CHE 532 Fall 2008 Tentative Schedule of Lecture Topics
August - September

(subject to *sudden and dramatic* change – be alert in class!)
Assigned preparatory reading should be completed prior to the lecture for which it is assigned.

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1. Thursday Aug 28
   Course introduction. The role of structure determination in the chemical sciences. Levels of structural detail: Elemental composition (analysis), functional groups, skeletal connectivity, stereochemistry, conformation. What is spectroscopy and spectrometry? Techniques to cover: elemental analysis, mass spectrometry, infrared spectroscopy, nuclear magnetic resonance spectroscopy, multidimensional NMR. Others (only if time permits): Raman, UV/vis, and chiroptical methods (circular dichroism, ORD, polarimetry)

2. Tuesday Sept 2
   Elemental Analysis. Not really spectroscopy, but useful as part of the toolbox for solving structural questions. What elements are present and in what relative quantities? Block diagram of a basic combustion analysis system. How to calculate the elemental composition from a molecular formula.

   Preparatory reading: PLK pages 1-14

3. Thursday Sept 4
   Mass Spectrometry I. Basic block diagram of an MS instrument. Ionization methods and mass analyzers. The parent ion, molecular weight, and high-resolution MS.

   Preparatory reading: PLK pages 418 - 438

4. Tuesday Sept 9
   Mass Spectrometry II. Interpreting MS data. Even/odd parent ions. Isotope issues (identification of halogens and total number of carbons). Fragmentation of the parent ion. The base peak (the most commonly formed fragment).

   Preparatory reading: PLK pages 438-451

   Problem set 1 assigned

5. Thursday Sept 11
   Mass Spectrometry III. Fragmentation patterns, problem solving.

   Preparatory reading: PLK pages 451 – 496.

6. Tuesday Sept 16
   Mass Spectrometry IV. Fragmentation patterns, problem solving.

   Problem set 1 due

   Wednesday Sept 17. Last day to drop a class or to change a grade option.

7. Thursday Sept 18
   Infrared Spectroscopy I. The Schroedinger equation and the vibrational component. Quantum phenomena, selection rules, transition dipole moments. IR active transitions and Raman active transitions. Jablonski diagrams. IR absorption frequencies correspond to energy *differences*, not to energies of specific vibrational states. Overtones.

   Key equations to know:
   $E\Psi=H\Psi$ (Schroedinger's equation)
   $E=h\nu$ (relates energy to frequency)
   $c=\lambda\nu$ (wavelength times frequency is a constant: the speed of light).

   Preparatory reading: PLK pages 15-28
   Infrared Spectroscopy II. The electromagnetic spectrum. Block diagram of an IR spectrometer. Common units in IR spectroscopy: microns or "millimicrons" (nanometers) (wavelength, archaic) Wavenumbers ($1/\lambda$, cm^{-1}): peculiar, but *linear with energy* ($E=hc/\lambda$)
   The appearance of IR spectra. Functional group identification through specific absorption band positions and intensities.
   Preparatory reading: PLK pages 28-58

8. Tuesday Sept 23
   Exam 1.

9. Thursday Sept 25
   Infrared Spectroscopy III. Gleaning additional information through subtle shifts in position.
   NH, OH, CH (sp^3, sp^2, sp) Bond length/strength and IR frequency
   C-C bonds (alkynes, alkenes, alkanes), C-O bonds (ethers and carbonyls),
   Effects of resonance, angle strain on IR spectra
   The "Fingerprint Region."
   Full spectra and problem solving.

   Preparatory reading: PLK pages 59-83

10. Tuesday Sept 30
    Infrared Spectroscopy IV. Full spectra and problem solving.