

Chemistry 4502

Rev. 1/14/2022

Introduction to Quantum Mechanics and Spectroscopy (3 cr.)

Spring 2022, 10:10 - 11:00 AM

Mon. & Wed. in Bruininks 220, Fridays by Zoom

Instructor: Prof. Doreen Leopold, Smith 211
Email: dleopold@umn.edu
"Office" Hours (Zoom): *Fridays 11:00 - 1:00 and other times by appointment*
(see Zoom link on our class Canvas site)

Teaching Assistant: Collin Clay
Email: clay0164@umn.edu
Mailbox: I -12 outside Smith 139
"Office" Hours: *Mondays 11:10 - 12:10 and Tuesdays 1:30 - 2:30*
in the 3rd floor Kolthoff study area (one floor above the main entrance)



Textbooks (Required):

1. "Physical Chemistry: A Molecular Approach" by Donald A. McQuarrie and John D. Simon (Univ. Science, 1997, ISBN 0935702997), 2nd or later printing
2. "Problems and Solutions to Accompany McQuarrie/Simon" by Heather Cox (Univ. Science Books 1997 ISBN 0935702431), 2nd or later printing

Prerequisites: 1 year each of college chemistry, physics and calculus, and a 3rd semester of calculus (can be taken concurrently) chosen from among these four courses: Math 2263 or 2374 (Multivariable) or Math 2243 or 2373 (Differential Equations). This course (Chem 4502) can be taken before, after or concurrently with Chem 4501 (Thermodynamics, Kinetics & Statistical Mechanics).

Midterm Exams: There will be **4 in-class, 50-minute exams on Wednesdays:**

Exam 1	Feb. 9
Exam 2	Mar. 2
Exam 3	Mar. 30
Exam 4	Apr. 20

Final Exam: **Wednesday, May 11, 8:00 - 10:00 AM**

Problem Sets (graded): We will have **4 problem sets due by noon on Wednesdays** the week before exams that will be graded. Together these count for a total of 40 points, or 6.7% of the course grade. Their due dates are the following:

Problem Set # 1	Feb. 2
# 2	Feb. 23
# 3	Mar. 23
# 4	Apr. 13

See p. 2 for a Table of Contents of this Syllabus (all 18 pages are posted on our Canvas site)

Syllabus (18 pp. including equation sheet, posted on Canvas - will be updated as needed)

- p. 1 Instructor, TA, Textbooks, Prerequisites, Exam Dates, Problem Set Due Dates
- p. 2 Table of contents
- p. 3 Student learning outcomes
 - ... official version
 - ... new and improved version
- p. 3 Canvas course website (list of items to be posted there)
 - ... Tech Helpline (612-301-4357, 1-HELP on campus)
- p. 4 Problem sets (due by noon on 4 Wednesdays, the week before exams)
Group work (studying together is great, but write up your answers independently)
Homework (not collected or graded, but very helpful for exam preparation)
Exams (in class - 4 midterms and a final)
 - ... Calculators (allowed on exams - must be non-graphing, non-programmable)
 - ... Notes (not allowed during exams - a formula sheet will be provided)
 - ... Distractions (try to avoid distractions to others during exams; use of earplugs)
- p. 5 Exams. continued
 - ... Remote exams (if student cannot attend in person for a valid reason)
 - ... Missed exams (due to illness, university-sponsored activities, etc.)
 - ... Make-up exams (not offered for the midterms; for the final, see "Incompletes")
 - ... Exam return policy (we can return the graded exams privately if requested)
 - ... Exam regrade policy (submit the "Regrade Request Form" with your exam, within 1 week of when it is returned in class)
- p. 5 Scholastic dishonesty (please avoid)
- p. 6 Chemistry Microlab (can print out upper-level chem course materials for free)
Class attendance on non-exam days (recommended but not required)
Lecture notes without blanks (displayed during live and recorded lectures)
Access and disability accommodations (DRC)
- p. 7 Grading (a combination of absolute thresholds and a grading curve applied after the final exam to raise some grades, if needed to bring the class average up to between B and B-)
- p. 7 Incompletes (if passing the class but unable to take the final for a valid reason)
- p. 8 Study suggestions
- p. 9 Exam strategies
- pp. 10 - 11 Additional links to recommended U of M syllabus policy statements
- pp. 12 - 16 Class schedule - topics, reading, exam dates, problem set due dates
- pp. 17 - 18 Equations, conversions and constants (portions will be included with each of our midterm exams, and all will be attached to the final exam.

Student Learning Outcomes:

Official version: Students will develop an understanding of the foundational principles of quantum theory (McQuarrie/Simon Chapters 1-5) and some of their applications to atomic and molecular structure (Ch. 6 - 9) and molecular spectroscopy (Ch. 13). Student learning outcomes will also include the development of students' abilities to identify, define and successfully solve chemical problems using appropriate methods of quantum mechanics.

New and improved version: Students will become fascinated by quantum mechanics, and will gradually find themselves incorporating its oddly counter-intuitive concepts into all aspects of their daily lives. They will find themselves using the language of quantum mechanics in matters ranging from philosophy and religion to romance, starting with writing an original Valentine's Day poem or lyrics to a tune (extra credit for performing it in class). Far into their future lives, and long after the equations have been forgotten, students will be excited to learn about breakthroughs that apply quantum mechanics to new technologies, such as quantum computing and quantum teleportation. When new discoveries are announced in various areas of science, and everyone else knowingly says, "that can't be right - it makes no sense!", students of the history of quantum mechanics will more wisely think, "... and yet, it may be true".

Canvas: <https://canvas.umn.edu/courses/290218>

The following materials will be available on our class Canvas website - please check it often.

- Announcements
- Syllabus (full version, 18 pages, will be updated as needed)
- Zoom links for our Friday class meetings and Doreen's "office" hours
- Lectures (will be recorded on Zoom before or after the lecture and posted by the next day)
- PowerPoint slides (with blanks that can be filled in during in-class or recorded lectures)
- Problem sets (4) and answer keys
- Homework (not collected or graded) - reading and end-of-chapter problems recommended to help learn the material and prepare for exams
- Review sheets for our exams
- Answer keys for our exams
- Practice exams with answer keys (given during two previous semesters of Doreen's classes)
- Grades on exams and problem sets
- Grade distributions for exams and (after the final) for end-of-semester scores and letter grades
- "Articles, Book Excerpts & Interesting Links" (mostly optional material to view if interested)

For help with computer-related problems:

Technology Helpline at **1-HELP** on campus, or **(612) 301-4357**.

Problem Sets (graded): (see p. 1 for due dates)

Problem sets are due by noon on Wednesdays, one week before our Wednesday midterms. They will be posted on our Canvas website by Monday of the week before the due date. Solutions will be posted by Friday after the due date, and the graded problem sets will be returned in class the following Monday. If you have only completed part of a problem set, it is fine to just turn in what you have. If you are not in class the day a problem set is due, please give it to another student to submit for you, or leave it in Collin's mailbox (I-12) outside Smith 139, or email it to him (clay0164@umn.edu) before noon. Each problem set can earn up to 10 points out of 600 points total (1.7%). Although the student can skip handing in one or more of these and still get an A in the class, their more important value is to help students keep up with the material, and to provide extra practice solving problems.

Group work: Students are encouraged to work together on problem sets and homework problems. Forming study groups is a great way to learn the material and prepare for exams. However, if two or more problem sets have identical answers for one or more problems for which the detailed worked-out solutions are required, those problem sets will be given grades of zero. The similar case of identical answers due to two or more students copying from solutions previously posted online will incur the same penalty. In summary, please

- do not copy someone's answers (or enable someone to copy yours), and
- do not copy from answers that may be available online.

Homework (not graded): In addition, we will have homework for each chapter which will include reading assignments in the text and selected end-of-chapter problems. Although these problems will not be collected or graded, they are very helpful to prepare for exams. Solutions to end-of-chapter problems are provided in the *Solutions Manual*. Several copies of the textbook and solutions manual are also available on Reserve in Walter Library.

Exams: (See page 1 for exam dates.) The four midterm exams will be a combination of multiple choice, short answer and longer problems requiring more detailed written solutions (for which partial credit will be given). Exams will cover the material discussed in lectures, in the assigned reading, end-of-chapter problems in the homeworks, and problem sets. Material in the text that has not been discussed in lecture or included in the homeworks or problem sets will not be covered on exams (except if it can be deduced from material that has been covered).

Calculators used for exams: You may use a **non-programmable, non-graphing calculator** on our exams (examples include the **TI-30Xa** or the two-line **TI-30X IIS**).

Notes during exams: **No notes** may be used during exams. All or part of the list of equations, constants and conversions on the last 2 pages of this syllabus, selected to be potentially helpful for each exam, will be provided with it, and the entire 2-page list will accompany the final.

Distractions during exams: Some students may feel distracted during exams by other students turning pages, leaving the exam early, clicking their pens, chewing gum, eating an apple, crinkling cellophane wrappers, etc. Please be considerate of the other students and do not eat during exams or contribute to other distractions. For some students, it may be helpful to use earplugs during exams, and we will have some available for those who request them.

Remote Exams: For students who are not able to be present in class for an exam (e.g., if feeling okay but required to quarantine due to a positive covid test, or unable to attend for another unavoidable reason), we will work out a way to administer that exam remotely via Zoom *at the same time that the rest of the class is taking it*. Please let Doreen or Collin know if this is your situation as soon as you know, and at least 2 prior to the start of the exam, so we can make arrangements to proctor your exam on Zoom. You will need to have a working camera on your laptop. Also, you will need to have the *Adobe Scan* (or a similar) app on your phone so you can photograph the papers on which you wrote your answers (you will need good lighting to give a clear image) and convert it to a PDF to submit for grading immediately after the exam. (This option does *not* substitute for DRC accommodations - see p. 6)

Missed Exams: **Students are required to take all 4 midterm exams and the final.** Unless an excused absence has been approved by Doreen, a score of zero will be given for missed exams. If a student cannot take a midterm exam due to illness, a personal emergency, or a university-sponsored activity, please email her prior to the start of the exam. For a student who has missed one exam for a valid reason and has obtained an excused absence, the course grade will be determined based on the other 3 midterm scores, the final exam and the problem sets (taking the percentage out of 500 points total instead of the usual 600 points). For information on excused absences from the final exam, see the section on "Incompletes" (p. 7).

Make-up Exams: ***No make-up exams will be given for the 4 midterm exams, nor will they be administered at times or on days other than those listed on p. 1.*** For make-up final exams, see "Incompletes" (p. 7).

Exam Return Policy: To ensure students' privacy, there will be a box to check on the first page of each exam if you want to request to pick it up from Collin privately during his office hours (see p. 1). Otherwise, students can pick up their midterms at the start of the following week's Mon. or Wed. class. from alphabetized piles on the front desk. (For privacy, your grade will be written on the second page of the exam, not on the front page.)

Exam Regrade Policy: If you wish to have your exam regraded, please indicate on the "Exam Regrade" form (posted on our Canvas page) which question(s) you feel were incorrectly graded and why, and what grade you think you deserved. If you plan to submit a regrade request for any question, please do not write anything on the graded exam after it is returned. Then, give the form and the exam to Doreen or Collin on or before the following Monday. We may also regrade other parts of your exam. (Of course, altering an exam in order to raise the score and then requesting a regrade is considered scholastic dishonesty.)

Scholastic Dishonesty: (Also see U of M policy item #3 on p. 10.)

In Chemistry classes, academic dishonesty in any portion of the academic work for a course is considered grounds for assigning a grade of F (or N if taking the class S/N) for the entire course. Scholastic dishonesty for our class would be acts like copying someone else's answers on an exam, surreptitiously using notes during an exam, having someone else take your exam, submitting a regrade request for a question after having changed its answer, etc. Here is a portion of the current CSE Policy on Scholastic Dishonesty:

If the instructor determines that a grade of F or N for the course should be awarded to a student because of scholastic dishonesty, the student cannot withdraw to avoid the F or N. If the student withdrew from the course before the scholastic dishonesty was discovered or before the instructor concluded that there was scholastic dishonesty, and the instructor (or the appropriate hearing body if the student requests a hearing) determines that the student should receive the F or the N, the student will be re-registered for the course and the F and N grade will be entered on the transcripts.

Chemistry Microlab:

<https://sites.google.com/umn.edu/studentpostdocintranet/computer-lab>

Students in our class can print out course-related materials for free in the Chemistry Microlab. As noted on their web site, "Welcome to the Chemistry Department's Microcomputer Lab (microlab). Its primary role is to support students working on upper-division chemistry coursework." The Microlab is in room 101D Smith Hall, phone 624-3372.

The computer-assisted instruction manager is Dan MacEwan chemcaim@umn.edu

The schedule (during the semester) is:

Monday - Thursday 9 AM - 9 PM, Friday 9 AM - 5 PM, Saturday 11 AM - 4 PM

The Microlab is closed when school is not in session, including University holidays and emergency days such as snow days.

Class Attendance: Due to covid and other factors, students will occasionally miss our in-person (M, W) or Zoom (F) class meetings. Lectures and problem-solving activities will also be made available on our Canvas site via Zoom recordings made before or after class meetings. Except for our four exam Wednesdays (see page 1), class attendance is voluntary. That is, attendance will not be recorded, and no points will be awarded or withheld for attendance or for working problems in our classroom or Zoom meetings. Nevertheless, it is hoped that many students will find that making a habit of attending our class meetings will help keep up with the material and enhance their learning. Students who do not attend a given class should check the "Chem 4502 Announcements" section of our Canvas page to view any current announcements.

Lecture Notes Without Blanks:

The PowerPoint lecture notes posted on Canvas include some blanked-out sections for students to fill in during class. This is done to help students remain attentive during lectures. Lecture notes with the blanks filled in will not be posted online after the lectures, but they can be viewed in the online lectures. These asynchronous recordings will also include the problems we work out on the whiteboard in class or during Friday Zoom meetings.

Access and Disability Accommodations (DRC):

<https://diversity.umn.edu/disability/>

The Chemistry Department supports providing accommodations for students who need them for equal access to exams, lectures and other class materials. To request the DRC's services, please contact the Disability Resource Center at 626 -1333, drc@umn.edu. They are located in 180 McNamara Alumni Center, 200 Oak Street SE. They will provide you with a letter to share with the instructor describing how the learning environment should be modified to work better for you.

If the DRC recommends extended exam times (and/or a private room), students are responsible for making arrangements with that office to take the exams under their supervision at the McNamara Alumni Center. The exams must be taken at times that overlap the usual times that the other students in the class will be taking them. The DRC requires at least one week advanced scheduling of exams in their testing center. Students can also make all of their reservations for the 4 midterms and the final exam early (e.g., when they make their reservation for the first midterm).

Grading: Course grades will be calculated as follows:

4 Hour Exams	100 points each	66.7% (16.7% each, 400 pts total)
Problem Sets	40 points	6.7% (1.7% each, 40 pts total)
Final Exam	<u>160 points</u>	26.7%
Total Points	600 points	

Absolute grading scale: Exam and problem set totals, expressed as a percentage of the 600 points are as follows. For example, if a student averages 82.0% (i.e., 504 points out of 615), that person is assured of getting at least a B+ in the course.

A	90 - 100 %	B+	80 - 84 %	C+	65 - 69 %	D+	45 - 49 %
A-	85 - 89 %	B	75 - 79 %	C	55 - 64 %	D	35 - 44 %
		B-	70 - 74 %	C-	50 - 54 %	F	0 - 34 %

Expressed as total points out of 600, the minimum number of points needed for each grade is:

A	540	B+	480	C+	390	D+	270
A-	510	B	450	C	330	D	210
		B-	420	C-	300		

Curved grading scale: Depending on the class performance, at the end of the semester (after the final exam), some of the numerical cutoffs listed above may be *lowered* (but they will not be raised), if needed to give an **average grade between B and B-** for the students in our class who completed the course. That is, the above "absolute" grading scale may be modified, but *only* in the favorable direction.

Incompletes:

Students who have an excused absence from the final exam (e.g., due to a serious illness or other personal emergency), and are passing the course with a C- or better based on their midterm scores, may be eligible to receive a temporary course grade of "I" (incomplete). (This option is rarely exercised.) If possible, the instructor should be notified of the problem before the start of the final exam.

An "Incomplete" form signed by the student (when able to do so) and the instructor is required. This form will describe the arrangements to make up the Incomplete, which must be done by the end of the following semester (Fall 2022). Generally, this will involve taking a different make-up final exam. (Make-up exams are not provided for midterms.)

Study Suggestions:

☼ **The lectures are intended to supplement the text, reading, homework and problem sets, not to substitute for them.** Students who want to do well in this course should plan to carefully study the assigned reading and to do all or most of the homework problems, in addition to the four problem sets.

☼ Before the class starts, it's a good idea to **read/skim the posted PowerPoint slides for that lecture and/or the relevant sections of the text.** You'll get more out of the lecture if you have some knowledge of what's to be discussed, and can anticipate what aspects you'd like clarified. After the lecture, you can go over the lecture notes and the reading in the text more carefully.

☼ When studying, **prioritize understanding the concepts.** You'll encounter a lot of material in the course, and its various topics may at first seem unrelated. Developing a good understanding of the underlying concepts that unify this material will make it much easier to remember specific applications, and to tackle problems that you haven't seen previously.

☼ **Work the assigned homework problems.** The concepts can best be learned by applying them to specific problems. Many of the assigned problems in the homeworks and problem sets are representative of the questions that may be asked on exams. Some may be virtually identical, while other exam questions may be simpler versions of more complicated homework or problem set questions. First, study the "Example" problems within the assigned reading, and the sample problems discussed in class, until you thoroughly understand them, and then work the assigned end-of-chapter homework problems. It is helpful to **use the same equation/formula sheets and the same calculator** when doing the homework and problem sets as will be used on our exams, to become familiar with them.

Resist the temptation to look at the answer in the *Solutions Manual* (for end-of-chapter problems) before you try to solve the problem yourself. This method may appear to be efficient, but it actually it can undermine your learning. If you glance at the *Solutions Manual* to see how to set up the problem and then do the subsequent math yourself, you may have lost the opportunity to practice the essential step – applying the concepts to figure out how to interpret the question correctly and to identify the initial steps of the solution.

☼ **Conceptual, qualitative problems** will often be taken directly from the PowerPoint lecture slides used in class. It's a good idea to study each slide carefully, asking yourself "what might I be asked about this?" Some students find a good memory aid to be preparing flash cards with potential exam questions, with answers on the other side. Just thinking up these questions and preparing the flash cards often helps to strengthen the concepts and methods in one's mind. It may be helpful to share these in study groups and quiz each other.

☼ Doing problems from **previous exams** (two of which will be posted on our Canvas site at least a week before each of our exams, along with their detailed answer keys) can also be very helpful in preparing for our exams. Some students may wish to save one practice exam to take in a classroom-like setting, timed for 50 minutes, with an approved calculator and no notes other than the equation sheet provided with the exam. Experiencing this exam-like rehearsal may make taking the actual exam feel less stressful.

Exam - Taking Strategies:

◆ The material in this course is inherently **cumulative**. To really understand what we are doing later in the course, you have to have understood some of what came before. The final exam will be cumulative over the whole course.

♣ Strategies for **multiple-choice** questions: Some of the questions on midterm exams will be multiple choice, and the final exam will be entirely multiple choice (so it can be graded quickly and the course grades submitted on time). Multiple choice questions with numerical answers may have up to 10 possible answers listed. So, the process of elimination isn't likely to give a high probability of identifying the correct answer. Some of the answers listed will include the results of doing calculations with common errors. So, even if you obtain a value that is included as one of the possible answers, you should still double-check your work.

To avoid missing quantitative problems for which you understand the concept but made errors in the calculation, pay special attention to the details of your calculations (including units) when doing the homework and problem set problems. Try to develop a sense of typical magnitudes, signs and units for various quantities, so you can make good estimates, and be able to spot unreasonable values that may result from calculation errors.

♥ Strategies for **True/False** questions: Since the chance of randomly guessing correctly is 50%, if a student circles the wrong answer, credit will be deducted. For example, if each True/False question in a set of five is worth 2 points, then the correct answer will earn 2 points, but an incorrect answer will be graded as -1 point (i.e., 1 point will be subtracted, with a minimum score of zero for the set). If neither true nor false is circled, there will be no penalty. So, if you have no idea what the answer is, it may be better to leave that question unanswered.

♠ Strategies to **optimize partial credit**: Few points are usually awarded if the problem is set up incorrectly but worked consistently from there on. So, pay close attention to **setting up the problem correctly**, and double check that you have answered the question that was actually asked. If a certain aspect of a problem differs from one that you have seen before in class or in the homework or problem sets, it is likely that our partial credit scheme will allocate significant points to being able to correctly incorporate this new variation. This is done to test whether the student has really understood the problem or is relying entirely on memorization.

♣ **Have confidence in your ability** to calmly think through the answer to an exam question that at first looks unfamiliar. Know that you can figure it out, based on your conceptual understanding of the material, and your experience doing similar (though not identical) problems in the homework and problem sets.

◆ **Regarding calculus skills**: You will not be asked to do math on an exam that you have not already seen during our class meetings, or in the problem sets or homework problems. A semester-long course in differential equations is *not* necessary to do well in this class. We'll use only one differential equation (the Schrödinger equation), and we'll solve only the simple cases completely. These solution methods are also described in the textbook's MathChapters. The integrals needed to solve exam problems are included on page 2 of the attached equation sheet, so you won't need to memorize them.

Additional Links to Recommended U of M Syllabus Policy Statements

WEBPAGE: <https://policy.umn.edu/education/syllabusrequirements-appa>

1. Academic freedom and responsibility: Students are encouraged to develop the capacity for critical judgment and to engage in a sustained and independent search for truth. For more on academic freedom, see:

https://regents.umn.edu/sites/regents.umn.edu/files/2019-09/policy_academic_freedom_and_responsibility.pdf

2. Student conduct code:

https://regents.umn.edu/sites/regents.umn.edu/files/2020-01/policy_student_conduct_code.pdf

3. Avoiding scholastic dishonesty:

<https://communitystandards.umn.edu/avoid-violations/avoiding-scholastic-dishonesty>

Scholastic Dishonesty is discussed under CSE's scholastic policies and is defined in the University Student Conduct Code as follows:

"Scholastic Dishonesty means plagiarizing; cheating on assignments or examinations; engaging in unauthorized collaboration on academic work; taking, acquiring, or using test materials without faculty permission; submitting false or incomplete records of academic achievement; acting alone or in cooperation with another to falsify records or to obtain dishonestly grades, honors, awards, or professional endorsement; altering, forging, or misusing a University academic record; or fabricating or falsifying data, research procedures, or data analysis."

Academic dishonesty in any portion of the academic work for a course shall be grounds for assigning the student a grade of F (or N) for the entire course.

4. Use of personal electronic devices:

<https://policy.umn.edu/education/studentresp>

5. Respecting Intellectual property:

"Students may not distribute instructor-provided notes or other course materials, except to other members of the same class or with the express (written) consent of the instructor. Instructors have the right to impose additional restrictions on course materials in accordance with copyright and intellectual property law and policy. Students may not engage in the widespread distribution or sale of transcript-like notes or notes that are close to verbatim records of a lecture or presentation."

6. Grading: (also see page 7 of this syllabus)

<http://policy.umn.edu/education/gradingtranscripts>

7. Makeup work for legitimate absences: (also see pages 5, 7 of this syllabus)

<http://policy.umn.edu/education/makeupwork>

8. Access and disability accommodations (see page 6 of this syllabus)

<https://diversity.umn.edu/disability/>

9. Student mental health and stress management:

To learn more about the range of confidential mental health services available on campus, see: <http://www.mentalhealth.umn.edu/>

10. Sexual harassment and related topics: The Chemistry Department strives to provide a safe and positive environment for everyone. Please review the policies regarding sexual harassment and related topics:

<https://policy.umn.edu/hr/sexharassassault>

For support and help please contact the Aurora Center:

<http://aurora.umn.edu>

11. Diversity, equity, inclusion: We welcome individuals of all ages, backgrounds, beliefs, ethnicities, genders, gender identities, gender expressions, national origins, religious affiliations, sexual orientations, ability, and other visible and nonvisible differences to this course. Instructors, teaching assistants, and peer students are expected to contribute to a respectful, welcoming and inclusive environment for every other member of the class. This is in agreement with university policy:

http://regents.umn.edu/sites/regents.umn.edu/files/policies/Equity_Diversity_EO_AA.pdf

12. Department of Chemistry Diversity, Equity and Inclusion (DEI) Committee:

Collaboration among people of all cultures and backgrounds enhances our experiences and contributes to excellence in teaching, learning, and research. We strive for a climate that celebrates our differences and strengthens our Department by embracing and working to increase diversity, equity, and inclusion. For more information about our departmental efforts and upcoming activities, see:

<https://cse.umn.edu/chem/diversity-inclusion>

For a list of diversity-related resources, see:

<https://sites.google.com/umn.edu/chemintranet/diversity-inclusion/department-initiatives>

Below is an approximate schedule of lectures and reading assignments from "Physical Chemistry: A Molecular Approach" by McQuarrie and Simon (University Science Books, 1997). Problem Sets will be posted on our Canvas web site at least a week before their due dates, and the Homeworks (not collected) will be posted before we start discussing that topic.

Review: If you have not thought about this material in a while, you might want to start by reviewing the relevant sections of the textbook that you used for introductory chemistry. In Silberberg's "Chemistry", these include Chapters 7 (Quantum Theory and Atomic Structure) and 8 (Electron Configuration and Chemical Periodicity). Excerpts are posted on our Canvas website under "Interesting Links".

Date	Topic	Reading & Homework (HW)
(1) Wed. Jan. 19	Introduction to Course; 2-slit experiment; wave/particle duality	(HW 1)
(Lectures 2 - 4) (2) Fri. Jan. 21 (3) Mon. Jan. 24 (4) Wed. Jan. 26	Chap. 1 - The Dawn of Quantum Theory Failures of classical physics: blackbody radiation, atomic spectra, photoelectric effect Particle nature of light (photons); de Broglie wavelengths of particles; Bohr theory of the H atom and the Rydberg formula; Heisenberg uncertainty principle; 2-slit experiment revisited	(HW 2) pp. 1-25
(Lecture 5) (5) Fri. Jan. 28	Chap. 2 - The Classical Wave Equation MathChapter A - Complex Numbers Solving this linear partial differential equation by separation of variables; Complex numbers and Euler's formula	(HW 3) 31-34 39-49
(Lectures 6 - 8) (6) Mon. Jan. 31 (7) Wed. Feb. 2 (P Set 1 due) (8) Fri. Feb. 4 (Mon. Feb. 7)	Chap. 3 - The Schrödinger Equation The time-independent Schrödinger equation; operators, eigenvalues and eigenfunctions; Hamiltonian operator; commuting operators Catch-up and review (Lecture 9 - See next page)	(HW 3) 73-79
Wed. Feb. 9	Exam 1 (Lectures 1 - 8)	

Date	Topic	Reading & Homework (HW)
(Lectures 9 - 11) (9) Mon. Feb. 7 (10) Fri. Feb. 11 (11) Mon. Feb. 14 <i>Valentine's Day</i> 	Chap. 3 (continued) The Particle-in-a-Box Problem The particle in a 1-D box, a model for electronic transitions in linear polyenes; quantized energy levels; zero point energy; normalized wave functions; calculating probabilities; correspondence principle The particle in a 3-D box, a model for translational motions of molecules; LaPlacian operator in Cartesian coordinates; degenerate energy levels	(HW 4) pp. 80-90 90-95
(Lectures 12 - 14) (12) Wed. Feb. 16 (13) Fri. Feb. 18 (14) Mon. Feb. 21	Chap. 5 - The Harmonic Oscillator The harmonic oscillator, a model for vibrational motions of molecules; wave functions, tunneling; energy levels; vibrational (IR and Raman) spectroscopy	(HW 5) 157-173
(Lectures 15, 16) (15) Wed. Feb. 23 (P Set 2 due) (16) Fri. Feb. 25 (Mon. Feb. 28)	Chap. 4 - Some Postulates and General Principles of Quantum Mechanics Interpretation of wavefunctions; quantum mechanical operators; observable properties as eigenvalues Time-dependent Schrödinger equation; orthogonality of eigenfunctions; commuting operators and the uncertainty principle Catch-up and Review (See next page)	(HW 5) 115-133
Wed. March 2	<div style="border: 2px dashed red; padding: 10px; display: inline-block;"> Exam 2 (to Lecture 16) </div>	

Date	Topic	Reading
(Lectures 17, 18) (17) Mon. Feb. 28 (18) Fri. Mar. 4	Chap. 5 (continued) The Rigid Rotator Model MathChapter D Spherical Coordinates The rigid rotator, a model for molecular rotations; Laplacian operator in spherical coordinates; relation between the rotational constant of a diatomic molecule and its equilibrium bond length; microwave spectroscopy	(HW 6) pp. 172-179 147-153
Mon. Mar. 7 through Fri. Mar. 11	<i>Spring Break</i>	
(Lectures 19 - 22) (19) Mon. Mar. 14 (20) Wed. Mar. 16 (21) Fri. Mar. 18 (22) Mon. Mar. 21	Chap. 6 - The Hydrogen Atom MathChapter C Vectors Use of the Schrödinger equation to solve for the <i>angular</i> parts (spherical harmonics) of the hydrogen atomic orbitals (and the rigid rotator wave functions); angular momentum as a vector property; angular momentum uncertainty relations <i>Radial</i> parts of the hydrogen orbitals; energy levels; quantum numbers n, ℓ, m ; s, p and d orbitals Schrödinger equation for the helium atom	(HW 7) 105-112 191-206 206-219
(Lectures 23, 24) (23) Wed. Mar. 23 (P Set 3 due) (24) Fri. Mar. 25 (Mon. Mar. 28)	Chap. 7 - Approximation Methods Variational method (Lecture 25 - See next page)	(HW 7) 241-249
Wed. March 30	Exam 3 (to Lecture 24)	

Date	Topic	Reading
(Lectures 25 - 29) (25) Mon. Mar. 28 (26) Fri. Apr. 1 (27) Mon. Apr. 4 (28) Wed. Apr. 6 (29) Fri. Apr. 8	Chap. 8 - Multielectron Atoms Atomic units; Hartree-Fock calculations and the self-consistent field method; electron spin; antisymmetric wave functions, the Pauli Exclusion Principle, and Slater determinants; orbital energies and Koopmans' theorem Electron configurations; atomic term symbols; J, quantum number for the total (orbital + spin) electron angular momentum; Hund's rules; atomic energy level diagrams	(HW 8) pp. 275-292 292-308
(Lectures 30 - 34) (30) Mon. Apr. 11 (31) Wed. Apr. 13 (P Set 4 due) (32) Fri. Apr. 15 (33) Mon. Apr. 18 (34) Fri. Apr. 22	Chap. 9 - The Chemical Bond: Diatomic Molecules Born-Oppenheimer approximation; H_2^+ and H_2 bonding described by molecular orbital theory; overlap, Coulomb and exchange integrals; bonding and antibonding orbitals; molecular orbitals (MO) as linear combinations of atomic orbitals (LCAO) σ , π and δ MOs and their energy ordering; understanding the ground state electron configurations and bonding properties of the homonuclear diatomics H_2 - Ne_2 and their positive and negative ions Photoelectron spectroscopy; heteronuclear diatomics; molecular term symbols; excited electronic states of molecules	(HW 9) 323-336 336-346 346-362
Wed. April 20	<div style="border: 2px dashed red; padding: 5px; display: inline-block;"> Exam 4 (to Lecture 32) </div>	

Date	Topic	Reading
(Lectures 35 - 37) (35) Mon. Apr. 25 (36) Wed. Apr. 27 (37) Fri. Apr. 29	Chap. 13 - Molecular Spectroscopy Molecular energy level diagrams including electronic, rotational and vibrational states; vibration-rotation spectra; pure rotational (microwave) spectroscopy; vibrational (infrared) spectra and anharmonicity Electronic spectroscopy (UV-visible); Franck-Condon Principle Polyatomic molecules; normal modes	(HW 10) 495-507 507-514 518-523
(Lecture 38) (38) Mon. May 2	Review	
Wednesday May. 11, 2022	<div style="border: 2px dashed red; padding: 10px; display: inline-block;"> <p>Final Exam 8:00 - 10:00 AM</p> </div>	

Possibly Useful Equations, Conversions and Constants

Chem 4502

$$\begin{aligned}
 c &= 2.998 \times 10^8 \text{ m/s} & k_B &= 0.695 \text{ cm}^{-1}/\text{K} \\
 h &= 6.626 \times 10^{-34} \text{ J}\cdot\text{s} & \hbar &= h/(2\pi) = 1.055 \times 10^{-34} \text{ J}\cdot\text{s} \\
 e &= 1.602 \times 10^{-19} \text{ C} \\
 1 \text{ eV} &= 1.602 \times 10^{-19} \text{ J} & & \text{(corresponds to } 8066 \text{ cm}^{-1}\text{)} \\
 m_e &= 9.109 \times 10^{-31} \text{ kg} & m_p &= 1.673 \times 10^{-27} \text{ kg} & \text{amu} &= 1.661 \times 10^{-27} \text{ kg} \\
 \tilde{\nu} &= 109,678 (1/n_1^2 - 1/n_2^2) \text{ cm}^{-1} \\
 E_n &= -\frac{m_e e^4}{8\epsilon_0^2 h^2} \frac{1}{n^2} & r &= \frac{\epsilon_0 h^2 n^2}{\pi m_e e^2}
 \end{aligned}$$

$$e^{ix} = \cos x + i \sin x$$

Classical wave equation $\partial^2 u(x,t)/\partial x^2 = (1/v^2) \partial^2 u(x,t) / \partial t^2$

Normal modes of a vibrating string of length ℓ : $u_n(x,t) = A_n \cos(\omega_n t + \phi_n) \sin(n\pi x / \ell)$

Schrödinger equation: $(-\hbar^2 / (2m)) d^2 \Psi / dx^2 + V(x)\Psi(x) = E\Psi(x)$

Momentum operator: $\hat{P}_x = -i \hbar \partial / \partial x$

PIB $\psi_n(x) = (2/a)^{1/2} \sin(n\pi x/a)$ $E_n = n^2 h^2 / (8ma^2)$

HO $\psi_0(x) = (a/\pi)^{1/4} e^{-ax^2/2}$ where $a = (\mu k)^{1/2} / \hbar$
 $E_v = (v+1/2) h\nu_0$ where $\nu_0 = (1/(2\pi)) (k/\mu)^{1/2}$ and $\mu = m_1 m_2 / (m_1 + m_2)$ (diatomic)

Rotational motion: $K = 1/2 I\omega^2 = L^2 / 2I$ $I = \mu r^2$ $L = I\omega = mrv$ $\omega = v/r$

Rigid rotator: $E_J = (\hbar^2 / 2I) J(J+1)$ $E \text{ (cm}^{-1}\text{)} = \tilde{B} J(J+1)$
 $B \text{ (Hz)} = h / (8\pi^2 I)$ $\tilde{B} \text{ (cm}^{-1}\text{)} = h / (8\pi^2 cI)$

Hydrogen atom: $\tilde{\nu} = 109,678 (1/n_1^2 - 1/n_2^2) \text{ cm}^{-1}$
 $E_n = -\frac{m_e e^4}{8\epsilon_0^2 h^2} \frac{1}{n^2} = -\frac{1}{n^2} \frac{e^2}{(4\pi\epsilon_0) 2a_0} = -\frac{1}{n^2} (13.6 \text{ eV})$

$$a_0 = \frac{\epsilon_0 h^2}{\pi m_e e^2} = 0.529 \text{ \AA}$$

$$\psi_{1s} = (1/\pi)^{1/2} (1/a_0)^{3/2} e^{-r/a_0} \quad \Phi_m(\phi) = (1/(2\pi)^{1/2}) e^{im\phi}$$

Angular momentum: $L^2 = \hbar^2 \ell(\ell+1)$ $L_z = m\hbar$ $\hat{L}_z = -i\hbar \partial / \partial \phi$

Spherical coordinates: $\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2}$

$$dV = r^2 \sin \theta dr d\theta d\phi$$

Boltzmann distribution: $N_j / N_i = (g_j / g_i) e^{-(E_j - E_i) / kT}$ $k = 0.695 \text{ cm}^{-1} / \text{K}$

Morse potential: $G(v) = (v + 1/2)\omega_e - (v + 1/2)^2 \omega_e x_e$ $D_e = \omega_e^2 / (4 \omega_e x_e)$

$G(v) - G(0) = v \omega_e - v(v + 1) \omega_e x_e$

$$\int u^n du = \frac{u^{n+1}}{n+1} + C \quad n \neq -1$$

$$\int \frac{du}{u} = \ln |u| + C$$

$$\int \sin(ax) dx = -\frac{1}{a} \cos(ax)$$

$$\int \sin^2(ax) dx = \frac{x}{2} - \frac{\sin(2ax)}{4a}$$

$$\int \cos(ax) dx = \frac{1}{a} \sin(ax)$$

$$\int \cos^2(ax) dx = \frac{x}{2} + \frac{\sin(2ax)}{4a}$$

$$\int \sin(ax) \cos(ax) dx = \frac{\sin^2(ax)}{2a}$$

$$\int x \sin^2 x dx = \frac{x^2}{4} - \frac{x \sin(2x)}{4} - \frac{\cos(2x)}{8}$$

$$\int_0^a \sin^2 \frac{n\pi x}{a} dx = \frac{a}{2}$$

$$\int_0^a x \sin^2 \frac{n\pi x}{a} dx = \frac{a^2}{4}$$

$$\int_0^a x^2 \sin^2 \frac{n\pi x}{a} dx = \left(\frac{a}{2\pi n}\right)^3 \left(\frac{4\pi^3 n^3}{3} - 2n\pi\right)$$

$$\int_0^\pi \sin x dx = 2$$

$$\int_0^{2\pi} \sin^2 x dx = \pi$$

$$\int \sin^2(ax) dx = \frac{x}{2} - \frac{\sin(2ax)}{4a}$$

$$\int_0^\pi \sin^3 x dx = \frac{4}{3}$$

$$\int \sin^3(ax) dx = -\frac{\cos(ax)}{a} + \frac{\cos^3(ax)}{3a}$$

$$\int_0^\infty x^n e^{-ax} dx = \frac{n!}{a^{n+1}} \quad (n \text{ positive integer})$$

$$\int_{-\infty}^\infty x^2 e^{-ax^2} dx = \frac{1}{2a} \sqrt{\frac{\pi}{a}}$$

$$\int_0^b x^2 e^{-ax} dx = \frac{2}{a^3} - \frac{2}{a^3} \left(1 + ba + \frac{b^2 a^2}{2}\right) e^{-ab}$$

$$\int_b^\infty x^2 e^{-ax} dx = \frac{2}{a^3} \left(1 + ba + \frac{b^2 a^2}{2}\right) e^{-ab}$$

Differential Equations

$$\frac{d^2 F(x)}{dx^2} + k^2 F(x) = 0 \quad \text{solution is:} \quad F(x) = A \cos(kx) + B \sin(kx)$$

$$F(x) = C_1 e^{ikx} + C_2 e^{-ikx}$$

$$\frac{d^2 F(x)}{dx^2} - k^2 F(x) = 0 \quad \text{solution is:} \quad F(x) = A e^{kx} + B e^{-kx}$$