UNIVERSITY OF CALGARY
FACULTY OF SCIENCE
DEPARTMENT OF CHEMISTRY
COURSE SYLLABUS
FALL 2019

1. Course: CHEMISTRY 373, Physical Chemistry II: Quantum Mechanics and Symmetry

LEC	DAYS	TIME	ROOM	PROFESSOR	OFFICE	EMAIL	OFFICE HOURS
L01	TR	11:00-12:15	ENG 224	Dr. Belinda Heyne	SB 419	bjmheyne@ucalgary.ca	TBA

To avoid IT problems, it is recommended that the students use their U of C account for all course correspondence. Please use "CHEM 373 inquiry" as the Subject of your e-mail.

Desire 2 Learn (D2L): CHEM 373 L01 - (Fall 2019) – Physical Chemistry: Quantum Chemistry
https://d2l.ucalgary.ca/d2l/home/278281

Departmental Office: Room SA 229, Tel: (403) 220-5341, e-mail: uginfo@chem.ucalgary.ca

2. Course Description: ***Lectures:*** Chem 373 presents an introduction to fundamental concepts in quantum chemistry. After a brief overview of the historical development of quantum theory, this course examines the Schrödinger equation and study how it depicts the behavior of very light particles. The quantum description of rotating and vibrating molecules is compared to the classical picture and the quantum description of the electronic structure of atoms is examined. Applications to chemical bonding including valence bond and molecular orbital theory is also covered. **Laboratory:** Experimental illustrations of quantum concepts will be combined with theoretical applications of quantum chemistry, such as computational modeling and selection rules in spectroscopy.

3. Recommended Textbook: Physical Chemistry, 3rd Edition, Thomas Engel and Philip Reid (available in the Bookstore)

4. Topics Covered and Suggested Readings:

Course Contents	**Chapter in Textbook** *(not all sections will be covered)*
Introduction to quantum theory	Chapters 12, 13 & 14
Historical development	
Wave nature, de Broglie wavelength	
Uncertainty principle	
Schrödinger equation	
Postulates of quantum mechanics	
Simple quantum mechanical systems	Chapters 15, 16 & 17
Particle in a box	
Probability, Expectation values	
Quantum tunneling	
Commuting and non-commuting operators	
Vibrations and rotations of diatomic molecules	Chapter 18
Harmonic oscillator	
Rigid Rotor (particle on a ring)	
Spherical harmonics	
Angular momenta	
Atomic structure and spectra	Chapters 20, 21 & 22
Hydrogen atom	
Hydrogen like atom	
Variation principle	
Helium atom	
Electron spin & Pauli principle	
Hartree-Fock, SCF	

5. Laboratory Experiments: (10 weeks, 3 hours/ week)

1. The Uncertainty Principle (2 weeks)
By performing a computer simulation, students will create wave packets using excel, providing a hands-on experience of Heisenberg uncertainty principle.

2. *The Absorption of Linear Polyene Dyes (2 weeks)*
Experimental illustration of the simple quantum mechanical system, the particle in a 1D box.

3. Harmonic Oscillator (2 week)
By performing a computer simulation, students will explore the classical forbidden region for the Harmonic Oscillator model.

4. Symmetry and Character Tables (2 weeks)
Student will learn to build a character table and to use it to assess the allowance of spectroscopic transitions.

5. Review project (1 week)
Students will critically assess and review a manuscript involving computational methods to investigate the spectroscopic properties of some molecules.

Department Approval Electronically Approved Date August 29, 2019