CHEM 747 – Molecular Spectroscopy and Structure
Dr. Fabien Goulay
Fall 2021

Lecture: CHEM747 Section 001, 3 credit hours

Lectures will be held on Monday, Wednesday and Friday between 1:30–2:20 in Clark Hall, Room 414.

Learning objectives: In this class we will use the basic principles of physical chemistry, quantum mechanics and classical electrodynamics to understand, analyze and predict the spectra of molecules. The material is intended to be relevant to those with an interest in spectroscopy of both gas- and condensed-phase systems. We will review the most relevant topics from quantum mechanics and classical electrodynamics before proceeding to molecular spectroscopy and its applications. The final unit of the course will be dedicated to lasers and laser spectroscopy. Real research problems will be used to illustrate the topics we cover in lectures.

Learning outcomes: After completing the course, the student will grasp the fundamental principles of quantum mechanics and be able to apply them to understand and predict the spectra of atoms and molecules over a very wide range of wavelengths.

Tentative Course Outline

1. Introduction and overview
   1.1. Macroscopic view of light-matter interaction
   1.2. Effect of energy quantization
   1.3. Units and dimensions
2. Light and its interaction with matter
   2.1. Electromagnetic waves
   2.2. Black body radiation and photon energy
   2.3. Quantum description of matter (Q-Chemistry review)
   2.4. Interaction of light with matter
3. Atomic spectroscopy
   3.1. The hydrogen atom (Review)
   3.2. Poly electronic atoms
   3.3. Atomic term symbols
   3.4. Selection rules and atomic spectra
4. Rotational spectroscopy
   4.1. The rigid rotor
   4.2. Rotational levels and transition rules
   4.3. Pure rotational spectra of molecules
5. Molecular symmetry (Review only)
   5.1. Symmetry operations
   5.2. Point groups
   5.3. Character tables
   5.4. Total representation of a group
   5.5. Symmetry and dipole moment
6. Vibrational spectroscopy
   6.1. Diatomic molecules
   6.2. Polyatomic molecules
7. Electronic transitions of polyatomic molecules
   7.1. Molecular orbitals and term symbols
   7.2. Rovibronic transitions
   7.3. The Franck-Condon principle
   7.4. Photoelectron spectroscopy
8. Laser spectroscopy
   8.1. Introduction and historic
   8.2. Principles of operation
   8.3. Different types of lasers
   8.4. Laser techniques

Recommended textbooks

No textbook is required for this course as no single text overlaps fully with the material that will be covered. The following books are recommended:
J. M. Hollas – *Modern Spectroscopy*, 4nd Edition (Wiley, 2009)
R. Kakkar – Atomic and Molecular Spectroscopy: Basic concepts and applications, Cambridge University Press, 2015
D. Harris and M. Bertolucci – *Symmetry and Spectroscopy: An Introduction to Vibrational and Electronic Spectroscopy*, Dover Publications, New York, 1978.
D. A. McQuarrie, *Mathematics for Physical Chemistry*, University Science Books.

Notable dates:

08/18	First day of class	11/15	Due date for homework 2
09/06	Labor day, no class	11/22	Thanksgiving break
09/20	Due date for homework 1	11/24	Thanksgiving break
10/06	No class	11/26	Thanksgiving break
10/08	Fall break	12/09	Last day of class
10/11	Midterm exam	12/8-10	Take home final exam

Grading

Attendance is mandatory for CHEM 747. Poor attendance may result in a lower grade for the course.

Grades are based on performance assessments that reflect achievement of learning outcomes outlined for this course.

Grade Formulation:

Homework 1	15 % of final grade
Homework 2	15 % of final grade
Midterm Exam	30 % of final grade
Final Exam	40 % of final grade

Homework assignments: Students are assigned two homework assignments throughout the duration of the semester. They are assigned one week before the due date. In order to receive credit, students must provide full detail, including unit analysis, mathematical derivation, and insightful justification (essay format) unless otherwise noted. Illegible work will be given a score of 0 %.

Homework submission: All homework assignments are to be submitted electronically, either via email or eCampus. Scans or photos of handwritten assignments are acceptable as long as they are readable. Further instructions will be provided before the due dates.

Midterm: The midterm exam will cover the first half of this course. It will consist of several problem sets. The exam will be written in class and last from 1 to 2 hours.

Final exam: The final exam will cover the integrality of this course. It will consist of several problem sets.

Homework assignments and exams are to be completed **independently**.

Make-up Policy: Absences/makeups will be dealt with on an individual basis. Please contact the instructor as soon as possible. No make-up exams will be given after the test has been discussed in class. Homework assignments are due on the specified date. Extensions will be given for appropriately excused absences as outlined above.

Plagiarism: Plagiarism in any of the assignments will results in a ***F grade*** for the entire class. See https://www.libraries.wvu.edu/instruction/plagiarism/ for further information on plagiarism.

Syllabus Statements

Inclusivity Statement:

The West Virginia University community is committed to creating and fostering a positive learning and working environment based on open communication, mutual respect, and inclusion.

If you are a person with a disability and anticipate needing any type of accommodation in order to participate in your classes, please advise your instructors and make appropriate arrangements with the Office of Accessibility Services. (https://accessibilityservices.wvu.edu/)

More information is available at the Division of Diversity, Equity, and Inclusion (https://diversity.wvu.edu/) as well. [adopted 2-11-2013]

Days of Special Concern: WVU recognizes the diversity of its students and the needs of those who wish to be absent from class to participate in Days of Special Concern, which are listed in the Schedule of Courses. Students should notify their instructors by the end of the second week of classes or prior to the first Day of Special Concern, whichever is earlier, regarding Day of Special Concern observances that will affect their attendance. Further, students must abide by the attendance policy of their instructors as stated on their syllabi. Faculty will make reasonable accommodation for tests or field trips that a student misses as a result of observing a Day of Special Concern.

Students withdrawing from courses: Students may withdraw from courses without a W being placed on their record through the end of the first week of the semester. They may withdraw with a W from the end of the first week through the end of the 10th week of the semester. Students must withdraw from courses themselves through the STAR system.