Chemistry 387 Syllabus

Chemistry 387
Dr. Badger

Text: "Spectrometric Identification of Organic Compounds," 7th edition, R. M. Silverstein, F. X. Webster and D. J. Kiemle John Wiley, New York, 2005.

We shall discuss material from the first six chapters of this text. However, you will be expected to spend significant independent study time reading and applying concepts presented in these chapters, in some cases before we have discussed it formally in class.

Generally I expect to spend the first hour of class time lecturing on new material and the second hour will be spent in small groups solving and presenting spectal problems.

Grading: We shall usually have some type of problem set each week worth 20 to 25 points. Most of these problems will be handout or web based spectra or problems from the text. However, some of them will involve the direct measurement of spectra on real compounds. There will also be a 50 point problem set to be submitted during the final exam time.

Problem sets 13 x 20 = 260
Final quiz 1 x 50 = <u>50</u>
Total = 310

Chemistry 387
Course Content

General

The course meets once a week for 110 minutes at a time. There is generally a 10 minute break about half way through. Class time is split about 50-50 between lecturing about new topics and solving spectral problems. In group class exercises we will solve/discuss almost all the chapter end spectral problems in Silverstein, Webster and Kiemle "Spectrometric Identification of Organic Compounds: seventh Edition" for chapters 1, 2, 3, 4 and 5. In addition, students are given approximately 13 take home problem sets consisting of at least 5 spectral problems each to be turned in and discussed the following week. These problems are taken from various sources. Students are usually required to integrate information from several spectroscopic techniques to determine and support their structure assignments.

Mass Spectroscopy

A simple electron impact magnetic sector mass spectrometrometer is discussed. The parent ion is discussed in detail concerning P, P+1, and P+2 ratios and their utility in indicating the presence of nitrogen, chlorine, bromine, and sulfur. Exact mass analysis is used to determine the chemical formula and the rule of 13 is applied for those cases where exact mass is not available. Students are expected to analyze daughter ions and propose fragmentation pathways for the more intense high mass ions. They are thus introduced to gas phase radical-cation, cation and radical stability. The loss of stable molecules such as water, HCl, CO_2 or other organic molecules via elimination or

MacLafferty rearrangement is discussed.

Infrared Spectroscopy

The characteristic functional group frequencies are reviewed. The effect of carboxylic acids, alcohols, amines and concentration on X-H stretching region is examined. The C-H stretching frequencies near 3000 cm^{-1} are analyzed in some detail to show how they may indicate the presence of alkyne, alkene, aromatic, alkane or aldehyde functionality. The aromatic C-H bending and overtone regions of aromatic compounds are analyzed to provide information on substitution patterns. The subtle effects of conjugation and different carbonyl containing functional groups on the carbonyl stretching frequency is examined. The C-O stretching region of alcohols is used to suggest primary, secondary or tertiary alcohols.

Proton Nuclear Magnetic Resonance

The analysis of integration, mulciplicity and chemical shift is briefly reviewed. Strong and weak coupling phenomena are discussed along with the effects of chiral centers. Students are introduced to deuterium exchange experiments, coupling constant analysis to determine cis/trans isomers, and homonuclear decoupling experiments to simplify spectra. The pulse NMR experiment is discussed in some detail to show students how the net magnetization vector is perturbed by the RF signal and NMR frequencies can be extracted from the FID by Fourier transform. The effect of pulse width and pulse delay on spectrum integration is used to introduce relaxation phenomena. Spectrum wrapping or folding is discussed.

Carbon Nuclear Magnetic Resonance

The simple pulse experiment with broad band decoupling is used to present the advantage of the pulse experiment in multiple acquisitions to improve the signal to noise. The nuclear Overhauser effect is briefly discussed to show why integration is generally not performed on carbon spectra. Various gated decoupling experiments are described that allow carbon integration or determination of hydrogens attached. The APT and DEPT experiments are presented as better methods of determining hydrogen attachment. The analysis and calculation of chemical shifts is used to assign carbons in relatively simple molecules.

Two Dimensional Nuclear Magnetic Resonance

The various 2D experiments such as COSY, NOESY, HETCOR, and INADEQUATE are briefly presented. Example spectra along with analysis methods used to assign each carbon in a structure are discussed.

Last update: Thursday, 25-Jan-2018 13:30:26 CST