Chem-T 530, Organic Spectroscopy

Instructor: Mohammad Hossain, Ph. D.
Indiana University Kokomo

Credit Hours: 3

Campus: IU Kokomo

Professor Name: Mohammad Hossain

Professor Contact Information: mohass@iuk.edu, 765-455-9482, Virtual office hours by appointment

Semester: Full Fall 2022

Dates of Course: 8/22/2022-12/16/2022

Course Format: Asynchronous Online

Course description:

Determination of molecular structure is one of the central themes of organic chemistry. For this purpose, chemists today rely almost exclusively on spectral methods or spectroscopy. Organic spectroscopy is introduced in undergraduate organic chemistry classes, but students only see the proverbial "tip of the iceberg" in their undergraduate classes. This course is intended to give students a more complete picture of how spectroscopic methods are used to elucidate the structure of complex organic molecules. Topics that will be covered include infrared (IR), mass spectroscopy (MS), nuclear magnetic resonance (NMR), and UV-visible spectroscopy. In this course, we will first develop basic understanding of various theories behind IR, MS, and NMR spectroscopy, and then we will concentrate on the interpretation of spectra and the information they can provide about details of molecular structure.

Student Learning Outcomes:

Upon completion of Organic Spectroscopy (Chem T530), students will be able to:

- Describe how the molecular formula of a compound is determined and how structural information may be obtained from that formula.
- Describe the physical and chemical changes that occur at the molecular level during a MS, IR, or NMR experiment.
- Identify different functional groups present in organic compounds using IR spectra.
- Describe major fragmentation patterns of organic compounds using mass spectra.
- Describe common terms in NMR spectroscopy such as chemical shift, coupling constant, and anisotropy, and describe how they are affected by molecular structure.

- Analyze and interpret 1D- ^{1}H and ^{13}C NMR as well as 2D NMR to determine chemical structure of organic compounds.
- Analyze and interpret UV-visible spectra for compounds containing conjugated double bonds.
- Integrate all spectral data (MS, IR, UV and/or NMR) of a compound to elucidate the structure of an organic molecule.

Course Contents:

In this semester, we will cover the followings:

- Vibrational spectroscopy techniques including IR and Raman spectroscopy.
- A much more detailed discussion of mass spectrometric methods will be presented. This includes discussion of various ionization and mass filter methods. In addition, treatment of high-resolution MS data and fragmentation pattern analysis will also be discussed in depth.
- A more detailed discussion of the nuclear magnetic resonance phenomenon at the molecular level.
- A variety of NMR spectroscopic methods will be discussed including more detailed treatments of basic 1H-NMR and ^{13}C-NMR spectroscopy, as well as other techniques, e.g. DEPT, COSY, HETCOR, HMQC, NOESY, and other more complex techniques. NMR spectroscopy of other common NMR-active nuclei (e.g. 19F & 31P) will also be discussed.
- Electronic (UV-visible) spectroscopic techniques.
- In addition, students will be given ample practice in the use of these spectroscopic techniques in determining the structure of complex organic molecules.

Course Materials:

Required Text:

- **Introduction to Spectroscopy**, 5th ed. by Pavia, et al. (ISBN 978-1-285-46012-3). The book can be purchased online at Amazon or any of the other usual places. A link to the Amazon page for the text is provided here.
- You also should have access to an undergraduate organic text (Brown, Solomons, etc.) to review basic organic concept.

Required Supplementary Readings:

- Supplementary readings from the chemical literature will be posted on canvas. You are expected to download these files and read them thoroughly.

Optional text:

- Spectrometric Identification of Organic Compounds, 8th ed. by Silverstein, et al. (ISBN 978-0-470-61637-6).

Assessment:

Student performance in this course will be evaluated through exams, quizzes, assignments, discussion, and a comprehensive final exam.

The approximate distribution for each category is as follows:

Category	**Weighted Percentage**
VoiceThread Introduction	2%
Exams	30%
Quizzes	15%
Assignments	20%
Discussion	15%
Final project and presentation	18%
Total	100%