Molecular Spectroscopy and Structure:
CHE 546

Dr. John M Franck office 2-008 CST, jmfranck@syr.edu. Open office hours Tues. 2-3pm and by appointment. If open office hours are not utilized, they will be cancelled, but office hours will *continue to be available by appointment.*

Overview of modules

Most students will take all 3 modules (each is 1 credit):

Overview of Spectroscopy, Scattering, and Structure Tu 8/29 – Tu 9/26

This section will survey various types of absorption and emission spectroscopy, both vibrational and electronic. Upon completion, the student should be familiar with most standard uses of spectroscopy, as well as some basic simulation techniques.

This module has a unique importance, since it will outline several mathematical tools that will be used in the next two modules.

2D Spectroscopy and Magnetic Resonance Th 9/28 – Th 10/26

This module will introduce the concept of modern two-dimensional spectroscopy. It will begin with the concept of pump-probe spectroscopy. After introducing magnetic resonance spectroscopy – both nuclear spin resonance (NMR) and electron spin resonance (ESR or EPR) – it will use magnetic resonance imaging (MRI) to demonstrate 2-dimensional (2D) spectroscopy.

In preparation for the next module, students will then begin to learn the quantum physics that underlies modern spectroscopy. In particular, they will begin by learning the mathematical framework used in magnetic resonance.

Into the Future with Quantum Mechanics Tu 10/31 – Tu 12/7

The framework outlined in the previous module will be expanded, leading to a survey of typical NMR techniques such as COSY, HSQC, and NOESY spectroscopy. This same framework, with some notational differences, will also be applied to two-dimensional laser spectroscopy.

Course Material

We will be using Fundamentals of Protein NMR Spectroscopy by Gordon S. Rule and T. Kevin Hitchens as the primary textbook. Even though this text emphasizes NMR, it clearly lays out fundamental concepts that are applicable to **all of spectroscopy**.

Students should expect to have to read the assigned material and to take notes during class (which will supplement the assigned reading) in order to keep pace with the class.

Demo handouts: when we will be performing an in-class demonstration, you will be provided with a tutorial handout that you will be asked to read and try out ahead of time.

Grading

Grading will be averaged from the following components:

60% of the grade will come from "quizzes" that will be due every Tuesday morning, at the start of class these "quizzes" will include the following:

- standard word problems
- basic simulations with the program Gaussian

- simple programming tasks with Python/Jupyter
- hands-on NMR or ESR experiments

The quizzes will test your retention and understanding of:

- The reading material for the week
- Additional topics covered during lecture
- Material covered in handouts.

40% Of the grade will come from a final problem set. The problem set will be handed out at least 2 weeks before the end of each module. You are encouraged to start work on the problem set **immediately**. The problem sets will be due in the morning one week after the end of each module (Tues Oct 3^{rd}, Thurs Nov 2^{nd}, Thurs Dec 14^{th}).

Tentative Syllabus for Module 1

Date	Day	Lecture #	Topic	Reading Assignment
8/29/2017	Tu	1	The tools, part 1: Linear algebra and dirac notation	Chpt. 4.1-4.5
8/31/2017	Th	2	The tools, part 2: Complex numbers and differential equations – also: numerical arrays	Appendix B, Diff. Eq. handout
Labor day – 4th				
9/5/2017	Tu	3	The toys: The rigid rotor, the harmonic oscillator, and the particle in a box → what's the point?	Chpt. 4.1-4.5
(5th is add deadline)				
9/7/2017	Th	4	Let's get started: IR absorption and Raman	
12th is pass/fail option				
9/12/2017	Tu	5	The rules: Absorption and emission spectroscopy, Beer's law, Einstein coefficients, and Boltzmann probabilities	paper:Hilborn2002
9/14/2017	Th	6	The field: Overview of vibrational techniques: Normal modes + what's the point of point groups?	Handout: Gaussian Simulations
9/19/2017	Tu	7	The tools, part 3: Detection methods, Fourier transform, and lifetime broadening	Appendix A
9/21/2017	Th	8	Crank up the energy and zoom out: UV-Vis and Fluorescence spectroscopy – It's Jablonski time!	
9/26/2017	Tu	9	(Buffer)	

Tentative Syllabus for Module 2

Date	Day	Lecture #	Topic	Reading Assignment
9/28/2017	Th	10	UV-Vis/Fluorescence part 2: pump-probe, time-dependence, and FRET	
10/3/2017	Tu	11	introduction to NMR	Chpt. 1.1-1.5, M+ handout
10/5/2017	Th	12	Quantum mechanical description of NMR	Chpt. 4.6-5.3
10/10/2017	Tu	13	2D imaging techniques – phase encoding and echo-planar	
10/12/2017	Th	14	Density matrix and product operators	Chpt 6
10/17/2017	Tu	15	Density Matrices, part 2	
10/19/2017	Th	16	J-Coupling	Chpt 7
10/24/2017	Tu	17	ESR	Weil + Bolton – Chpt 1-2 (selected)
10/26/2017	Th	18	(Buffer)	

Tentative Syllabus for Module 3

Date	Day	Lecture #	Topic	Reading Assignment
10/31/2017	Tu	19	Coupled spins = product operators	Chpt 8
11/2/2017	Th	20	Derivation of the rotation rules, and introduction of raising and lowering operators	
11/7/2017	Tu	21	COSY and friends	Chpt 9
11/9/2017	Th	22	Overview of 2D spectroscopy techniques: enhanced resolution – tutorial in identification. HSQC, HMQC, NOESY, PRE, DOSY	
11/14/2017	Tu	23	HSQC and friends	Chpt 10
11/16/2017	Th	24	Pulse sequence elements and polarization transfer	Appendix D
11/21/2017	Tu	no class		
11/23/2017	Th	no class		
11/28/2017	Tu	25	Relaxation and cross-relaxation	Chpt 19
11/30/2017	Th	26	Relaxation, part 2	
12/5/2017	Tu	27	What about Lasers? The setup of a 2D experiment – replacing phase cycling with k-vectors.	Handout
12/7/2017	Th	28	(Buffer)	
last day of classes 9th				
final grades due 21st				

Prerequisites

The following prerequisites are strongly recommended:

(1) Two semesters of calculus-based physics

(2) Organic chemistry with an introduction to spectroscopy (CHE 325 /335) or equivalent experience

(3) Physical chemistry that includes an introduction to quantum mechanics

General Information

If you believe that you need accommodations for a disability, please contact the Office of Dis-

ability Services (ODS) located at 804 University Avenue, third floor or go to the ODS website at `disabilityservices.syr.edu` and click current students tab to register on-line. You may also call 315.443.4498 to speak to someone regarding specific access needs. ODS is responsible for coordinating disability-related accommodations and will issue 'Accommodation Letters' to students as appropriate. Since accommodations may require early planning and are not provided retroactively, please contact ODS as soon as possible.

Syracuse University's Academic Integrity Policy reflects the high value that we, as a university community, place on honesty in academic work. The policy defines our expectations for academic honesty and holds students accountable for the integrity of all work they submit. Students should understand that it is their responsibility to learn about course-specific expectations, as well as about university-wide academic integrity expectations. The policy governs appropriate citation and use of sources, the integrity of work submitted in exams and assignments, and the veracity of signatures on attendance sheets and other verification of participation in class activities. The policy also prohibits students from submitting the same work in more than one class without receiving written authorization in advance from both instructors. Under the policy, students found in violation are subject to grade sanctions determined by the course instructor and non-grade sanctions determined by the School or College where the course is offered as described in the Violation and Sanction Classification Rubric. Syracuse University students are required to read an online summary of the University's academic integrity expectations and provide an electronic signature agreeing to abide by them twice a year during pre-term checkin on MySlice. The Violation and Sanction Classification Rubric establishes recommended guidelines for the determination of grade penalties by faculty and instructors, while also giving them discretion to select the grade penalty they believe most suitable, including course failure, regardless of violation level. **Any established violation in this course may result in course failure regardless of violation level.**

Students must notify instructors by the end of the second week of classes for regular session classes (such as this one) when they will be observing their religious holiday(s).

Educational use of student work: I intend to use academic work that you complete this semester for educational purposes in this course during this semester. Your registration and continued enrollment constitute your permission.

In the event of an emergency

- Phone emergency line from on-campus: 711
- Phone emergency line from off-campus: 315.443.2224
- Phone emergency line from cell phone providers ATT/Verizon/Nextel: #78

For complete details on emergency procedures, visit: `http://emergencyguide.syr.edu/`.