POINT LOMA NAZARENE UNIVERSITY	**Chemistry Department** **CHE3026** **Units: 3**
Fall 2021	

Meeting days: Tuesday, Thursday	**Instructor: Dr. David Gleason-Rohrer**
Meeting times: 11:00-12:15	**Phone: 619-757-8138**
Meeting location: Latter Hall 2	**Email: dgleaso1@pointloma.edu**
Final Exam: Thurs. Dec 16, 10:30 AM – 1:00 PM, Latter Hall room 2	**Zoom Office hours: Thursday, Sunday 7-9PM**
Additional info:	**Office Hours link:** https://pointloma.zoom.us/j/98298110301

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.

COURSE DESCRIPTION

Study of reaction dynamics and complex reaction mechanisms and an investigation of matter from a quantum chemistry perspective with particular emphasis on the theoretical concepts and their implications for molecular spectroscopy.

COURSE LEARNING OUTCOMES

Upon completing this course you will:

1. Have developed more sophisticated mental models of wave functions, energy levels, atomic structures, chemical bonding, spectroscopy, computational chemistry, and statistical mechanics as grounded in the fundamentals of quantum theory.
2. Be able to use fundamental exact and approximate physical systems as models for understanding more complex molecular structure and behavior.
3. Be able to apply the concepts, methods, and techniques of quantum chemistry to chemical systems and make predictions for these systems.

REQUIRED TEXTS AND RECOMMENDED STUDY RESOURCES

Quantum Chemistry & Spectroscopy, Fourth Edition, Thomas Engel, Pearson Education, 2019.

COURSE CREDIT HOUR INFORMATION: In the interest of providing sufficient time to accomplish the stated Course Learning Outcomes, this class meets the PLNU credit hour policy for a 3 unit class delivered over 16 weeks. It is anticipated that students will spend a minimum of 37.5 participation hours per credit hour on their coursework. For this course, students will spend an estimated 112.5 total hours meeting the course learning outcomes. Expect to spend significantly more time if your mathematical foundations are weak.

ASSESSMENT AND GRADING

Mid-term exam 1	20%
Mid-term exam 2	20%
Final exam	25%
Homework	10%
Quizzes	15%
Participation	10%

A	90%	C	70%
A-	88%	C-	68%
B+	86%	D+	66%
B	80%	D	60%
B-	78%	D-	58%
C+	76%	F	< 58%

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.

INCOMPLETES AND LATE ASSIGNMENTS

All assignments are to be submitted by the beginning of the class session when they are due. Assignments will be posted in class and on Canvas and uploaded to Canvas. Assignments may be resubmitted for a maximum of half of the missed points. Problem sets are a record of the practice that you put into the mathematical techniques. As such, all homework should be

handwritten either on paper or a tablet and uploaded. Calculations will be performed on Excel or comparable spreadsheet and uploaded.

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.

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. Copying solutions to homework problems from another student or an online service (Chegg, Bartleby, etc.) prevent students from practicing the mathematical concepts needed to understand physical chemistry. There are usually tell-tale signs of copying, and if it is detected, the student will receive a zero for the assignment, and a zero for the participation portion of the overall grade. 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. Faculty should follow and students may appeal using the procedure in the university Catalog. See Academic Policies for definitions of kinds of academic dishonesty and for further policy information.

PLNU ACADEMIC ACCOMMODATIONS POLICY

PLNU is committed to providing equal opportunity for participation in all its programs, services, and activities. 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 619-849-2486). Once a student's eligibility for an accommodation has been determined, the EAC will issue an academic accommodation plan ("AP") to all faculty who teach courses in which the student is enrolled each semester.

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 and/or if they do not wish to utilize some or all of the elements of their AP in that course.

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.

PLNU ATTENDANCE AND PARTICIPATION POLICY

Regular and punctual attendance at all class sessions is considered essential to optimum academic achievement. If the student is absent for more than 10 percent of class sessions, the faculty member will issue a written warning of de-enrollment. If the absences exceed 20 percent, the student may be de-enrolled without notice until the university drop date or, after that date, receive the appropriate grade for their work and participation.

SPIRITUAL CARE

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

If students have questions, a desire to meet with the chaplain or have prayer requests you can contact the Office of Spiritual Development.

CLASS SCHEDULE

Sessions	**Topics**	**Readings**
Sept 2	Introduction: From Classical to Quantum Mechanics	Chapter 1, sections 1.1-1.7
Sept 2 1:30-4:30PM	Calculus boot camp	
Sept 7, 9	The Schrödinger Equation	Chapter 2, sections 2.1-2.8
Sept 14	The Quantum Mechanical Postulates	Chapter 3, sections 3.1-3.5
Sept 16, 21	Using Quantum Mechanics on Simple Systems	Chapter 4, sections 4.1-4.4
Sept 23	The Particle in a Box and the Real World	Chapter 5, sections 5.1-5.3,5.5-5.6
Sept 28, 30	Commuting and Non-commuting Operators	Chapter 6, sections 6.1, 6.3-6.5
Oct 5	**Midterm Exam 1 (Chapters 1-6)**	

Oct 7, 12	Models for the Vibrations and Rotations of Molecules	Chapter 7, sections 7.1-7.7
Oct 14	The Vibrational and Rotational Spectroscopy of Diatomics	Chapter 8, sections 8.1-8.6
Oct 19, 21	The Hydrogen Atom	Chapter 9, sections 9.1-9.6
Oct 26, 28	Many-Electron Atoms	Chapter 10, sections 10.1-10.6 (also section 6.2)
Nov 2	Quantum States for Many-Electron Atoms and Atomic Spectroscopy	Chapter 11, sections 11.1-11.4, 11.11
Nov 4, 9	The Chemical Bond in Diatomic Molecules	Chapter 12, sections 12.1-12.9
Nov 11	**Midterm Exam 2 (Chapters 7-12)**	
Nov 16, 18	Molecular Structure and Energy Levels for Polyatomic Molecules	Chapter 13, sections 13.1-13.2, 13.4-13.5, 13.7
Nov 23	Electronic Spectroscopy	Chapter 14, sections 14.1-14.4, 14.6-14.8
Nov 30 Dec 2	Computational Chemistry	Chapter 15, sections 15.1-15.8, 15.10
Dec 7, 9	Molecular Symmetry	Chapter 16, sections 16.1-16.4
Dec 16, 10:30 AM – 1:00 PM	**Comprehensive Final Exam** Final Exam: Thurs. Dec 16, 10:30 AM – 1:00 PM, Latter Hall room 2	