(Last update 9/2/2025)

Chemistry 4502

Introduction to Quantum Mechanics and Spectroscopy (3 cr.)

Fall 2025, MWF 10:10 - 11:00 AM in Bruininks 230

Instructor:	Prof. Doreen Leopold, Smith 211
Email:	dleopold@umn.edu
Mailbox:	B1 (outside Smith 139)
Office Hours:	Fridays 11:15 - 12:45 in Smith 111 and other times by appointment

Teaching Assistant:	Mikayla Fahrenbruch
Email:	fahre063@umn.edu
Mailbox:	I16 (outside Smith 139)
Office Hours:	Tues. 2:30 – 3:30 and Thurs. 1:30 – 2:30 in the Kolthoff 3rd floor study area facing the mall and other times by appointment

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: 4 x 50-minute exams on Wednesdays in Bruininks 230

Exam 1	**Sept. 24**
Exam 2	**Oct. 15**
Exam 3	**Nov. 5**
Exam 4	**Dec. 3**

Final Exam: Thurs. Dec. 18 at 1:30 – 3:30 pm in Bruininks 230

Problem Sets (graded): 4 problem sets due on Wednesdays by 5 PM:

Problem Set # 1	**Sept. 17**
# 2	**Oct. 8**
# 3	**Oct. 29**
# 4	**Nov. 26**

Syllabus (Also posted on Canvas)

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 (Chapters 6 - 9) and molecular spectroscopy (Chapter 13). Learning outcomes will also include developing students' abilities to identify, define and solve chemical problems using the 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. Far into their future lives, and long after many of 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 cryptography. When new discoveries are announced in various areas of science, and everyone else knowingly says, "that can't be right - it's illogical and makes no sense!", students of the history of quantum mechanics will wisely think, "... and yet, it may still be true".

Canvas: `https://canvas.umn.edu/courses/517828`

Our Canvas site will include the following items:

- ***"Home"*** (class location and times, instructor and TA contact information and office hours)
- ***"Syllabus"*** (this document; can also be provided in different formats)
- ***"Announcements"*** (additional announcements and reminders will be announced in class)
- ***"Modules"*** section includes the following items:
  - Lecture slides
  - Problem Sets (four, see p. 1 for due dates) and answer keys
  - Homework (not collected) - recommended reading and end-of-chapter problems
  - "Our Exams (Fall 2025)" (four, see p. 1 for due dates) -
    review sheet posted before each exam (helpful study guide)
    answer keys posted after exams, class grade statistics, regrade request form
  - "Old Exams (Spring 2025)" - exams given last semester (answer keys will be posted)
  - "Articles, Book Excerpts & Interesting Links" (mostly supplementary material, but the first 8 items are recommended reading in Homework 1 on the 2-slit experiment)

- ***"Media Gallery"*** has lecture videos for the whole course recorded in 2022 on Zoom (captions have been edited only for the first half of the semester)

- ***"Grades"*** - each student's scores on problem sets, exams, and ChimeIn questions

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)

The four problem sets are due by 5:00 pm on Wednesdays, one week before each of the four midterms. They will be posted on our Canvas site by the start of the preceding week. Answer keys will be posted the next day, 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 morning a problem set is due, please leave it in Mikayla Fahrenbruch's mailbox (I16 outside Smith 139) by 5:00 pm or email it to her at fahre063@umn.edu by 5:00 pm. Please include the word “quantum” in the subject line.

Each problem set is worth 10 points out of 600 points total (1.7%). Although the four problem sets contribute only a small percentage (6.8%) of the total points, doing them is a good way to keep up with the material and to prepare for exams.

In general, problem sets will not be graded in as much detail as will exams. So, it is possible to get a higher score for a question on a problem set than would be given for the same answer to the same (or similar) problem on an exam. Therefore, it is a good idea to review the posted answer key carefully when studying for exams, rather than assuming that the score received for a problem in a problem set is an accurate measure of the correctness of the answer submitted.

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, each student should out write their own answers to the problem sets independently.
If two or more problem sets have identical worked-out answers for one or more problems for which detailed solutions are required, those problem sets will be given grades of zero.

Homework (not graded):

In addition to the four problem sets, we will have "homework" (study guides) for each chapter with reading and selected end-of-chapter problems. Although these problems will not be collected, they are very helpful to learn the material. Detailed solutions to end-of-chapter problems are worked out in the *Solutions Manual*. Several copies of the text and its Solutions Manual are available in the Reserve Room of Walter Library.

Exams:

The four midterm exams (see p. 1 for dates) 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, problem sets, and additional end-of-chapter problems in the homeworks. Material in the text that has not been discussed in lecture or included in the problem sets or homeworks will not be covered on exams (except insofar as 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 are the two-line **TI-30X IIS** or the one-line **TI-30Xa**).

(No) Notes During Exams: No notes may be used during exams. Pages 19-20 of this syllabus include equations, constants and conversions, of which the potentially useful sections will be provided with each midterm exam, and the complete equation sheet will be included with the final exam.

Excused Absences from Midterm Exams:

Students are required to take all 4 midterm exams and the final exam. However, if you cannot take an exam due to illness, a personal emergency, or a university-sponsored activity, please email Doreen prior to the start of the exam. For a student who has missed an exam for a valid reason and has obtained an *excused absence*, the course grade will be determined based on the other three midterm scores, the final exam, and the problem sets (taking the percentage out of 500 points total instead of the usual 600 points, since an exam is worth 100 points). For information on excused absences from the final exam, see the section on "Incompletes" below.

(No) 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 a make-up final exam, see "Incompletes" below.

Remote Midterm Exams: For students who are not able to be present in class for an unavoidable reason, we will try to work out a way to administer that exam remotely via Zoom *at a time that overlaps when the rest of the class is taking it*. Please let Doreen know if this is your situation as soon as you know so we can make arrangements to proctor your exam on Zoom. You will need to have a working camera and microphone 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 clear images) and convert these to a single PDF file to submit to Doreen or Mikayla for grading immediately after the exam. (This option does *not* substitute for DRC accommodations - see p. 7)

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 exam and problem set 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 (Spring 2026). Generally, this will involve taking a different make-up final exam.

Note that the University has policies already in place to permit students called to military service, or unexpectedly disabled by major medical issues, to petition for withdrawal (and potential full or partial tuition remission) without prejudice.

Exam Return Policy: There will be a box to check on the first page of each exam if you want to request to pick it up privately. Otherwise, students can pick up their graded midterms from alphabetized piles in the classroom on the day they are returned or during the following week's classes. (For privacy, the grade will be written on the second page of the exam.)

Exam Regrade Policy:

A "Regrade Request" form is posted on our Canvas site in the "Our Exams" section, and printed copies will also be available in class. If you wish to have your exam regraded, please indicate on this form which question(s) you feel were incorrectly graded and why, and what you believe the grade(s) on those question(s) should have been. Please review the posted answer key that includes partial credit breakdowns before you submit your regrade request form, to verify that the grading of your exam was in error and/or was not consistent with the grading guidelines.

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 graded exam to Doreen or Mikayla within one week of when the graded exams were returned. We may also regrade other parts of your exam. (Needless to say, altering an exam to improve the score and then requesting a regrade is considered scholastic dishonesty.)

Scholastic Dishonesty: (Also see U of M policy item #3 on p. 11.)
In Chemistry classes, academic dishonesty in any portion of the academic work for a course is considered grounds for assigning a grade of zero for that work, or even a failing course grade. Scholastic dishonesty for our exams would include copying someone else's answers, having someone else take your exam for you, using supplementary notes not provided with the exam, submitting a written regrade request for a question whose answer was changed after the exam was returned, etc. On problem sets, scholastic dishonesty would include copying someone else's answers, copying answers provided by Gemini, ChatGPT or another AI program, etc.

Class Attendance: Except for our four Wednesday exams (see dates on page 1), class attendance is not required. It is hoped that most students will find that making a habit of attending our class meetings, and participating in ChimeIn and other problem-solving activities in class, helps them keep up with the material and enhances their learning.

Prerecorded lectures (from Spring 2022) are available in the "Media Gallery" on Canvas. These are already posted for the entire semester. (Captions have been edited by the instructor only for the first half of the semester and those for the second half are not reliable.)

Students who do not attend class may find it useful to check the pdf file to be posted on the home page of our Canvas site for a running list of in-class announcements and updates on which topics were covered in that week's lectures.

Chemistry Microlab: https://sites.google.com/umn.edu/chemintranet/computer-lab

Students in our class can print out course-related materials for free in the Chemistry Microlab. Quoting from their web site, "Welcome to the Chemistry Department's Computer Lab, AKA 'The Microlab.' Its primary role is to support students working on upper-division chemistry coursework." The Microlab is located in room 101D Smith Hall, phone 624-3372.
It is managed by Dan MacEwan chemcaim@umn.edu
Hours are: Monday-Thursday 9 a.m.-9 p.m., Friday 9 a.m.-5 p.m., Saturday 11 a.m.-4 p.m.
The Microlab is closed when school is not in session.

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 the instructor with a letter with recommendations for how the learning environment can be modified to work better for you.

For exams, if the DRC recommends extended times or other special accommodations, students are responsible for making arrangements to take the exams at the DRC testing center. ***Exams taken at the DRC must occur at times that overlap when 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 make all of their reservations for the four midterm exams and the final exam early (e.g., when making the first reservation).

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	**160 points**	26.7%
Total Points	**600 points**	

Exam and problem set totals, expressed as a percentage of 600 points, are as follows.

A	85 - 100 %	B+	75 - 79 %	C+	60 - 64 %	D+	40 - 44 %
A−	80 - 84 %	B	70 - 74 %	C	50 - 59 %	D	35 - 39 %
		B−	65 - 69 %	C−	45 - 49 %	F	0 - 34 %

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

A	510	B+	450	C+	360	D+	240
A−	480	B	420	C	300	D	210
		B−	390	C−	270		

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

ChimeIn - Extra Credit In-Class Questions:

To respond to ChimeIn questions conveniently using your phone, install the Canvas app.

Students can earn up to 10.0 points of extra credit by answering questions in class through ChimeIn. These questions can be answered using the student's laptop, iPad, phone, or other device that can access Canvas. No or other external device (such as a clicker) is needed. In addition to providing this small amount of extra credit, these ChimeIn questions will provide real-time feedback on students' understanding of concepts and calculations covered relatively recently in class. Studies have shown that in-class participation in a course generally increases students' learning and engagement.

Earning 80% (or more) of the maximum ChimeIn credit will earn the full 10.0 points of extra credit. For each question that can earn credit, half credit will be given if it is attempted but the answer is incorrect. No credit will be given if there is no response. (Some questions may be survey questions and will not earn credit.)

There will not be make-up options for the ChimeIn questions. However, the 80% threshold (rather than 100%) to earn the full 10.0 points is intended to roughly compensate for class absences and other situations that occasionally prevent a student from participating in ChimeIn.

Each student's cumulative score will appear on their Canvas grades list in a single column labeled "ChimeIn". This score will be listed as the percentage of ChimeIn credit earned out of the maximum credit possible for all of the questions since the start of the semester. The Canvas Grades list will be updated a few hours after each class.

For example, if during the first week of class, 4 ChimeIn questions that can earn credit have been asked and a student answered all of them correctly, then the percentage listed would be 100%. Say that during the second week of class, 4 more questions were asked and the student answered 2 of them correctly and 2 incorrectly, giving a total of 6 questions answered correctly and 2 incorrectly out of 8 total questions asked. Then, the percentage earned would be updated as

$$(6 + 2 \times ½) / 8 = 7/8 = 87.5\%.$$

At the end of the semester, a student with a cumulative ChimeIn percentage of 80.0% or more will earn the full 10.0 points of extra credit, whereas a percentage of 40.0% will earn 5.0 points, etc. That is, the number of extra credit points earned by a student with a ChimeIn percentage of x % will be

$$(10.0 \text{ points}) (x\ \%) / 80\%$$ (with a maximum of 10.0 points).

These extra credit points will be added to the total points earned on the problem sets and exams to determine the student's letter grade in the course. Since this is an extra credit option, it is not necessary for students to participate in ChimeIn to earn the course grades guaranteed by the thresholds listed on p. 7. For example, even without any extra credit, a total score of 450.0 points (i.e., 75.0% of 600.0 points) will guarantee a minimum course grade of B+.

Study Suggestions:

✸ ***The lectures are intended to supplement reading the text and doing the homework and problem sets, not to substitute for them.*** To do well in this course, it is helpful to ...

- attend lectures and/or review the prerecorded lecture videos and posted lecture slides,
- study (or at least skim) the assigned reading in the text,
- answer the questions on the four problem sets (and subsequently check these answers against those on the answer keys),
- do many of the additional end-of-chapter problems recommended in the homeworks (and check answers against those in the Solutions Manual),
- answer the questions on the old exams (from Spring 2025) that will be posted prior to each of our exams (and check answers against their posted answer keys),
- keep a list of questions about material you would like to have clarified, and ask these in class or during Doreen's or Mikayla's office hours (p. 1) or email one of us with your questions.

✸ Before the class starts, it is a good idea to ***read/skim the posted PowerPoint slides for that lecture and/or the relevant sections of the text***. You will get more out of lectures if you have an idea of what is going to be discussed, and can anticipate what aspects you would like clarified. After the lecture, you can go over the lecture slides and the reading more carefully.

✸ When studying, ***prioritize understanding the concepts***. You will 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 have not seen previously.

✸ ***Work the assigned problems on the problem sets and homeworks.*** 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. It is helpful to study the "Example" problems in the reading, and the problems discussed in class, until you thoroughly understand them.

It is also helpful to ***use the same equation sheet and the same calculator*** when doing the homework and problem sets as you will be using 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 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 in the solution.

✸ **Conceptual, qualitative problems will often be taken directly from the PowerPoint lecture slides** used in class, which are also posted on our Canvas site. It is a good idea to study each slide carefully and ask yourself, "What might I be asked about this?" Some students find a good memory aid is preparing "flash cards" with potential exam questions. Just thinking of these questions and preparing the flash cards (e.g., as physical index cards or preparing digital ones using an online template) can help strengthen the concepts and methods in one's mind. It may be helpful to share these in study groups and quiz each other.

Exam - Taking Strategies:

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

♥ Doing problems from ***previous exams*** can be *very* helpful in preparing for our exams. The Spring 2025 exams will be posted at least a week before each of our exams (Exam 1 is already posted), along with their detailed answer keys. Some students may wish take the old exam 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, zero-stakes rehearsal may make taking the actual exam less stressful.

♣ Strategies for **multiple-choice** questions: Some of the questions on midterm exams will be multiple choice, and our 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 alone is not likely to succeed in 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 problems on problem sets and homeworks. 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 (or calculator use) 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.

♦ **Regarding calculus skills:** A course in differential equations is *not* necessary to do well in this class. Math methods that are useful in this course are described, with end-of-chapter problems for practice, in the text's MathChapters. The integrals and differential equations that may be useful are included on the second page of the attached equation sheet (p. 20) and will be provided with exams that involve that type of math, so you will not need to memorize them.

♣ **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 problems in class, for the problem sets and in the homework.

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:
Link to a pdf file of the Student Conduct Code (last amended June 2022):
https://regents.umn.edu/sites/regents.umn.edu/files/2020-01/policy_student_conduct_code.pdf

3. Avoiding scholastic dishonesty: (also see p. 6 of this syllabus)
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."

Additional Links to Recommended Syllabus Policy Statements (continued):

6. Grading: (also see p. 7 of this syllabus)
http://policy.umn.edu/education/gradingtranscripts

7. Makeup work for legitimate absences: (also see p. 5 for excused absences)
http://policy.umn.edu/education/makeupwork

8. Access and disability accommodations (also see p. 7 of this syllabus)
https://disability.umn.edu/
https://disability.umn.edu/student-access

9. Student mental health and stress management:
To learn more about the range of confidential mental health services available on campus, see:
https://mentalhealth.umn.edu/
https://usgumn.com/mental-health-resources

10. Safe Campus resources https://safe-campus.umn.edu/personal-wellbeing

11. 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

12. 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

13. Department of Chemistry Diversity, Equity and Inclusion (DEI) Committee:
The DEI Committee's mission is "to serve all members of the chemistry department by advocating and creating opportunities for accessibility, inclusivity, equity, and diversity across our teaching, research, and service responsibilities." The committee, chaired by Professor Edgar Arriaga and Professor Sapna Sarupria, is made up of 20 chemistry community members, including students, staff, and faculty. For more information about our departmental efforts and upcoming activities, see:
https://cse.umn.edu/chem/diversity-equity-inclusion

Chem 4502 Intro to Quantum Mechanics & Spectroscopy Fall 2025

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 (to be collected and graded) will be posted on Canvas by Monday of the week before their due dates, and Homeworks (not collected or graded) are already posted.

Exam dates and problem set due dates are firm, but the lecture schedule is only approximate.

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

Date	Topic	Reading & Homework (HW)
(1) Wed. Sept. 3	**Introduction to Course**; 2-slit experiment; wave/particle duality	(HW 1)
(Lectures 2 - 4) (2) Fri. Sept. 5 (3) Mon. Sept. 8 (4) Wed. Sept. 10	**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. Sept. 12	**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 - 7) (6) Mon. Sept. 15* **(7) Wed. Sept. 17 (P Set 1 due)** (8) Fri. Sept. 19 (9) Mon. Sept. 22	**Chap. 3 - The Schrödinger Equation** The time-independent Schrödinger equation; operators, eigenvalues and eigenfunctions; Hamiltonian operator; commuting operators (Lecture 8 - See next page) Catch-up and review for Exam 1	(HW 3) 73-79 * Mon. Sept. 15 Last day to *drop* a class without W on transcript
Wed. Sept. 24	**Exam 1**	

Date	Topic	Reading & Homework (HW)
(Lectures 8,10,11) (8) Fri. Sept. 19 (10) Fri. Sept. 26 (11) Mon. Sept. 29	**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. Oct. 1 (13) Fri. Oct. 3 (14) Mon. Oct. 6	**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. Oct. 8 (P Set 2 due)** (16) Fri. Oct. 10 (17) Mon. Oct. 13	**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 (Lecture 16 - See next page) Catch-up and Review for Exam 2	(HW 5) 115-133
Wed. Oct. 15	**Exam 2**	

Date	Topic	Reading
(Lectures 16, 18) (16) Fri. Oct. 10 (18) Fri. Oct. 17	**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
(Lectures 19 - 22) (19) Mon. Oct. 20 (20) Wed. Oct. 22 (21) Fri. Oct. 24 (22) Mon. Oct. 27	**Chap. 6 - The Hydrogen Atom** MathChapter C Vectors Use of the Schrödinger equation to solve for the *angular* parts (spherical harmonics) of the hydrogen atomic orbitals (and the rigid rotator wave functions); angular momentum as a vector property; angular momentum uncertainty relations *Radial* 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
(Lecture 23) **(23) Wed. Oct. 29 (P Set 3 due)** (24) Fri. Oct. 31 **(25) Mon. Nov. 3**	**Chap. 7 - Approximation Methods** Variational method (Lecture 24 - See next page) Catch up and Review for Exam 3	(HW 7) 241-249
Wed. Nov. 5	**Exam 3**	

Date	Topic	Reading
(Lectures 24 - 28)	**Chap. 8 - Multielectron Atoms**	(HW 8)
(24) Fri. Oct. 31 (26) Fri. Nov. 7	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	pp. 275-292
(27) Mon. Nov. 10 (28) Wed. Nov. 12	Electron configurations; atomic term symbols; J, quantum number for the total (orbital + spin) electron angular momentum; Hund's rules; atomic energy level diagrams	292-308
(Lectures 29 - 33)	**Chap. 9 - The Chemical Bond: Diatomic Molecules**	(HW 9)
(29) Fri. Nov. 14 (30) Mon. Nov. 17	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)	323-336
(31) Wed. Nov. 19 (32) Fri. Nov. 21	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	336-346
(33) Mon. Nov. 24	Photoelectron spectroscopy; heteronuclear diatomics; molecular term symbols; excited electronic states of molecules	346-362
(34) Wed. Nov. 26 **(P Set 4 due)**	(Lecture 34 - See next page)	
(35) Mon. Dec. 1	Catch-up and Review for Exam 4	
Wed. Dec. 3	**Exam 4**	

Date	Topic	Reading
(Lectures 34 - 37)	**Chap. 13 - Molecular Spectroscopy**	(HW 10)
(34) Wed. Nov. 26	Molecular energy level diagrams including electronic, rotational and vibrational states; vibration-rotation spectra;	495-507
[Fri. Nov. 28 Thanksgiving Break]		
(36) Fri. Dec. 5	Rotational (microwave) spectroscopy; vibrational (infrared) spectra and anharmonicity	507-514
(37) Mon. Dec. 8	Electronic spectroscopy (UV-visible); Franck-Condon Principle Polyatomic molecules; normal modes	518-523
(38) Wed. Dec. 10	Catch Up and Review for Final Exam	

Final Exam

Thursday Dec. 18 at 1:30 – 3:30 pm

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c = 2.998 x 10^8 m/s k_B = 0.695 cm^{-1}/K

h = 6.626 x 10^{-34} J·s $\hbar = h/(2\pi)$ = 1.055 x 10^{-34} J·s

e = 1.602 x 10^{-19} C

1 eV = 1.602 x 10^{-19} J (corresponds to 8066 cm^{-1})

m_e = 9.109 x 10^{-31} kg m_p = 1.673 x 10^{-27} kg amu = 1.661 x 10^{-27} kg

H atom $\tilde{\nu} = 109{,}678\ (1/n_1^2 - 1/n_2^2)\ cm^{-1}$

$$E_n = -\frac{m_e e^4}{8\varepsilon_0^2 h^2}\frac{1}{n^2} \qquad r = \frac{\varepsilon_0 h^2 n^2}{\pi m_e e^2}$$

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

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

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

HO $\psi_0(x) = (a/\pi)^{1/4} e^{-a x^2/2}$ where $a = (\mu k)^{1/2}/\hbar$

$E_v = (v+1/2)\, h\nu_o$ where $\nu_o = (1/(2\pi))\,(k/\mu)^{1/2}$ and $\mu = m_1m_2/(m_1+m_2)$ (diatomic)

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

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

$B\ (Hz) = h/(8\pi^2 I)$ $\tilde{B}\ (cm^{-1}) = h/(8\pi^2 cI)$

Hydrogen atom: $\tilde{\nu} = 109{,}678\ (1/n_1^2 - 1/n_2^2)\ cm^{-1}$

$$E_n = -\frac{m_e e^4}{8\varepsilon_0^2 h^2}\frac{1}{n^2} = -\frac{1}{n^2}\frac{e^2}{(4\pi\varepsilon_0)\, 2a_o} = -\frac{1}{n^2}\ (13.6\ eV)$$

$$a_o = \frac{\varepsilon_0 h^2}{\pi m_e e^2} = 0.529\ \text{Å}$$

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

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

Morse potential: $G(v) = (v+½)\,\omega_e - (v+½)^2\,\omega_e x_e$ $D_e = \omega_e^2 / (4\,\omega_e x_e)$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Differential Equations

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

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

$$\frac{d^2F(x)}{dx^2} - k^2F(x) = 0 \qquad solution\ is: \qquad F(x) = Ae^{kx} + Be^{-kx}$$