CHE 532 Fall 2007 Tentative Schedule of Lecture Topics

(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 23
   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: 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 Aug 28.
   Elemental Analysis. Not really spectroscopy, but useful as part of the tool box 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 1-12

3. Thursday Aug 30
   Mass Spectrometry I. Basic block diagram of an MS instrument. Ionization methods, mass analysers. The parent ion, molecular weight, and high-resolution MS.

   Preparatory reading: PLK pages 390 - 415

4. Tuesday Sept 4
   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 416-445

   Problem set 1 assigned

5. Thursday Sept 6
   Mass Spectrometry III. Fragmentation patterns, problem solving.

   Preparatory reading: PLK pages 446 – 465.

6. Tuesday Sept 11
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.

Key equations to know:
$E\Psi=H\Psi$, how the wavefunction separates into different components (in the Born-Oppenheimer situation, at least.)
$E=h\nu$ (relates energy to frequency)
$c=\lambda\nu$ (wavelength times frequency is a constant: the speed of light).

Preparatory reading: PLK pages 13-18

Problem set 1 due

Wednesday Sept 12. Last day to drop

7. Thursday Sept 13
Infrared Spectroscopy II. The electromagnetic spectrum. Block diagram of an IR spectrometer. Diffraction gratings (dispersive) instruments versus FT instruments. IR absorption frequencies correspond to energy *differences*, not to energies of specific vibrational states. Overtones.

Common units in IR spectroscopy: microns or "millimicrons" (nanometers) (wavelength, archaic)
Wavenumbers ($1/\lambda$, cm^{-1}): peculiar, but *linear with energy* ($E=hc/\lambda$)

Preparatory reading: PLK pages 19-27

8. Tuesday Sept 18
Exam 1.

9. Thursday Sept 20
Infrared Spectroscopy III. The appearance of IR spectra. Functional group identification through specific absorption band positions and intensities. The "Fingerprint Region."

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), full spectra and problem solving.

Preparatory reading: PLK pages 26-83