Chemistry 532
Advanced Physical Chemistry II
Spring 2021 Course Syllabus

Instructor:
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401-874-5516

Office hours:
Any time

Lecture:
TR 9:30-10:45 am, Beaupre 215

Required texts:
Jeanne L. McHale, *Molecular Spectroscopy* (2nd edition)
Daniel C. Harris & Michael D. Bertolucci, *Symmetry and Spectroscopy* (New Edition)

Other recommended texts:
Donald A. McQuarrie, *Quantum Chemistry*
J. Michael Hollas, *Modern Spectroscopy*
F. A. Cotton, *Chemical Applications of Group Theory*
Russell S. Drago, *Physical Methods for Chemists*

Prerequisites:
CHM 531 or permission of instructor

Overview:
This course aims to provide a comprehensive introduction to time-dependent phenomena and molecular spectroscopy, with a focus on vibrational and electronic spectroscopy. We will also cover several advanced topics, including nonlinear and time-resolved spectroscopies.

Grades:

a.	Homework (lowest grade dropped)	100 pts
b.	Two 75-minute exams	200 pts
c.	Paper	50 pts
d.	Presentation	50 pts
e.	Final exam	200 pts
	Total:	**600 pts**

Please note that changes to the syllabus may be made to account for unforeseen circumstances (weather, etc.), but students will be notified in advance of any changes.

Exams:
All exams will be held in class and will be open book and open notes. If a student cannot take an exam because of a medical or other emergency, documentation must be provided before a make-up exam will be given.

Homework:
New problem sets will be uploaded most weeks, and you will always have at least one full week to complete each assignment. Homework should ideally be submitted in class, but submissions will be accepted until 5pm on the due date. Late submissions are NOT accepted. Note that the lowest grade is dropped. You are strongly encouraged to work on the problem sets together, but remember that you will need to be able to solve similar problems independently during exams. If you would like additional practice, the primary textbooks have many excellent problems at the end of each chapter.

Final project:
Each student will be responsible for writing a paper and giving an in-class presentation on a particular spectroscopic method. Suggested topics include but are not limited to: Mössbauer spectroscopy, nuclear resonance vibrational spectroscopy, time-domain/time-resolved terahertz spectroscopy, surface enhanced Raman spectroscopy, coherent anti-Stokes Raman spectroscopy, femtosecond stimulated Raman spectroscopy, time-resolved microwave conductivity, X-ray absorption near-edge structure, extended X-ray absorption fine structure, X-ray emission spectroscopy, magnetic circular dichroism, two-dimensional infrared or electronic spectroscopy, electron nuclear double resonance, electron spin echo envelope modulation, saturation transfer difference nuclear magnetic resonance. If you would like to choose a topic not listed, please ask me first. Papers should be 8-10 pages (double spaced), plus additional pages for references, and cover the following:

a. Historical development
b. Theoretical basis
c. Technical description
d. Major applications
e. Two examples from the last 24 months
f. References (at least 20)

Presentations should cover similar material but must be no more than 30 minutes.

Readings:
All readings are listed in the course outline below. “MS” refers to *Molecular Spectroscopy*, while “S&S” refers to *Symmetry and Spectroscopy*. In some cases, the readings will be supplemented with handouts, which will be uploaded to Brightspace. MS Chapter 1 and S&S Chapter 2 provide general reviews of quantum mechanics and will NOT be covered in class. You are encouraged to read these independently and/or revisit Chapters 1-8 of McQuarrie’s *Quantum Chemistry* (QC) for a refresher before this class begins.

The CHM 532 Brightspace page:
All supplementary notes, problem sets, problem set solutions, and exam solutions will be posted on the course Brightspace page.

Extra help:
You may find that you need additional in-person assistance to master the course material. I will be available for office hours throughout the week. Please stop by my office or email me to set up an appointment.

Disability Services for Students:
Your access in this course is important. Please send me your Disability Services for Students (DSS) accommodation letter early in the semester so that we have adequate time to discuss and arrange your approved academic accommodations. If you have not yet established services through DSS, please contact them to engage in a confidential conversation about the process for requesting reasonable accommodations in the classroom. DSS can be reached by calling: 401-874-2098, visiting http://web.uri.edu/disability or emailing dss@etal.uri.edu.

Anti-Bias Statement:
We respect the rights and dignity of each individual and group. We reject prejudice and intolerance, and we work to understand differences. We believe that equity and inclusion are critical components for campus community members to thrive. If you are a target or a witness of a bias incident, you are encouraged to submit a report to the URI Bias Response Team at http://www.uri.edu/brt. There you will also find people and resources to help.

COVID-19 statement:
The University is committed to delivering its educational mission while protecting the health and safety of our students. At this uncertain time, those concerns include minimizing the potential spread of COVID-19 within our community. While the University has worked this summer to create a healthy learning environment, it is up to all of us to ensure our campus stays that way.

As members of the URI community, students are required to comply with standards of conduct and take precautions to keep themselves and others safe. Students are required to comply with Rhode Island state laws, including the Rhode Island Executive Orders related to health and safety, ordinances, regulations, and guidance adopted by the University as it relates to public health crises, such as COVID-19.

An addendum on policies and guidelines concerning your obligations during this crisis has recently been integrated into the Student Handbook. These obligations include:

- Wearing of face masks when on a URI campus in the presence of others
- Maintaining physical distancing of at least six feet at all times
- Following state rules on the number of individuals allowed in a group gathering
- Completing a daily health self-assessment before coming to campus
- Submitting to COVID-19 testing as the University monitors the health of our community
- Following the University's quarantine and isolation requirements

If you answer yes to any of the questions on the daily health assessment, do not come to class. YOU MUST STAY HOME/IN YOUR ROOM and notify URI Health Services via phone at 401-874-2246 immediately.

If you are already on campus and start to feel ill, you need to remove yourself from the public and notify URI Health Services via phone immediately at 401-874-2246 and go home/back to your room and self-isolate while you await direction from Health Services.

If you are unable to attend class on the day of an exam for any of these reasons, please notify me by email (dugan@uri.edu) at your earliest convenience.

In general, lectures will be delivered in person and will also be filmed and posted to the Brightspace page later the same week. However, during the first week of classes (01/26 – 01/29), all course content at URI must be delivered virtually. The two lectures for this week will be filmed and posted to the Brightspace page; they will not be live streamed. In the event that classes must shift to online-only instruction for an extended period, future lectures will be live streamed via Zoom.

Course outline:

Date	Material	Readings
Before class	Review of quantum mechanics	MS1, S&S2, QC1-8
01/26 – 01/28	Fourier series/transforms and probability (**ONLINE ONLY)**	QC-B/C, handout
01/02 – 02/09	Electromagnetic radiation	MS2, Hollas 2
02/09 – 02/16	Electric and magnetic properties of molecules	MS3
02/18 – 02/23	Time-dependent perturbation theory of spectroscopy	MS4
02/25 – 03/02	The time-dependent approach to spectroscopy	MS5
03/04	**EXAM 1 (MS1-4)**	---
03/09 – 03/11	Experimental considerations	MS6, Hollas 3
03/16 – 03/23	Molecular symmetry and group theory	S&S1, Hollas 4
03/25 – 04/01	Vibrational spectroscopy	MS9-10, S&S3
04/06	Electronic spectroscopy	MS11, S&S5
04/08	**EXAM 2 (MS5-6, MS9-10, S&S3)**	---
04/13 – 04/15	Electronic spectroscopy (continued)	MS11, S&S5
04/20 – 04/22	Nonlinear spectroscopy	MS13
05/04	**FINAL EXAM (comprehensive), 8am**	---