# SPECTROSCOPIC METHODS AND ANALYSIS OF SPECTRA

**The University of Toledo**

**Department of Chemistry & Biochemistry, College of Natural Sciences**

**CHEM 4330/6330/8330**

**CRNs 17272/11225/14469**

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**Office Hours**: By Appt (In Office or Blackboard)

**Office Location**: WO 3266B

**Instructor Phone**: (419)530-1524

**Offered**: Spring 2021

**Class Location**: BO 2059 **Class Day/Time**: TR 8:00-9:50 AM

**Lab Location**: N/A

**Lab Day/Time**: N/A **Credit Hours**: 4

 **CATALOG/COURSE DESCRIPTION**

*A comprehensive study of theory and instrumentation. Applications of spectroscopic methods including spectral interpretation. Topics include a study of absorption, emission, Raman, NMR, ESR, mass spectrometry, and related subjects. Important methodology and strategy in organic synthesis including disconnection and retrosynthetic analysis.*

**STUDENT LEARNING OUTCOMES**

*By the end of the course, you should:*

* *Be familiar with the instrumentation available for performing characterization of (predominately) organic molecules, with emphasis on those instruments available at UToledo.*
* *Be capable of explaining in lay terms how different instruments function.*
* *Understand the different types of experiments capable from the various characterization instruments.*
* *Be capable of diagnosing and applying the appropriate characterization techniques for a specific sample.*
* *Demonstrate competence in spectral data interpretation.*

## PREREQUISITES AND COREQUISITES*For those in CHEM 4610: CHEM 2410 WITH MIN. GRADE OF C*

*None for CHEM 6610/8610*

## “REQUIRED” INSTRUCTIONAL MATERIALS (TEXTS AND ANCILLARY MATERIALS)

*Silverstein, R. M.; Webster, F. X.; Kiemle, D. J.; Bryce, D. L. Spectrometric Identification of Organic Compounds, 8th Ed., Wiley; 2015. ISBN 978-0-470-61637-6.*

**TECHNOLOGY EXPECTATIONS**
*We will work problems during class, which will require having access to a laptop (or to dial in from a desktop). Software will be provided as needed for these activities.*

### UNIVERSITY POLICIES

### *Policy Statement on Non-Discrimination on the basis of Disability (ADA): The University is an equal opportunity educational institution. Please read* [*The University’s Policy Statement on Nondiscrimination on the Basis of Disability Americans with Disability Act Compliance*](http://www.utoledo.edu/policies/administration/diversity/pdfs/3364_50_03_Nondiscrimination_o.pdf)*.*

**ACADEMIC ACCOMODATIONS***The University of Toledo is committed to providing equal access to education for all students. If you have a documented disability or you believe you have a disability and would like information regarding academic accommodations/adjustments in this course please contact the* [*Student Disability Services Office*](http://www.utoledo.edu/offices/student-disability-services/index.html)*.*

## COURSE EXPECTATIONS

*Grades for this course will be based on three exams. There will be several in-class activities, so your attendance will be beneficial to your success in this course. If you would prefer to “dial-in” you may do so.*

## OVERVEW OF COURSE GRADE ASSIGNMENT

*Everyone’s grade in this course will be based on three exams (200 pts each) and classroom participation (100 pts). Worksheets will be provided with extra practice opportunities, but these will not be for a grade. For CHEM 6330/8330 students, an additional requirement will be to provide an evaluation of reported experimental data (50 pts).*

***Midterm Grading****Midterm grades will be based on the first mid-term.*

***Final Grading****A: >85% A-: 80-84% B+: 75-79% B: 70-74% B-: 66-69% C+: 63-65%
C: 60-62% C-: 57-59% D+: 54-56% D: 51-53% D-: 48-50% F: <48%*

## DATES FOR GRADED ITEMS

*Exam I: February 11th (8:00-9:50)
Exam II: March 25th (8:00-9:50)
Exam III: May 4th (8:00-10:00)
Experimental Evaluation Due: May 7th (23:59)*

## ACADEMIC SUPPORT SERVICES

*The University of Toledo has many resources for those in need, including the Learning Enhancement Center, the Counseling Center, and the Disability Services Office. If you are in need of any additional support during this course, please feel free to see me, and I can direct you to the appropriate resource.*

## SAFETY AND HEALTH SERVICES FOR UT STUDENTS

*For a comprehensive list of these, please see the following document online: (*[*http://www.utoledo.edu/offices/provost/utc/docs/CampusHealthSafetyContacts.pdf*](http://www.utoledo.edu/offices/provost/utc/docs/CampusHealthSafetyContacts.pdf)*).*

**Tentative Lecture Schedule**

**Date Lecture Topic**

January 19 Mass Spectrometry (Intro, Ionization, Fragmentation)

January 21 Mass Spectrometry (Ionization Cont., Experiments)

January 26 Mass Spectrometry (Experiments Cont., Reporting)

January 28 Vibrational Spectroscopy: Infrared and Raman

February 2 UV/Vis Spectroscopy

February 4 Fluorescence, Chirality and Spectroscopy (Circular Dichroism)

February 9 X-Ray and Microwave Spectroscopies

February 11 **Exam I**

February 16 *Instructional Break*

February 18 Nuclear Magnetic Resonance (Introduction, Simple 1D Experiments)

February 23 Nuclear Magnetic Resonance (Advanced 1D Experiments)

February 25 Nuclear Magnetic Resonance (Breaking Down NMR Spectra/Interpretation)

March 2 Nuclear Magnetic Resonance (Solvents)

March 4 Nuclear Magnetic Resonance (Advanced Coupling Analysis)

March 9 Nuclear Magnetic Resonance (Quantitation)

March 11 Nuclear Magnetic Resonance (Reporting)

March 16 Nuclear Magnetic Resonance (Biomolecules)

March 18 Nuclear Magnetic Resonance (Dynamics)

March 23 Nuclear Magnetic Resonance (Dynamics Continued)

March 25 **Exam II**

March 30 2D NMR (COSY)

April 1 2D NMR (NOESY/ROESY)

April 6 2D NMR (TOCSY)

April 8 2D NMR (HSQC)

April 13 2D NMR (HMBC)

April 15 2D NMR (Other Heterocorrelations)

April 20 2D NMR (DOSY)

April 22 Make-Up (or Other Topics)

April 27 Make-Up (or Other Topics)

April 29 *Instructional Break*