CHE 3026L

Quantum Chemistry Lab

Syllabus, Fall 2025, Sep. 2 – Dec 19

POINT 1902 LOMA
NAZARENE UNIVERSITY
Department of Chemistry

This is a lab course that accompanies the Quantum Mechanics semester of Physical Chemistry. The fundamental goals are to apply concepts you learn in lecture to the analysis of chemical data, to gain experience with specialized equipment and techniques, and to develop skills in formal scientific communication.

Dr. Sam Stoneburner
Office: Rohr Science 322 (enter 330)
Email: sstonebu@pointloma.edu
Phone: 619-849-2788
Lecture location: Sator Hall 208
Section 1: T: 1:30 pm – 5:00 pm

Drop-in Office Hours*:
Mondays, 2:45pm – 3:45pm
Tuesdays, 9:00am – 10:30am
Wednesdays, 2:45pm – 3:45pm
Thursdays, 9:00am – 11:30am
Fridays, 11:00am – 1:00pm
2:45pm – 3:45pm
*Changes to be announced on Canvas

You do not need an appointment to meet with me during my Drop-in Office Hours. I am often available at other times, so you can also email me to schedule an appointment.

Course Description: Designed to accompany CHE 3026. Emphases on spectroscopic methods and computational chemistry. (1 unit)
Corequisite(s):CHE 3026 (lecture, graded separately)

Required Materials:

- The required texts from CHE 3025. (Lab instructions will be provided on Canvas.)
- Safety glasses.
- A scientific or graphing calculator
- A computer and Microsoft Excel (not Google Sheets or LibreOffice Calc). You should have access to Microsoft Office 365 as a PLNU student.

About your professor: I am a computational chemist with a deep appreciation and respect for "wet lab" experimental chemistry. I have spent much more of my teaching career in lab than in lecture, which has given me considerable opportunity to share from my library of lab safety horror stories, including…

- How I was in the building at the University of Minnesota at the time of the infamous lab hood explosion of 2014 (and related thoughts on the relevance to chemistry of Edmund Burke's "Reflections on the Revolution in France").
- My mostly unsupervised summer with cadmium.
- Possibly second-hand accounts involving elemental sodium, uranium hexafluoride, and/or misused chemical solvents.

Course Learning Outcomes: Upon completion of this course, students will be able to:

- Understand the theories and applications of quantum chemistry as they relate to molecular structure and spectroscopy
- Understand the utility of spectroscopy in revealing the nature and properties of molecular systems
- Use theoretical chemistry software to predict chemical properties
- Analyze and interpret data using appropriate software
- Communicate scientific ideas and results in writing using appropriate software
- Articulate limits and assumptions in experimental methodology and data analysis.

Safety:

Safety is THE top priority in the lab. You will be required to sign a safety agreement form before you can take part in the lab. The agreement form delineates safety rules set forth by the department. Make sure to review the full safety rules on Canvas, but note especially the dress code before coming in the first day:

- Long pants (pants that **fully** cover all skin down to the top of your shoes or socks)
- Shoes that cover the feet (closed-toed and closed-heel)
- Shirts that cover the shoulders, back, and stomach

Grading and Assessment

Letter grades will be assigned according to the following scheme after all scores are finalized. Any changes to these ranges will be only in your favor.

<table>
<tr><th>A-range</th><th>B-range</th><th>C-range</th><th>D-range</th><th>F-range</th></tr>
<tr><td rowspan="2">A:
93.00% or above.</td><td>B+:
87.00-89.99 %</td><td>C+:
77.00-79.99 %</td><td>D+:
67.00-69.99 %</td><td rowspan="3">F:
Below 60.00%</td></tr>
<tr><td>B:
83.00-86.99 %</td><td>C:
73.00-76.99 %</td><td>D:
63.00-66.99 %</td></tr>
<tr><td>A−:
90.00-92.99 %</td><td>B−:
80.00-82.99 %</td><td>C−:
70.00-72.99 %</td><td>D−:
60.00-62.99 %</td></tr>
</table>

Percent	Component
5 %	Tutorial writing activities (2)
5 %	Prelab safety quizzes (3, drop lowest 1)
15 %	Data Spreadsheets (3, drop lowest 1)
5 %	Partial Report (has revision)
70 %	Research project, percentage includes all points below
5 %	Project: Annotated bibliography
10 %	Project: Proposal
5 %	Project: Data updates (3)
10 %	Project: Introduction draft (has revision)
10 %	Project: Oral presentation
5 %	Project: Formal Report draft
20 %	Project: Formal Report (has revision)
5 %	Project: Press Release (has revision)
Professionalism modifier: A multiplier applied at the end of the semester	
100 %	Total

There is no final exam for CHE 3026L.

Each category is explained further in the subsections below.

Professionalism

Most students in chemistry are planning to work in either a clinical or laboratory environment, where professional conduct can be a matter of life and death. (Students who show unprofessional behavior in med school have been shown to be more likely to have state board disciplinary action after they graduate.) Learning good habits early can give you the best chance at success in your career.

In the Physcial Chemistry lab, "professionalism" includes the following categories:

- Did you arrive fully prepared to participate? For example…
  - Were you on time?
  - Did you read and understand the instructions?
  - Were you appropriately dressed?
- Did you comply with all safety requirements without needing reminders? For example…
  - Did you wear eye protection until everyone was done with chemicals?
  - Did you wear gloves (if needed)?

    - Did you wear a mask if you were experiencing respiratory symptoms?
- Did you correctly clean and dispose of everything? For example…
    - Did you make sure any waste went in the appropriate container?
    - Did you clean all of your glassware?

You will be assessed each week according to each of the three categories:

	Every week	−1 week	−2 weeks	−3 weeks	−4 weeks	−5+ weeks
On time / prepared	105 pts	100 pts	90 pts	75 pts	50 points	0 points
Safety w/o reminders	105 pts	100 pts	90 pts	75 pts	50 points	0 points
Cleaning / disposal	105 pts	100 pts	90 pts	75 pts	50 points	0 points

Your professionalism grade is an average of the three scores above, and you can get extra credit if your professionalism is consistently good throughout the semester. For example, if you get full credit on arriving on time and prepared (105 pts), and for cleaning and disposal (105 pts), but you had to be reminded one time to put on your safety glasses (100 pts), you would have 103/100 on your professionalism grade, which would work out to extra credit of 3% on your final score.

Tutorial writing activities: CHE 3026L is a writing-instructive course. Formal scientific writing takes time, practice, and repetition, so there are some activities early in the semester designed to help you get ready for formal write-ups.

There will be two activities: One to train you in preparing data and graphs, and one in which you will "grade" a set of AI-written components of a formal lab report.

Prelab quizzes: Three of the experiments will have a quiz at the beginning to ensure you are familiar with the lab, the associated concepts from lecture, and any relevant safety risks. The quizzes will be closed-book, closed-notes, no-internet, but they will not involve complicated math. The quizzes will begin immediately at the section start time.

Data: Physical chemistry experiments often require less time on the experiments, but much more time *after* the lab work for calculations and analysis. As time permits, parts of some lab periods will be devoted to working through analysis. For three of your experiments, you will turn in an Excel spreadsheet with all of your results and calculations clearly labeled. These are individual and should not be identical between students.

Partial Report: For **one** of your earliest two experiments, you will write up an Abstract, a Methods section, and a Conclusion. This is to give you some practice with the requirements for these sections before you write a complete formal report for the Research Project (see below). You may choose which of these two experiments you write up. You will have the opportunity for a revision after your initial submission is graded.

Research Project: You will spend several weeks on a research project of your own design. There will be some broad guidelines as far as topic and methodology, but this is a much more open assignment than most lab experiments. The intent is for you to have an opportunity to put into practice the concepts and skills you have been learning and experience a miniature version of what you might do as a practicing scientist. The project is scaffolded out into a series of assignments:

- **Annotated Bibliography:** A list of literature sources that you will use as you are designing your project, along with brief explanations of how you plan to use them.
- **Proposal:** A description of your project plans, including a specific timeline.
- **Data updates:** You will have about 5 lab periods to perform experiments on your project. Throughout that time, you will turn in three Data Spreadsheets summarizing your results thus far.
- **Introduction draft:** During your experimental Project weeks you will also be writing up a draft of the Introduction for your final Formal Report. The Introduction usually takes the longest to write, so it's important to get an early start. Your Annotated Bibliography and your Proposal will serve as a foundation. You will have an opportunity for a revision.
- **Oral presentation:** Near the end of the semester, you will present your project to the class. This is to simulate internal group or department presentations, so you will be assuming a certain level of expertise.
- **Formal Report:** You will write up your Project in the style of a complete research paper that one might submit to a peer-reviewed journal, including an Abstract, Introduction (which will already have been drafted), Methods, Results and Discussion, and Conclusion. You will have an opportunity for revision.
- **Press Release:** Good science often languishes in the shadows because none of the people who could benefit from it are aware that the work was done. Communicating with the broader public is an important scientific skill, and you will practice it by writing up a mock Press Release for your project. Your target audience will be the general public, so it will be like a simplified version of your Abstract with more emphasis on broader impact and motivation.

For all assignments with revisions, note that first and second submissions are graded independently of each other. It is possible I might catch something one the second submission that I missed on the first one. Be sure to pay careful attention to ALL aspects of the rubric on the second submission, not just the items that I flagged on the first submission.

Additional Notes and Policies

PLNU Attendance and Participation Policy:
Regular and punctual attendance at all class sessions is considered essential to optimum academic achievement. In keeping with PLNU policy, if the student is absent for more than 10 percent of class sessions (i.e., 2 absences for this course), the faculty member will issue a written warning of de-enrollment. If the absences exceed 20 percent (i.e., 3 absences for this course), the student may be de-enrolled without notice until the course withdrawal date or, after that date, receive an "F" grade. Note that ALL absences are counted toward this total, including "excused" absences. Absences do not count towards this total if they are made up.

Laboratory sections will meet on a weekly basis unless specified otherwise. Some lab periods are devoted to exams from the lecture course. A tentative schedule is provided at the end of the syllabus, but see Canvas for the most up-to-date information.

PLNU academic honesty policy:
Students should demonstrate academic honesty by doing original work and by giving appropriate credit to the ideas of others. Academic dishonesty is the act of presenting information, ideas, and/or concepts as one's own when in reality they are the results of another person's creativity and effort. A faculty member who believes a situation involving academic dishonesty has been detected may assign a failing grade for that assignment or examination, or, depending on the seriousness of the offense, for the course. For all student appeals, faculty and students should follow the procedures outlined in the University Catalog. See Academic Policies for definitions of kinds of academic dishonesty and for further policy information.

Artificial Intelligence (AI) Policy:
You are allowed to use Artificial Intelligence (AI) tools (e.g., ChatGPT, Gemini Pro 1.5, GrammarlyGo, Perplexity, etc) **ONLY** to generate ideas and computer code. You are not

allowed to use AI tools (e.g., ChatGPT, iA Writer, Marmot, Botowski, GrammarlyGo, Perplexity, etc.) to generate content (text, video, audio, images) that will end up in any work submitted to be graded for this course, including drafting, editing, or final submissions. This course is designed to assess your independent critical thinking, writing, and research skills without the assistance of AI technologies. Violations of this policy will be treated as breaches of academic integrity. If you have any doubts about using AI, please gain permission from the instructor.

Loma Writing Center

The Loma Writing Center exists to help all members of the PLNU community cultivate transferable writing skills to engage their academic, professional, personal, and spiritual communities. We work toward this goal by conducting one-on-one consultation sessions, supporting writing education across the PLNU community, and participating in ongoing writing center research.

Getting feedback from the Loma Writing Center while you're in the process of working on an assignment is a great way to improve the quality of your writing and develop as a writer. You are encouraged to talk with a trained writing consultant about getting started on an assignment, organizing your ideas, finding and citing sources, revising, editing for grammar and polishing final drafts, and more. For information about how to make in-person or online appointments, see Loma Writing Center webpage or visit the Loma Writer Center on the first floor of the Ryan Library, room 221.

- Appointment Calendar
- Website
- Email: writingcenter@pointloma.edu

PLNU copyright policy: Point Loma Nazarene University, as a non-profit educational institution, is entitled by law to use materials protected by the US Copyright Act for classroom education. Any use of those materials outside the class may violate the law.

Spiritual care: PLNU strives to be a place where students grow as whole persons. To this end, we provide resources for our students to encounter God and grow in their Christian faith.

If you have questions, a desire to meet with the chaplain, or if you have prayer requests, you can contact the Office of Student Life and Formation.

PLNU academic accommodations policy

PLNU is committed to providing equal opportunity for participation in all its programs, services, and activities in accordance with the Americans with Disabilities Act (ADA). Students with disabilities may request course-related accommodations by contacting the Educational Access Center (EAC), located in the Bond Academic Center (EAC@pointloma.edu or 619-849-2533). Once a student's eligibility for an accommodation has been determined, the EAC will work with the student to create an Accommodation Plan (AP) that outlines allowed accommodations. Professors are able to view a student's approved accommodations through Accommodate.

PLNU highly recommends that students speak with their professors during the first two weeks of each semester/term about the implementation of their AP in that particular course. Accommodations are not retroactive so clarifying with the professor at the outset is one of the best ways to promote positive academic outcomes.

Students who need accommodations for a disability should contact the EAC as early as possible (i.e., ideally before the beginning of the semester) to assure appropriate accommodations can be provided. It is the student's responsibility to make the first contact with the EAC. Students cannot assume that because they had accommodations in the past, their eligibility at PLNU is automatic. All determinations at PLNU must go through the EAC process. This is to protect the privacy of students with disabilities who may not want to disclose this information and are not asking for any accommodations.

Note that the "hands-on" nature of the lab class limits how accommodations can be applied without fundamentally altering the academic standards of the course. Please discuss the specific accommodations you are interested in applying to this course with the lab coordinator as early as possible.

Language and Belonging

Point Loma Nazarene University faculty are committed to helping create a safe and hospitable learning environment for all students. As Christian scholars we are keenly aware of the power of language and believe in treating others with dignity. As such, it is important that our language be equitable, inclusive, and prejudice free. Inclusive/Bias-free language is the standard outlined by all major academic style guides, including MLA, APA, and Chicago, and it is the expected norm in university-level work. Good writing and speaking do not use unsubstantiated or irrelevant generalizations about personal qualities such as age, disability, economic class, ethnicity, marital status, parentage, political or religious beliefs, race, gender, sex, or sexual orientation. Inclusive language also avoids using stereotypes or

terminology that demeans persons or groups based on age, disability, class, ethnicity, gender, race, language, or national origin. Respectful use of language is particularly important when referring to those outside of the religious and lifestyle commitments of those in the PLNU community. By working toward precision and clarity of language, we mark ourselves as serious and respectful scholars, and we model the Christ-like quality of hospitality.

If you (or someone you know) have experienced other forms of discrimination, you can find more information on reporting and resources at www.pointloma.edu/nondiscrimination.

Sexual misconduct and discrimination:
In support of a safe learning environment, if you (or someone you know) have experienced any form of sexual discrimination or misconduct, including sexual assault, dating or domestic violence, or stalking, know that accommodations and resources are available through the Title IX Office at pointloma.edu/Title-IX. Please be aware that under Title IX of the Education Amendments of 1972, faculty and staff are required to disclose information about such misconduct to the Title IX Office.

If you wish to speak to a confidential employee who does not have this reporting responsibility, you can contact Counseling Services at counselingservices@pointloma.edu or find a list of campus pastors at pointloma.edu/title-ix

If you (or someone you know) have experienced other forms of discrimination or bias, you can find more information on reporting and resources at www.pointloma.edu/bias

State authorization: State authorization is a formal determination by a state that Point Loma Nazarene University is approved to conduct activities regulated by that state. In certain states outside California, Point Loma Nazarene University is not authorized to enroll online (distance education) students. If a student moves to another state after admission to the program and/or enrollment in an online course, continuation within the program and/or course will depend on whether Point Loma Nazarene University is authorized to offer distance education courses in that state. It is the student's responsibility to notify the institution of any change in his or her physical location. Refer to the map on State Authorization to view which states allow online (distance education) outside of California.

PLNU Recording Notification

In order to enhance the learning experience, please be advised that this course may be recorded by the professor for educational purposes, and access to these recordings will be limited to enrolled students and authorized personnel. Note that all recordings are subject to copyright protection. Any unauthorized distribution or publication of these recordings without written approval from the University (refer to the Dean) is strictly prohibited.

PLNU Mission: To Teach ~ To Shape ~ To Send

Point Loma Nazarene University exists to provide higher education in a vital Christian community where minds are engaged and challenged, character is modeled and formed, and service is an expression of faith. Being of Wesleyan heritage, we strive to be a learning community where grace is foundational, truth is pursued, and holiness is a way of life.

Schedule:

This schedule is accurate as of the posting of this syllabus.
Canvas will have the most up-to-date information.

Date		Experiment
Sep. 2	0	Math Workshop
Sep. 9	1	Particle In A Box
Sep. 16	2	Fluorescence
Sep. 23		Exam 1 (for lecture course)
Sep. 30	3	Quantum Computers
Oct. 7	4	Infrared Spectroscopy
Oct. 14		Exam 2 (for lecture course)
Oct. 21	5	Research project experiment day
Oct. 28	6	Research project experiment day
Nov. 4	7	Research project experiment day
Nov. 11		Exam 3 (for lecture course)
Nov. 18	8	Research project experiment day
Nov. 25	*9	Research project experiment day
Dec. 2	10	Oral presentations
Dec. 9		Exam 4 (for lecture course)
Dec. 16		No lab (Finals week, no lab final)

* Thanksgiving Recess is Nov. 26-28, which does not include the Mondays or Tuesdays before or after Thanksgiving. There is a scheduled lab period on Nov. 25.