# CHM6490:
# Introduction to Molecular Spectroscopy

Spring 2019 3 credit hours

T Period 4 R Periods 3-4 FLI109

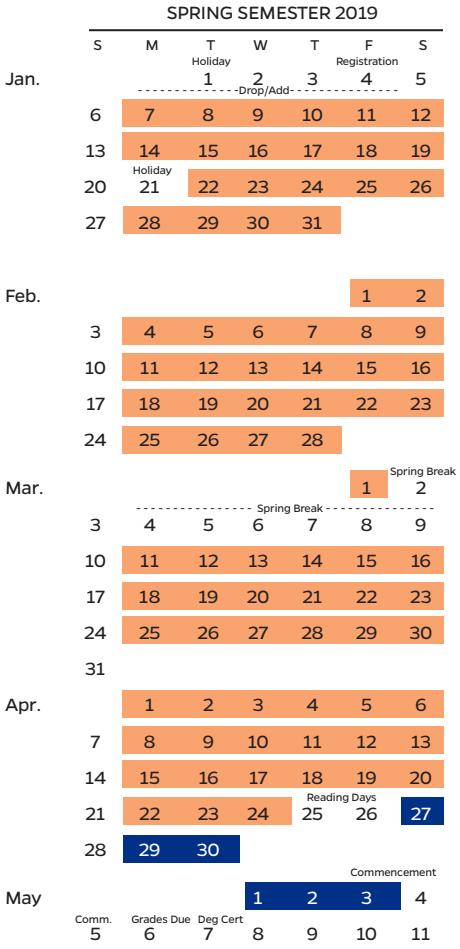
**Instructor**: PJ Brucat

- Office location: CLB311
- Scheduled (group) office hours (tentative):
  Mondays 11:15-12:30 CLB313,
  Wednesdays 13:55-14:45 CLB313
- Private office hours:
  by Appointment, offer *three* choices (see below)
- Contact method: *Canvas Messaging only*

**Course Website**: https://ufl.instructure.com/courses/359368/
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.

**Accommodations**: Students with disabilities may request special accommodations through the Dean of Students. https://drc.dso.ufl.edu/




**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 availbale 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 Anaylsis 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 ourside of these meeting times, asynchronously reading papers and textbooks, solving problems, and analysing 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 indended 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.

**Exams** There will be two in-class exams during the term. These are typically 5-6 page white-space closed-book tests, with a page or two of given information (fact sheet) to assist your work. These Exams will be graded and reviewed in class by your instructor.

All activity dates and grades are posted in Canvas. Assignments *must* be submitted in full by the assignment deadline for credit.

**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 | 40 |
| Exams | 50 |

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**: http://www.registrar.ufl.edu/grades/gradepolicy.html
**Honesty and Truthfullness**: Students, faculty, and all participants in UF's Academic activities are bound by the Honor Code. Moreover, ethical, moral, and professional behavior is expected and required of all participants in this course.
**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/

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 01/03/2019 —