# 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**: M 11-12, T 10-12, R 10-12 (In Office or Blackboard)

**Office Location**: WO 3266B

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

**Offered**: Spring 2022

**Class Location**: BO 2059 **Class Day/Time**: TR 8:30-9:50 AM\*

**Lab Location**: N/A

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

\*Course Is Partially Flipped

**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 able to:*

* *Describe the instrumentation available for performing characterization of (predominately) organic molecules, with emphasis on those instruments available at UToledo.*
* *Explain in lay terms how different instruments function.*
* *Describe the different types of experiments capable from the various characterization instruments.*
* *Diagnose and apply the appropriate characterization techniques for a specific sample.*
* *Demonstrate mastery in spectral data interpretation.*
* *Apply characterization data towards the elucidation of crude reaction mixtures.*
* *Quantitate pure or compound mixtures based on available spectrometric data.*

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

*For those in CHEM 6610/8610: Admission to the appropriate graduate program.*

## “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.*

### FLIPPED CLASS

### *To facilitate problem solving, much of the lecture material for this course will be recorded and posted, leaving time in class to work problems together. As a result of this shift away from traditional lecture utilization, we will begin class at 8:30 rather than 8:00 am. It is expected that you will watch the lectures ahead of time, as our classroom activities will frequently make use of material from the previous lectures.*

### 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, in-class activities, and watching the lecture videos ahead of time. There will be several in-class activities, for which you will receive participation credit. If you lose points for any reason on these activities, you will be informed so that you may improve your performance. Missing the lecture period without an excused absence will result in loss of points. Due to COVID-19, lecture activities can be performed using Blackboard Collaborate to ensure you can participate safely while in quarantine.*

## OVERVEW OF COURSE GRADE ASSIGNMENT

*Everyone’s grade in this course will be based on three exams (100 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 10th (8:00-9:50)  
Exam II: March 24th (8:00-9:50)  
Exam III: May 3th (8:00-10:00)*

## 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 18 Mass Spectrometry (Intro, Ionization, Fragmentation)

January 20 Mass Spectrometry (Ionization Cont., Experiments)

January 25 Mass Spectrometry (Experiments Cont., Reporting)

January 27 Vibrational Spectroscopy: Infrared and Raman

February 1 UV/Vis Spectroscopy

February 3 Fluorescence, Chirality and Spectroscopy (Circular Dichroism)

February 8 X-Ray and Microwave Spectroscopies

February 10 **Exam I**

February 15 Nuclear Magnetic Resonance (Introduction, Simple 1D Experiments)

February 17 Nuclear Magnetic Resonance (Advanced 1D Experiments)

February 22 Nuclear Magnetic Resonance (Breaking Down NMR Spectra/Interpretation)

February 24 Nuclear Magnetic Resonance (Solvents)

March 1 Nuclear Magnetic Resonance (Advanced Coupling Analysis)

March 3 Nuclear Magnetic Resonance (Quantitation)

March 8 *No Class (Spring Break)*

March 10 *No Class (Spring Break)*

March 15 Nuclear Magnetic Resonance (Reporting)

March 17 Nuclear Magnetic Resonance (Biomolecules)

March 22 Nuclear Magnetic Resonance (Dynamics)

March 24 **Exam II**

March 29 2D NMR (COSY)

March 31 2D NMR (NOESY/ROESY)

April 5 2D NMR (TOCSY)

April 7 2D NMR (HSQC)

April 12 2D NMR (HMBC)

April 14 2D NMR (Other Heterocorrelations)

April 19 2D NMR (DOSY)

April 21 Make-Up (or Other Topics)

April 26 Make-Up (or Other Topics)

April 28 Make-Up (or Other Topics)