



## CHEM 322/422: Quantum Mechanics

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Discussion: M 7:50 PM - 8:40 PM

Lab: W 6:55 PM - 9:55 PM

Lecture/Lab Location: SCH 616

Web: <https://blackboard.roosevelt.edu>

Lecture: M 6:00 PM - 7:45 PM

W 6:00 PM - 6:45 PM

Office Hours: MW 5:00 - 6:00 PM

or by appointment

Office: SCH 600R

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### Textbooks

#### Required

The following items are required for this course. They are available at the bookstore unless noted otherwise:

- Atkins and de Paula, "**Physical Chemistry**", 9th ed. ISBN-10: 9781429218122  
ISBN-13: 978-1429218122
- Heine, Joswig, Gelessus, "**Computational Chemistry Workbook: Learning through Examples**" ISBN: 978-3-527-32442-2

#### Suggested

- McQuarrie, "**Mathematics for Physical Chemistry: Opening Doors**" University Science Books ISBN: 978-1-891389-56-6

## Grading

### CHEM 322

	Weight
Homework	21.0%
In class work	11.0%
Exam I	15.0%
Exam II	15.0%
Final Exam	20.0%
Lab <sup>a</sup>	18.0%

<sup>a</sup>Omitted, if you are not registered.

### CHEM 422

	Weight
Project	12.5%
Homework	14.0%
In class work	5.5%
Exam I	15.0%
Exam II	15.0%
Final Exam	20.0%
Lab <sup>a</sup>	18.0%

<sup>a</sup>Omitted, if you are not registered.

Please note that even though you register for both lecture and lab, the same grade will be assigned for both courses.

## Final grade distribution by total points

Letter grades will be assigned based on the following lower thresholds.

A		B		C		D		F	
	Threshold		Threshold		Threshold		Threshold		Threshold
A	≥ 92.0%	B+	≥ 86.0%	C+	≥ 76.0%	D+	≥ 66.0%	F	≥ 0.0%
A-	≥ 89.0%	B	≥ 82.0%	C	≥ 72.0%	D	≥ 62.0%		
		B-	≥ 79.0%	C-	≥ 69.0%	D-	≥ 59.0%		

## Lecture

### Policies and procedures

Note that the final exam is cumulative, with weighted preference to the new material covered after exams 1 and 2.

**Late homework assignments will not be accepted. There will be no make up exams.**

Working in groups is encouraged. However, **copying work for homework assignments is unacceptable. Any such assignments will not be accepted and will receive a score of zero points.**

Homework is generally due one week after assigned (unless otherwise noted) and solution sets will be posted on blackboard.

Please turn off all cell phones before class. No texting, laptops or iPods allowed.

**There are no makeup labs.**

Discussion will cover both lab and lecture material, depending on the particular situation. See BlackBoard for each week's discussion topic.

## Course expectations

Chemistry 321 is not a prerequisite for this class.

Students will be required not only to have taken the calculus prerequisite, but also to have a working knowledge of it. If you have problems remembering the mathematics, review it now before it becomes too late.

Read ahead. Ask questions.

We will spend time in class on each chapter working on problems in groups supplied by the instructor. Participation in groups of 2-3 students is required, and 1-2 of the problems will be assigned and turned in the next class period. They will account for 11% of the final grade. (5.5% for 422)

Chem 422 students will have a short paper (5-7 pgs) on an article published in a peer-reviewed journal. The topic should be something covered in class and must meet my approval. The paper is due on the last day of classes.

The course material will closely follow the text, so it is to the students' advantage to read the text. Students should read the appropriate material **before** lecture.

Note: exams will closely follow homework assignments, so it is to the students' advantage to understand the material covered in homework sets.

## Laboratory

Note that the laboratory grade is factored into the lecture grade—they are not totally separate classes. There is only one grade issued for lab and lecture.

## Policy and procedures

The lab portion is computational. All "experiments" will be performed on a computer using the deMon software. There are no make up labs. Unless otherwise stated, labs are due at the start of lab one week after they are performed.

Working in your lab groups is encouraged. However, **copying work for lab assignments is unacceptable. Any such assignments will not be accepted and will receive a score of zero points.**

Lab questions are generally due one week after assigned (unless otherwise noted) and solution sets will be posted on blackboard.

## Lab Report Guidelines

Lab reports will be electronically uploaded to the designated Turnitin folder. The proper file format is MS Word, which will allow the instructor to add comments. The submission folder will show the deadlines. **No late submissions will be accepted.**

### Overall guidelines for good lab reports:

- Write in the 3rd person, past tense and use passive voice. Do not use the words 'students,' 'individuals,' or 'persons' to get around writing in the third person.

Saying, “Students were asked to mass a sample,” is the same as saying, “We were asked to mass a sample.”

- Use scientific language. Avoid flowery descriptions and conversational language. Don’t write as if you were speaking to a friend.
- Pay attention to the instructions of the professor.

**Lab reports should include the following sections:**

1. **Title page.** Experiment number, title, date, your name and student ID number. Rubric page should proceed the the title page.
2. **Purpose.** Give a concise description of the overall point of the laboratory in 1-2 sentences. Address the goals of the experiment or the problem that was being solved. Give a brief description of the theory only as it relates to the experiment. Describe how your data were used to solve the problem or reach a conclusion. It is generally a good idea to state a hypothesis or make predictions about how the experiment will turn out. This often leads to a good starting point for writing your discussion section.
3. **Procedure.** Always cite the experimental procedure as shown in the lab manual. Probably you will be referring to manual overall (i.e. the chapter) so you may cite as follows:

CHEM 322 Experiment 1, Physical Chemistry II Lab, Spring Semester 2017-2018, Roosevelt University. [Online] <https://blackboard.roosevelt.edu> (accessed February 14, 2018).

Alternatively,

CHEM 322 Experiment 1, Physical Chemistry II Lab, Spring Semester 2017-2018, Roosevelt University. Heine, Joswig, Gelessus, “**Computational Chemistry Workbook: Learning through Examples**” ISBN: 978-3-527-32442-2. (p. 1-20).

4. **Results.** The results are actually your responses to each problems. Number the questions accordingly (i.e. **1** or **1a**) and show your solutions. You may use screen shots or program outputs to support your responses. The data must be presented in a well-organized manner. It is in your best interest to include short paragraphs (i.e. a narrative) in your results section that summarize the data that were collected.
5. **Discussion.** The discussion should be written in paragraph form with complete sentences. Restate your calculated results and discuss their agreement with true values. Never number your discussion section. The answers to questions need not appear sequentially; you may answer the questions in any order you like as long as the order makes sense and your discussion reads well. Always write discussions in the third person, past tense.

## Rubric for Lab Reports

The following items with designated points will be used as basis for grading:

	Points
Title	1
Rubric	1
Purpose	4
Procedure	2
Results	8
Discussion	4
Total	20

Overall scale for evaluations of items:

	Points
Excellent	5
Above Average	4
Average	3
Below Average	2
Poor	1
Absent	0

## Policies

### Academic dishonesty

The university's policies on issues such as plagiarism, recycling, cheating and other forms of academic dishonesty can be found in the undergraduate catalog at <http://catalog.roosevelt.edu/undergraduate/policies/academic-integrity-policy> and the graduate catalog at <http://catalog.roosevelt.edu/graduate/policies/academic-integrity>. Additional guidelines for avoiding plagiarism are available here: <https://www.roosevelt.edu/current-students/academics/academic-integrity>.

### Disability

Roosevelt University complies fully with the Americans with Disabilities Act. Details about ADA and Roosevelt's policies and practices are found in the following link: <https://www.roosevelt.edu/student-experience/disability-services>. If you have a condition or disability that requires reasonable accommodation, please alert your instructor or the Academic Success Center as soon as possible, certainly before any assignment or classroom activity that requires accommodation. The Academic Success Center is located in AUD1050 (inside the Library) in Chicago, and the phone number is 312-341-3818. In Schaumburg, the office is in room 125, and the phone number is 847-619-7978. Email Adam Wouk or Danielle Smith at [dsmith51@roosevelt.edu](mailto:dsmith51@roosevelt.edu).

## Withdrawal/Incomplete Grades Rules

### Incomplete (I)

A grade of Incomplete may be given only with the consent of the instructor and appropriate notification to the registrar. An Incomplete grade specifies to the student and to the registrar that only a small portion of the total semester's work needs to be completed (e.g., the student must take a final examination, complete a paper, or similar

requirements), that the student is academically able to complete the work, and that the student has presented a satisfactory reason to the instructor for not completing the work within the deadline of the regular semester. Students must complete the course requirements prior to the end of the following term. A student may also be given an extension of an Incomplete due to extraordinary circumstances, for example if the instructor will not be available during the following semester to ensure that the work is completed. Under such circumstances, the instructor will submit an extension date in writing to the registrar. The Incomplete grade will be removed when the instructor submits a letter grade evaluating academic progress (A, B, C, D, P, F) within the above deadline. If no grade is submitted and no extension granted, the registrar will automatically convert the Incomplete grade on the deadline date to the default grade (B, C, D, or F) submitted by the faculty member at the time of granting the original Incomplete grade.

### **Withdrawal (W)**

The final date for an official withdrawal from this class (meaning a “W” would appear on your transcript) is 23-Mar. In order to withdraw after that date, you must petition for a late withdraw with the registrar. Petitions are granted only for non-academic reasons after the deadline. You should consult your academic advisor if you are considering withdrawing from a course. If you receive financial aid, also check with your financial aid counselor to assure that aid isn’t affected by withdrawing from a class. The complete withdrawal policy is here: <https://www.roosevelt.edu/current-students/academics/register-classes>.

### **Religious holidays**

Roosevelt University policy requires written notification to the instructor within the first two weeks of the term. Any work you miss because of a religious holiday can be made up. You can see the full policy here: <https://www.roosevelt.edu/policies/religious-holidays>.

### **Student code of conduct**

Students enrolled in the university are expected to conduct themselves in a manner compatible with the university’s function as an educational institution. <https://www.roosevelt.edu/current-students>.

### **Title IX**

Roosevelt University cares greatly about the health and well-being of our students, staff, faculty, and guests to our campuses. Federal law, specifically Title IX, and the University Sexual Misconduct Policy require that all employees are mandated reporters of incidents involving sexual or gender-based violence or harassment.

Disclosures made to faculty or teaching assistants (TAs) about sexual or gender-based harassment, sexual assault, dating violence, domestic violence, and/or stalking

on or off campus must be forwarded to the Title IX Coordinator. The above listed staff are Responsible Employees and therefore are mandated to report. The Title IX office will contact any student who discloses an incident regarding student rights, including the option to request an investigation, interim safety measures, and/or academic accommodations. In certain circumstances, the Title IX Coordinator may need to proceed with an investigation, even if none is requested, if there are safety risks to the student or campus community. Participation in the process is voluntary.

If you want a confidential place to disclose sexual assault, sexual harassment or intimate partner violence, there are two confidential advisors on campus who are not mandated reporters. They are: Audrey Guy (312)244-0577, LaDonna Long (312)244-0426. Both are available via phone all hours. The Counseling Center (430 S. Michigan Avenue Room 470 Phone: 312-341-3548) staff are also NOT mandatory reporters and therefore not required to report a disclosure to the Title IX Office.

## Tentative Schedule (Subject to Change)

Week	Day	Date	Course Overview	Discussion/Lab	HW Due
1	M	15-Jan	No Class	No Class	No Class
	W	17-Jan	Introduction	-	-
2	M	22-Jan	Lecture 1, 2	Group work #1	-
	W	24-Jan	Lecture 3	Lab Lecture	-
3	M	29-Jan	Lecture 4, 5	Group work #2	Group work #1
	W	31-Jan	Lecture 6	Lab Ch. 2	
4	M	5-Feb	Lecture 7, 8	Group work #3	Group work #2; HW #1
	W	7-Feb	Lecture 9		Lab Report Ch. 2
5	M	12-Feb	Lecture 10, 11	Group work #4	Group work #3;
	W	14-Feb	Lecture 12		
6	M	19-Feb	Lecture 13, 14	Group work #5	Group work #4
	W	21-Feb	Lecture 15		
7	M	26-Feb	Lecture 16, 17	Group work #6	Group work #5
	W	28-Feb	Exam #1 Review	-	
8	M	5-Mar	No Class	No Class	No Class
	W	7-Mar	No Class	No Class	No Class
9	M	12-Mar	Exam #1	Group work #7	Group work #6
	W	14-Mar	Lecture 18		
10	M	19-Mar	Lecture 19, 20	Group work #8	Group work #7; HW #2
	W	21-Mar	Lecture 21	Lab Ch. 4	Lab Report Ch. 3
11	M	26-Mar	Lecture 22, 23	Group work #9	Group work #8; HW #3
	W	28-Mar	Lecture 24	Lab Ch. 5	Lab Report Ch. 4
12	M	2-Apr	Lecture 25, 26	Group work #10	Group work #9; HW #4
	W	4-Apr	Lecture 27	Lab Ch. 6	Lab Report Ch. 5
13	M	9-Apr	Lecture 28, 29	Group work #11	Group work #10
	W	11-Apr	Lecture 30	Lab Ch. 7	Lab Report Ch. 6
14	M	16-Apr	Lecture 31, 32; Exam #2 Review	-	Group work #11; HW #5
	W	18-Apr	Exam #2	Lab Ch. 8	Lab Report Ch. 7
15	M	23-Apr	Lecture 33, 34	-	HW #6
	W	25-Apr	Lecture 35	Lab Ch. 9	Lab Report Ch. 8
16	M	30-Apr	No Class	No Class	HW #7 Ch. 13
	W	2-May	No Class	No Class	Lab Report Ch. 9
17	M	7-May	Final Exam	-	-

Changes to this syllabus may be made when deemed appropriate.



**Lecture Content**

	Topic
Lecture 1	Quantization of energy
Lecture 2	Wave-particle duality
Lecture 3	The Schrödinger equation
Lecture 4	Math for quantumchemistry
Lecture 5	The Born interpretation
Lecture 6	Hermitian operators
Lecture 7	The uncertainty principle
Lecture 8	The particle in a box
Lecture 9	The particle in a well
Lecture 10	The harmonic oscillator
Lecture 11	The particle on a ring
Lecture 12	The particle on a sphere
Lecture 13	Space quantization and spin
Lecture 14	Time-independent perturbation theory
Lecture 15	Time-dependent perturbation theory
Lecture 16	Tunneling
Lecture 17	Hydrogenic atoms
Lecture 18	Atomic spectra
Lecture 19	Helium and heavier atoms
Lecture 20	Spin multiplicities
Lecture 21	Spin-orbit coupling
Lecture 22	The Born-Oppenheimer principle
Lecture 23	VB theory
Lecture 24	MO theory I
Lecture 25	MO theory II
Lecture 26	Point-group symmetry I
Lecture 27	Point-group symmetry II
Lecture 28	Point-group symmetry III
Lecture 29	General theory of spectroscopies I
Lecture 30	General theory of spectroscopies II
Lecture 31	Rotational spectroscopy I
Lecture 32	Rotational spectroscopy II
Lecture 33	Vibrational spectroscopy
Lecture 34	Electronic spectroscopy
Lecture 35	Nuclear magnetic resonance