

Interpretation of Organic Spectra

Chm 515/415 - Fall 2016

Instructor: Dr. Ralf Warmuth

Office: W380; Phone: (848) 445 8432; E-mail: warmuth@rutgers.edu

Time: Monday and Wednesday, 10:20 am – 11:40 am; Room WL-260

(1st lecture: 9/7/16; last lecture: 12/12/16)

Required Text: ‘Organic Structural Spectroscopy, Lambert, Gronert, Shurvell, Lightner, Prentice Hall, 2nd Ed., 2011; ISBN: 9780321592569

Overview: Use of nuclear magnetic resonance, mass spectrometry, infrared and ultraviolet spectroscopy for the identification of organic compounds and the elucidation of organic reaction mechanisms. A basic understanding of mechanistic and structural organic chemistry is required.

Exams: Three exams will be given during a lecture period. Each contributes 25% to your grade (200 points, total 800 points for the course). The first exam will cover mass spectrometry and some 1D-NMR spectroscopy. The second exam will cover 1D & 2D NMR spectroscopy and will also require knowledge in mass spectrometry. To solve the problems of the third exam, knowledge in all techniques discussed during the semester is needed (MS, NMR, IR, UV/Vis). You may use a calculator during the exams, but not a computer device or the internet.

Exam I	10/10	10:20 am – 11:40 am	Lectures 1-8	9/7 – 10/3
Exam II	11/7	10:20 am – 11:40 am	Lectures 9-16	10/5 – 11/2
Exam III	12/14	10:20 am – 11:40 am	Lectures 17-25	11/9 – 12/12

Quizzes: Five unannounced quizzes (15 min; 10 points each) will be given at the beginning of a lecture period. The lowest score will be dropped. These quizzes will cover the material discussed in the previous lecture. You may use a calculator during the quizzes, but not a computer device or the internet. No make-up quizzes.

Take Home Quizzes: Several take home quizzes will be given (150 points total). They can be downloaded after a Thursday lecture (announcement during class and via e-mail) and are due at the beginning of the following Monday lecture. The answers to the questions will be discussed during the Monday lecture (with student participation). For the take home quizzes, you may use any library resource (books, journals), your lecture notes or text book, or any resource on the www. But you can't take help from others and have to solve the problems on your own.

Course Web Site: sakai.rutgers.edu; ‘INTERP OF ORG SPECTR 01 F16’

Handouts: Handouts that accompany the lectures can be downloaded from the course web page as they become available. A copy of this syllabus also has been posted

Practice Problems: A number of problems that can be found at the end of each book chapter will be assigned. It is recommended, that you work through these problems, which will aid your understanding of the material and will help prepare you for the exams. Some of these problems may be part of a lecture quiz or take home quiz.

Topics of Interpretation of Organic Spectra

<i>Topic</i>	<i>Chapter</i>	<i>Pages</i>	<i>Suggested Problems*</i>
Mass Spectrometry		224-324	
Instrumentation	7		7.1-4
Fragmentation and Ionization	8		8.1-4; 8.5a,b
Interpretation of Mass Spectra	9		9.1b,9.2-4
NMR Spectroscopy		1-221	
Basics & Theory	2		2.1-4
Chemical Shift	3		3.1-5, 3.6a-f
Coupling Constants	4		4.1-5,7-8,12-13,15a-c,16,18,21
1D NMR spectroscopy	5		5.1,2,4,5,8,10-12,14,16,17
2D NMR spectroscopy	6		6.1a-g; 6.2-6,10
Infrared Spectroscopy		326-395	
Basics & Theory	11		11.1-3
Group Frequencies	12		12.1-10
UV/Vis Spectroscopy		398-444	
Basics & Theory	13		13.1-8
Structural Analysis	14		14.1-3,6-8,9a-e,12,13,16,19,20
Circular Dichroic Spectroscopy (if time permits)		Handout	
Combined Methods	15	446-518	15.1-24

*) Answers to problems will be posted on sakai course site. Selected problems will be solved during a lecture period