinent IR absorption bands were assigned.
- Work in groups of 4: Each group should come up with proposed structures for each of the 4 unknowns whose IR spectra and molecular formulas were handed out. For your observations for this experiment:
  1. First, determine the IHD for each unknown compound and draw at least 2 possible structures for each compound based solely on the compound’s molecular formulas and calculated IHD values. Do this before you look at/try to interpret the IR spectra.
  2. Examine the IR spectra for each unknown and assign pertinent IR absorption bands in the functional group region (1400 – 4000 cm⁻¹) for each compound by using the IR Absorption Table-2012 that has been provided to you.
  3. Using both IHD values and the IR absorption band assignments you proposed in step 2, propose a viable structure(s) for each unknown.
  4. Do any IR absorptions in the fingerprint region (600-1400 cm⁻¹) of the IR Spectra help to reinforce the structures you proposed for each unknown? If so, what are the fingerprint absorption peaks and what structural features in your proposed molecule do they correspond to?
  5. For each unknown, does your proposed structure correspond with any of the structures you initially proposed based solely on your IHD value in from Step 1?
  6. Can you eliminate any of your initially proposed structures (based solely on IHD, step 1) by showing an absence of IR bands for structural features in the functional group region?
  7. In your write-ups for this experiment, you should include copies of the IR spectra of the unknowns A thru D with absorption peaks labeled as to the structural features they represent.
  8. Your conclusions should include the structures you determined for each unknown and a summary of how you arrived at the proposed structures. If there is more than 1 structure possible for an unknown based on your interpretation of the IHD and IR data, you should list the alternate structures.