Organic II lecture Review for exam 1 Spectroscopy

- 1. What is the relationship between energy, wavelength, frequency and wavenumbers in terms of proportional or inversely proportional? Write equations that interconvert these values.
- 2. Be familiar with the electromagnetic spectrum from radio waves to ultra violet region -Which region is more energetic than another, and what molecular influence is brought by that region? For example: IR = molecular vibration and bending.
- 3. What factors influence the frequency at which a bond vibrates?
- 4. What type of species can be observed by mass spectrometry?
- 5. Predict the base peak for 2-methylpentane.
- 6. For 1-butanol, what is the mass corresponding the peak with the highest m/z value?
- 7. Using a 90 MHz NMR, a doublet was obtained at 5.5 ppm with a coupling constant of J=10 Hz.
 - a) What is the probable functionality indicated by this proton?
 - b) What is the geometric orientation between this proton and the proton inducing the splitting?
 - c) Calculate the chemical shift and the gap between the doublet in Hz if the sample is run in a 360 MHz NMR.

8. Consider *sec*-butyl acetate:

a) Label all chemical environments and predict their spin-spin splitting and chemical shift within 1 ppm.

- b) Which proton(s) appear farthest upfield, and which are farthest downfield?
- c) What is meant by "shielded"?
- 9. What causes spin-spin splitting? Explain why the methyl group in propane is split into a triplet.
- 10. In off resonance ¹³C NMR, how would the peak representing the methyl group of propane appear?
- 11. What is the relationship between the energy difference of α and β nuclear spins and H₀?
- 12. What elements can be specifically identified by mass spectrometry, and tell how?