CHM6490:
Introduction to Molecular Spectroscopy

Spring 2020 16H7(11137) 3 credit hours

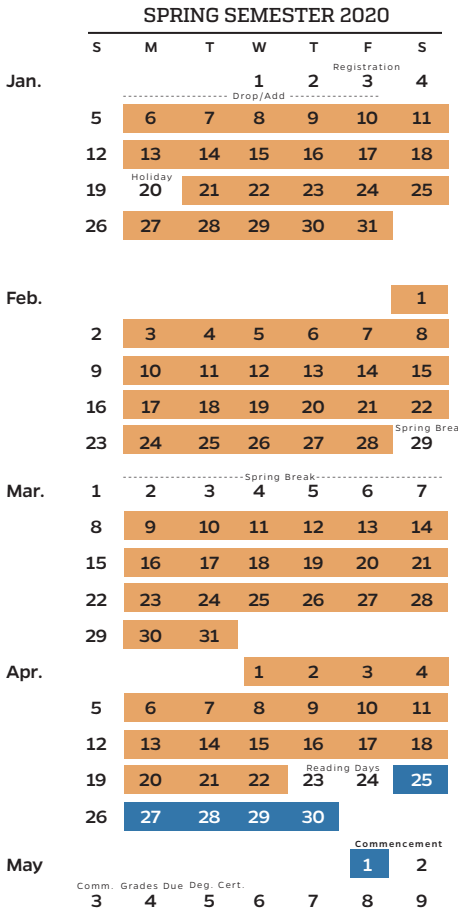
T Period 2 R Periods 2-3 FLI109

Instructor: PJ Brucat

- Office location: CLB311
- Scheduled (group) office hours (tentative):
  Tuesdays per 4 (10:40-11:30)
  Thursdays per 6-7 (12:50-14:45)
- Private office hours:
  by Appointment, offer *three* choices (see below)
- Contact method: *Canvas Messaging only*

Course Website: https://ufl.instructure.com/courses/387460/
All course materials, course communications, and many assessments will be delivered from within UFs eLearning system (Canvas) at the URL above. Please become familiar with our course website as soon as possible. Note that some of the materials there will be subject to change, so pay attention to all announcements. It is suggested that printing or static downloads of the content be avoided.

Attendance Your prompt attendance at all our scheduled class times is required. If you are unable to make a class for some reason, please message the Instructor (within Canvas) before the scheduled class time. Excused absences are defined by University attendance policy. Unexcused absences will result in grade penalties at the discretion of the Instructor.



Requirements:

- Students are expected to have a mastery of Physical Chemistry, (Quantum Mechanics specifically) at a level concomitant with a Bachelor of Science degree in Chemistry. Students without a strong background will be expected to self-remediate under the guidance of the instructor.
- Basic programming skills and familiarity with computational platforms such as Python, *Mathematica*, or equivalent will be assumed. Alternate equivalent technologies may be chosen but are not supported by the course material. Students lacking this requirement will be expected to acquire these skills with the assistance of the instructor.

No specific textbook is required. However, students are expected to have access to text resources of the following types

- An undergraduate PChem text such as: Physical Chemistry, P. W. Atkins, or similar titles by McQuarrie & Simon, Levine, Raff, Castellan, *etc.*
- Classic texts on the topic of molecular spectroscopy (These all should be available on course reserve at Marsten Library.
  - Steinfeld, J. I., "Molecules and Radiation: An Introduction to Modern Molecular Spectroscopy", 2ed, (Dover, 2005).
  - Herzberg, Gerhard, "Molecular Spectra and Molecular Structure, Vol I-III", (D. Van Nostrand Company, 1950)
  - Townes and Schawlow, "Microwave Spectroscopy" (Dover, 2012)
  - McHale, J.L., "Molecular Spectroscopy" (Prentice Hall, 1999).
  - Hollas, J.M., "Modern Spectroscopy", 4ed (Wiley, 2004).
  - Engel, T., "Quantum Chemistry and Spectroscopy" (Prentice Hall, 2010).
  - Banwell, C.N., McCash, E.M., "Fundamentals of Molecular Spectroscopy" 4ed., McGraw-Hill, 1994).
- An advanced (graduate level) Quantum text
  - C. Schatz and M. A. Ratner Quantum Mechanics in Chemistry, (Prentice Hall, 1993). Chapter 9 of this book provides an introduction to the time-dependent approach to spectroscopy.
  - Levine, I.N., "Quantum Chemistry", 6ed (Prentice Hall, 2009).
  - Fayer, M.D., "Element of Quantum Mechanics" (Oxford University Press, 2001).
  - Atkins, P.W. and Friedman, R.S., "Molecular Quantum Mechanics" (Oxford University Press, 2005).

Course Goals: Successful completion of this course will enable the learner to

- Diagnose and Exploit the underlying Quantum Mechanical Principles in the Analysis of Molecular Spectra
- Utilize a new Perspectives on the Concepts of Coherence, the Act of Measurement, Entanglement, and other Quantum phenomena to properly apply existing, and potentially develop new, Spectroscopic Techniques.
- Become a Better Scientist

Course Objectives: Mastery of the course material will be assessed in the following areas

- Derive Quantitative Relationships in the context of the Semiclassical Interaction of Light with a Quantized Molecular System
- Apply the Approximate Separability of Motion to the Simplification the Description of Molecular Properties.
- Utilize Point Group Symmetry to Derive Spectroscopic Selection Rules.
- Master the Analysis of Common Spectroscopic Methods (UV-Vis, IR/Raman, $\mu\lambda$, NMR, *etc.*)
- Identify and apply appropriate approximate methods to QM Problems

Course Operation and Philosophy The structure of the course consists of physical meetings twice a week. Some of this time will be used for traditional lecture, some for group discussion, and some for working problems. However, the most significant portion of our efforts (2/3) will be apportioned outside of these meeting times, asynchronously reading papers and textbooks, solving problems, and analyzing and simulating spectra.

Communication with your Instructor All course communications with your Instructor are to occur within the Canvas environment using the embedded Announcement, Discussion, or Messaging tools (all grade-related discussion should exclusively use Canvas Messaging directly to the Instructor). Your Canvas account profile must be configured for immediate automatic notification of course announcements and course communications via the individuals preferred communication/email method. Do this now. Responsibility for receiving and responding to electronic course communication in a timely fashion is entirely that of the student.

Office Hours and Scheduled Meetings Regularly-recurring office hours are intended for general and group discussion so of course concepts. Individual student-scheduled office hours are intended for one-on-one discussion of a students standing in the class (grades), learning strategy and habits, remediation of specific hindrances to individual learning, and any other things not appropriate for group discussion. These latter, private discussions will be held at times you arrange. If you want a meeting of this sort, message (from within Canvas, only) **3 options** for meeting times that are convenient for you, and your instructor will reply with a choice that works best with a location for the meeting. *Make sure to include at least three distinct time options in your request message.*

Regrades You have the right to ask for any assignment to be regraded if you suspect an error. Regrade requests must be received by the Instructor within 72 hours of the grade posting. Regrades will be performed only on the entire assignment. Since the process of regrading is to correct errors and make all grading consistent and fair, the grade may either increase or decrease as a result. Regrade requests must all be accompanied by a Canvas message.

Course Activity Types

Lecture Review After each lecture, there will be a Community Review assignment delivered in VoiceThread. The assignment will typically be to post comments on the lecture notes displayed, but other activities may be requested. Read the assignment instructions for details.

CourseWork (CW) Illustrative examples and problems related to the course content will be regularly assigned and turned in for a grade. Some of these will require graphing or computation.

Course Grade Computation: Course grades will be computed from the weighted-average of the earned percentages of each graded item submitted by the student. The weighting factors are as follows:

Category Weights

Grade Category	weight %
Lec Review	10
CourseWork	90

Grade Percentages

Grade	A	A−	B+	B	B−	C+	C	D	E
Minimum percentage	87.5	80.0	77.5	72.5	70.0	67.5	60.0	50.0	< 50.0

UF's Grading Policy: See http://www.registrar.ufl.edu/grades/gradepolicy.html and https://catalog.ufl.edu/ugrad/current/regulations/info/grades.aspx

Honesty and Truthfullness: Ethical, moral, and professional behavior is expected and required of all participants in this course. Moreover, all participants in UF's Academic activities are bound by Rules of Conduct, from which can be found:
"UF students are bound by The Honor Pledge which states,
'We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honor and integrity by abiding by the Honor Code.'
On all work submitted for credit by students at the University of Florida, the following pledge is either required or implied:
'On my honor, I have neither given nor received unauthorized aid in doing this assignment'
The Honor Code (http://www.dso.ufl.edu/sccr/process/student-conduct-honor-code/) specifies a number of behaviors that are in violation of this code and the possible sanctions. Furthermore, you are obligated to report any condition that facilitates academic misconduct to appropriate personnel. If you have any questions or concerns, please consult with the instructor or TAs in this class"

Accommodations: Students with disabilities requesting accommodations should first register with the Disability Resource Center (352-392-8565, www.dso.ufl.edu/drc/) by providing appropriate documentation. Once registered, students will receive an accommodation letter which must be presented to the instructor when requesting accommodation. Students with disabilities should follow this procedure as early as possible in the semester.

Counseling: Useful non-academic services are available in many forms at UF. A good source of information is the Counseling and Wellness Center: http://www.counseling.ufl.edu/cwc/

GatorEvals:"Students are expected to provide professional and respectful feedback on the quality of instruction in this course by completing course evaluations online via GatorEvals. Guidance on how to give feedback in a professional and respectful manner is available at https://gatorevals.aa.ufl.edu/students/. Students will be notified when the evaluation period opens, and can complete evaluations through the email they receive from GatorEvals, in their Canvas course menu under GatorEvals, or via https://ufl.bluera.com/ufl/. Summaries of course evaluation results are available to students at https://gatorevals.aa.ufl.edu/public-results/."

All course policies and procedures are subject to change at any time at the sole discretion of Brucat

We, the members of the University of Florida Community, pledge to hold ourselves and our peers to the highest standards of honesty and integrity

— PJ Brucat 01/01/2020 —