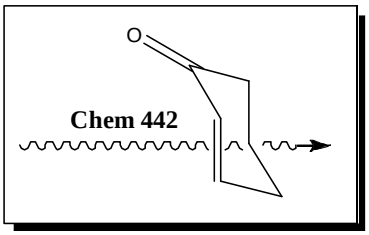
Lycoming College **Spectroscopy and Molecular Structure** **Fall 2011**



Course Description - This course examines the various spectral and chemical techniques used by organic chemists to identify and characterize organic molecules. The laboratory component of the course will utilize the spectral techniques discussed in class.

Faculty - Dr. Chriss McDonald, HBC 233, 998-8647 (home, call up to 10 pm), 321-4186 (work), email *mcdonald@lycoming.edu*, no specific office hours but I'm usually around.

Texts and Other Stuff

a. *Spectrometric Identification of Organic Compounds*, 7th Edition, by Silverstein and Webster
b. Old 220-221 lab manual
c. Bound laboratory notebook by Freeman
d. Lab safety glasses
e. Calculator (add, subtract, multiply, divide, logs)

Course Format

a. Lectures - MWF, 2:00 PM.

b. Assigned homework - problems designed to enhance your understanding and prepare you for testing situations. A key will be passed out immediately after collection of the assignment. No late homework will be accepted.

c. Laboratory - 7:45 - 11:35 Th. The experiments are listed on the last page.

d. Recitations – none scheduled, If you wan some, let me know and we'll find a time to get together. We do a lot of in class problem solving as you will see.

e. Colloquium – Almost all of our colloquia have some spectroscopic component. Therefore a small portion of your grade will be based on your attendance at colloquium. You must attend 5 colloquia to obtain full credit. If you are unable to attend colloquium due to a schedule conflict, you may obtain these points by summarizing appropriate journal articles from the primary chemical literature. Let me know if you intend to do this and I will share guidelines for these summaries.

Course Objectives

Upon completion of this course each student should be able to:

1. Use MS to determine MW, molecular formula, and some connectivity.
2. Use IR to determine the presence of functional groups.
3. Use ^{1}H-NMR to elucidate the structure of low molecular weight organic molecules.
4. Use ^{13}C-NMR to elucidate the structure of low molecular weight organic molecules.
5. Use 2-dimensional NMR techniques to elucidate the structure of low molecular weight organic molecules.

Grading Scheme

a. The final grade is based on the number of points obtained out of a possible 650 points. The points will be distributed as follows:

quizzes	45 points
hour exams	300 points
final exam (cumulative)	135 points
laboratory	120 points
homework	35 points
colloquium	15 points
total	**650 points**

b. Assignment of letter grades is based on the following scale: 650-585 **A**, 584-520 **B**, 519-455 **C**, 454-390 **D**, < 390 **F**. A higher score on the cumulative final (adjusted to a 100 point scale) can be used to replace the lowest exam score.

Policy on Attendance for Exams and Quizzes Makeups will be administered only if I deem the reason for absence to be legitimate **and I am notified of the absence beforehand.** Absence due to transportation difficulties is not considered legitimate.

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Week	date	topic	reading	quiz/test
1	8/29	introduction	both prefaces	
	8/31	EIMS instrumentation and initial considerations	1.1-4	
	9/2	elemental analysis, IHD, and hydrocarbon fragmentation	1.5,6	
2	9/5	EIMS of various functionality	1.6	
	9/7	as above	1.6	
	9/9	MS probz	-	
3	9/12	IR theory	2.1-4	
	9/14	IR of hydrocarbons	2.5-6	Quiz 1
	9/16	IR of other functional groups	3.6	
4	9/19	as above	3.6	
	9/21	as above *(in lab Thursday*)	3.6	
	9/23	practice problems	-	
5	9/26	practice problems	-	
	9/28	Q/A	-	Exam 1
	9/30	NMR review	221 lab manual	(in lab)
6	10/3	practice problems	3.1	
	10/5	quantum NMR theory	3.2	
	10/7	classical NMR theory	3.2,3	
7	10/10	chemical shift (CH)	3.4	
	10/12	coupling phenomena	3.5	Quiz 2
	10/14	chemical shift equivalence and molecular topology	3.8,9,12	
8	10/17	more coupling issues	3.10,11	
	10/19	Karplus, long range coupling	3.13,14	
	10/21	protons on heteroatoms	-	

9	10/24 practice problems	3.6	
	10/26 ^{13}C basic principles	3.17	
	10/28 Long Weekend	4.1,2	
10	10/31 ^{13}C-decoupling	4.3-5	
	11/2 Q/A	-	Exam 2
	11/4 calculation of ^{13}C chemical shifts	4.7	(in lab)
11	11/7 calculation of carbon chemical shifts	4.7	
	11/9 ^{13}C resonances for various functionality	4.7	
	11/11 same, DEPT	4.7,6	
12	11/14 problems	-	
	11/16 problems	-	
	11/18 2-D NMR theory	5.1,2	Quiz 3
13	11/21 2-D NMR techniques.....	5.3-6	
	11/23 Tgiving		
	11/25 Tgiving		
14	11/28 more 2D techniques	5.3-6	
	11/30 more 2D techniques	5.3-6	Exam 3
	12/2 spectral problems using 2D techniques	7	(in lab)
15	12/5 spectral problems using 2D techniques	7,8	
	12/7 spectral problems using 2D techniques	8	
	12/9 review	-	

12/12-12/16 **f i n a l e x a m s**

442 LAB SCHEDULE (FALL 2011)

Starting Date	Experiment [points], (due date)	Reference	Required Characterization
9/1	Check-in, Spectral Identification of an Unknown [40 points], (Th, 9/22)	handout	EIMS, CIMS, IR, ^{1}HNMR
9/8	as above		
9/15	as above		
9/21 (Wednesday)	Rxns of Alcohols with Calcium Hypochlorite [40 points], (Th, 10/24)	handout	IR, ^{1}HNMR, ^{13}CNMR, EIMS CIMS
9/28	**Exam 1**	-	-
10/6	more Rxns of Alcohols….		
10/13	as above		
10/20	Experimental Smorgasbord[@] [40 points], (Th, 12/8)	handouts	IR, ^{1}HNMR, EIMS, CIMS COSY, DEPT
10/27	more Smorgasbord	-	-
11/3	**Exam 2**		
11/10	more Smorgasbord		
11/17	more Smorgasbord		
11/24	Tgiving	-	-
12/1	**Exam 3**		
12/8	Check-out	-	-

[@] One from:

1. The Reaction of Cinnamyl Alcohol with Triethyl Orthoacetate
2. A View to Acrylate.
3. The Reaction of Oct-3-en-1-ol with Triethyl Orthoacetate
4. The Reaction of Styrene with Formaldehyde in Acid
5. The Reaction of Furfuraldehyde with Cyclopentanone
5. The Reaction of Tetrahydrofuran with Acetyl Bromide
6. The Reaction of Non-3-yn-1-ol with Formic Acid and p-Touenesulfonic Acid
7. The Reaction of Non-3-yn-1-ol with Formic Acid
8. The Reaction of 1-Methylcyclohexanol with Bromine and Potassium Carbonate

details will follow.....