

Physical Chemistry – Quantum Chemistry and Spectroscopy

CHEM 3461

Fall 2021

MWF 12:00 pm – 12:50 pm

CAV 223

Dr. Gregory Smith

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Office Hours: MTWRF 11 am – 12 pm, or by appointment

Required Material

Modified Mastering Chemistry with Pearson eText -- Instant Access -- for Physical Chemistry: Thermodynamics, Statistical Thermodynamics, and Kinetics, 4th Edition
Engel & Reid

ISBN: 9780134813806

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(This includes the Quantum Chemistry portion in the eText)

A hardcopy of the text is available. Please let me know if you wish to purchase one and I can help you get the correct version.

A scientific calculator is strongly recommended.

Course Description

To quote a textbook, “Physical chemistry is the study of the underlying physical principles that govern the properties and behavior of chemical systems.” In this class, we will be studying quantum chemistry and spectroscopy, two important areas of physical chemistry. Quantum chemistry describes the link between quantum mechanics and chemical properties and behavior. Spectroscopy utilizes the interaction between electromagnetic radiation and atoms, ions, and molecules for study. These topics are complex and we will use calculus extensively in our studies.

Technology Requirements

Students are required to have access to:

- A computer with internet access.
- Access to **Modified Mastering Chemistry**.
- Access to **Slack**. Join our Slack workspace using this link:
https://join.slack.com/t/pchemfall21/shared_invite/zt-udq8mnd3-ZL1mDkJVfQ70ZWLACuiLMw. Slack is an easy way to get in touch with me or other students to discuss homework and form study groups.

Lecture Schedule

Week of	Topic
Aug. 23	Chapter 1 <i>From Classical to Quantum Mechanics</i>
Aug. 30	Chapter 2 <i>The Schrödinger Equation</i>
Sept. 6	Holiday, Aug. 6: No class. Chapter 3 <i>The Quantum Mechanical Postulates</i>
Sept. 13	Chapter 4 <i>Applying Quantum-Mechanical Principles to Simple Systems</i> Exam 1: Tuesday, September 14 5:00 – 7:00 pm
Sept. 20	Chapter 5 <i>Applying the Particle in a Box Model to Real-World Topics</i>
Sept. 27	Chapter 6 <i>Commuting and Non-commuting Operators and the Surprising Consequences of Entanglement</i>
Oct. 4	Chapter 7 <i>A Quantum Mechanical Model for the Vibration and Rotation of Molecules</i>
Oct. 11	Chapter 8 <i>The Vibrational and Rotational Spectroscopy of Diatomic Molecules</i>
Oct. 18	Chapter 9 <i>The Hydrogen Atom</i> Exam 2: Tuesday, October 19 5:00 – 7:00 pm
Oct. 25	Chapter 10 <i>Many-Electron Atoms</i>
Nov. 1	Chapter 11 <i>Quantum States for Many-Electron Atoms and Atomic Spectroscopy</i>
Nov. 8	Chapter 12 <i>The Chemical Bond in Diatomic Molecules</i>
Nov. 15	Chapter 13 <i>Molecular Structure and Energy Levels for Polyatomic Molecules</i> Exam 3: Tuesday, November 16 5:00 – 7:00 pm
Nov. 22	Chapter 14 <i>Electronic Spectroscopy</i> Holiday, Nov 24-26: No class.
Nov. 29	Chapter 14 <i>continued</i> Chapter 15 <i>Computational Chemistry</i>
Dec. 6	Final Exams

Course Delivery

This is a face-to-face class, however I will be recording our lectures and posting them on Blackboard.

Attendance

You are expected to attend all class meetings. You are expected to arrive on time and to stay until the end of the lecture. Activities such as worksheets and quizzes cannot be made up. You will not be automatically dropped if you stop attending class.

If you feel sick, please stay home. Keep your professor informed as to your status by email (preferred) or telephone (if necessary). Your faculty will work with you to keep up to date in the class.

Lecture Grading Scale:

Mastering Homework	10%
Weekly Quizzes	10%
Exam 1	20%
Exam 2	20%
Exam 3	20%
Final Exam	20%
Total	100%

Laboratory Grading Scale:

Worksheet	14.2%
Lab Reports	71.4%
Presentation	14.2%
Total	100%

Total Grading Scale:

Lecture	75%
Laboratory	25%
Total	100%

The lecture section counts for a total of 75% of the final grade with the remainder from the laboratory section.

The Mastering Homework will be assigned on a by chapter basis and will cover material from that chapter. Late work will generally *not* be accepted. Registration for Mastering can be done at this website: [Pearson Mastering](#). Use the course ID smith95164 to enroll in this course. I have also posted instructions on Blackboard.

There will be approximately 12 weekly quizzes throughout the semester. The content of these quizzes will be based on lectures and weekly homework assignments.

The exams will cover material since the last exam, although many concepts carry throughout the course. The final will be comprehensive.

Student Learning Outcomes

After completion of this course, students will be able to:

- Demonstrate technical and analytical skills in the area of physical chemistry
 - Students will be able to calculate the results of quantum mechanical phenomena on photons and particles.
 - Students will be able to predict spectra for various types of spectroscopic techniques on molecules.
- Analyze complex chemical problems and draw logical conclusions.
 - Students will be able to calculate probability distribution functions for electrons.
 - Students will be able to use the postulates of quantum mechanics to predict behavior of photons and particles.
- Employ mathematics in the analysis of chemical problems.

- Students will be able to use the Schrödinger equation to derive wavefunctions and eigenvalues.
- Students will be able to use operators to calculate experimental observables for systems.

Evaluation of Student Learning Outcomes

The student learning outcomes will all be evaluated by performance on online homework, Friday quizzes, and exams.

Honor Code / Academic Dishonesty

Angelo State University expects its students to maintain complete honesty and integrity in their academic pursuits. Students are responsible for understanding the Academic Honor Code, which is to be found in the Student Handbook (www.angelo.edu/cstudent/). The penalty for ANY sort of dishonesty, cheating, or plagiarism can range from a grade of zero on the assignment to an F in the course and disciplinary action warranted in accordance with university guidelines. Don't even consider it.

Accommodations for Students with Disabilities

ASU is committed to the principle that no qualified individual with a disability shall, on the basis of disability, be excluded from participation in or be denied the benefits of the services, programs or activities of the university, or be subjected to discrimination by the university, as provided by the Americans with Disabilities Act of 1990 (ADA), the Americans with Disabilities Act Amendments of 2008 (ADAAA) and subsequent legislation.

Student Disability Services is located in the Office of Student Affairs, and is the designated campus department charged with the responsibility of reviewing and authorizing requests for reasonable accommodations based on a disability. It is the student's responsibility to initiate such a request by contacting an employee of the Office of Student Affairs, in the Houston Harte University Center, Room 112, or contacting the department via email at ADA@angelo.edu. For more information about the application process and requirements, visit the [Student Disability Services website](#).ⁱ The employee charged with the responsibility of reviewing and authorizing accommodation requests is:

Dr. Dallas Swafford
Director of Student Disability Services
Office of Student Affairs
325-942-2047
dallas.swafford@angelo.edu
Houston Harte University Center, Room 112

Information About COVID-19

Please refer to ASU's [COVID-19 \(Coronavirus\) Updates](#)ⁱⁱ web page for current information about campus guidelines and safety standards as they relate to the COVID-19 pandemic.

Physical Chemistry Laboratory

The laboratory sections are complimentary to the lecture section and offer a more hands-on experience. We will use ideas and concepts from the lecture to probe the relationship between theory and experiment.

Laboratory Sections

Section	Days	Meeting Time	Instructor	Lab Room	Class Room
02Z	T	2:00 pm – 4:50 pm	Dr. Smith	CAV 209	TBA

Laboratory Schedule

Week of	Laboratory
Aug. 23	Calculus review, error, and error propagation lecture and worksheet (<i>dry lab</i>)
Aug. 30	Intro to Gaussian
Sept. 6	Intro to Gaussian
Sept. 13	Conjugated Dyes
Sept. 20	Conjugated Dyes
Sept. 27	<i>TBD</i>
Oct. 4	<i>TBD</i>
Oct. 11	HCl-DCI Ro-Vibrational Spectra
Oct. 18	HCl-DCI Ro-Vibrational Spectra
Oct. 25	Water Overtones and Anharmonicity
Nov. 1	Water Overtones and Anharmonicity
Nov. 8	I ₂ Spectroscopy
Nov. 15	I ₂ Spectroscopy
Nov. 22	Oral Presentations
Nov. 29	Oral Presentations
Dec. 6	Finals: no labs

Lab Reports

One week after finishing the lab work, calculations are due for that lab. One week after that, the full lab report is due. Each lab report should read like a journal article, each with an abstract, introduction, experimental, discussion, and conclusion section. We will

talk more about this in class. Late work will not be accepted, except for extenuating circumstances.

The final week we will have oral presentations. These will be 10-15 minute presentations on a laboratory of your choice. You will not have to turn in a written report on your chosen lab.

Each lab, worksheet, and presentation count equally for your final grade in the lab.

Laboratory Attire

Beginning on the first day of lab, everyone **MUST** have **approved goggles, long-sleeved shirts which cover the midriff, long pants, and shoes with closed toes and heels** (no sandals, slides, etc.). (Basically, you should have as little exposed skin as possible.) Anyone not wearing the appropriate attire will not be allowed into lab.

ⁱ <https://www.angelo.edu/current-students/disability-services/>

ⁱⁱ <https://www.angelo.edu/covid-19/>