Chemistry 617 Organic Structural Spectroscopy Fall 2012 Dr. Honeychuck

This syllabus can be found at http://mason.gmu.edu/~rhoneych/617syllb.pdf

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Class meets Wednesday 7:20-10:00 pm in Engineering 1110

Required text: Silverstein, R. M.; Webster, F. X.; Kiemle, D. J. *Spectrometric Identification of Organic Compounds*; 7th ed., Wiley: New York, 2005.

Required course packet: Honeychuck, R. V. *Chemistry 617 Organic Structural Spectroscopy*; Fall 2012.

Date	Pages	Subjects
Aug 29	72-86	IR basics, FT IR
Sep 5	87-103	Functional group modes, sample handling, IR CD-ROM & web resources, IR lab demo
Sep 12	104-110	Functional groups, pseudosymmetry
Sep 19		Midterm 1
Sep 26	127-139, 157-160	NMR basics, FT NMR, ^{1}H NMR, multiplicity, equivalent groups
Oct 3	139-147	Shielding, deshielding, Pascal's triangle
Oct 10	135-138, 147-150	Deuterated solvents, lock signal, shimming, spin systems, nondistorted & distorted multiplets
Oct 17	147-151	Pople notation
Oct 24	162-169	Magnetic equivalence, magnetic nonequivalence, H-bonding, NMR lab demo
Oct 31	150-162, 169-177	Exchange, NH & NH_2, spin number, quadrupole moment, vicinal Karplus correlation
Nov 7		Midterm 2
Nov 14	204-229	^{13}C NMR, composite pulse decoupling, Nuclear Overhauser enhancement, ^{13}C-^{1}H coupling constants, distortionless enhancement via polarization transfer
Nov 21		Day before Thanksgiving. No 617.
Nov 28	316-317, 323-326, 327-333, 245-254	^{19}F NMR, ^{31}P NMR, 2 D NMR
Dec 5	1-38	MS basics, instrument types, molecular ions, fragmentation patterns, chemical classes, UV/VIS basics, Raman basics

Dec 12 Comprehensive Final Exam, 7:30-10:15 pm, Engineering 1110

Grading:
25% Midterm 1
25% Midterm 2
10% Assigned Problems
40% Final Exam
100%

On Reserve in the Johnson Center:
Silverstein, R. M.; Webster, F. X.; Kiemle, D. J. *Spectrometric Identification of Organic Compounds*; 7th ed., Wiley: New York, 2005.
Shriner, R. L. *The Systematic Identification of Organic Compounds*; 7th ed., Wiley: New York, 1998.
Breitmaier, E. *Structure Elucidation by NMR in Organic Chemistry: A Practical Guide*; 3rd ed., Wiley: New York, 2002.

Chemistry 617 covers the spectroscopic determination of organic molecular structure using dispersive and Fourier transform infrared spectroscopy, multinuclear NMR, mass spectrometry, ultraviolet/visible spectroscopy, and Raman spectroscopy. The prerequisite for Chemistry 617 is Chemistry 314 or an equivalent second semester undergraduate organic chemistry lecture taken by science majors, pre-medical students, or chemistry majors.

Mostly oriented toward the elucidation of the structure of organic compounds whose makeup is not known, Chemistry 617 might be classified as an analytical organic chemistry course. It is devoid of heavy mathematical and theoretical treatments. Sometimes the point will be to develop an understanding of a spectrum itself, and the structure will be provided. This is often the case in the real world; a structure or much of a structure might already be known. Also, an IR or UV/visible spectrophotometer is often used to assay for a known compound in a reaction in progress, or in a natural product extraction, because of the small amount of time required for spectrum collection. Here background knowledge acquired in 617 becomes useful in screening out peaks due to starting materials and solvents.

There will be one lecture per week, with a laboratory demonstration component during certain weeks. Not every technique will have a laboratory demonstration. The main nuclei in the NMR part of the course will be ^{1}H, ^{13}C, ^{19}F, and ^{31}P. The focus will be on a broad range of structures, from small synthetic organics and small organic molecules occurring in biological systems, to medium-sized molecules and polymers. With this course the need for elucidation of organic structures in various research labs on campus, as well as verification of known structures in use as starting materials, will be satisfied. Matching algorithms are part and parcel of elucidation-oriented spectroscopy because of the associated high speed and accuracy, so spectral databases with matching software on CDs and web sites will be in use and encouraged. There will be many assigned problems containing spectra of different types but no given structure, and it will be up to the student to determine the structure of the compound, or at least a part of it. At the end of the course the student will be able to take the information in several spectra and turn it

mentally into a molecule, or give a qualitative interpretation of a spectrum taken on a known compound, or have a computer do these things instead.

If you are a student with a disability and you need academic accommodations, please see me and contact the Office of Disability Services at 993-2474. All academic accommodations must be arranged through that office.