UNIVERSITY OF CALGARY
FACULTY OF SCIENCE
DEPARTMENT OF CHEMISTRY
COURSE SYLLABUS
FALL 2017

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

LEC	DAYS	TIME	ROOM	PROFESSOR	OFFICE	EMAIL	OFFICE HOURS
L01	TR	11:00-11:50	ST 147	Dr. B. 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 333 inquiry" as the Subject of your e-mail.

Desire 2 Learn (D2L): CHEM 373 L01 - (Fall 2017) - CHEM 373 – Quantum Chemistry
https://d2l.ucalgary.ca/d2l/home/171384

Departmental Office: Room SA 229, Tel: (403) 220-5341, e-mail: chem.undergrad@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 Historical development Wave nature, de Broglie wavelength Uncertainty principle Schrödinger equation Postulates of quantum mechanics	Chapters 12, 13 & 14
Simple quantum mechanical systems Particle in a box Probability, Expectation values Quantum tunneling Commuting and non-commuting operators	Chapters 15, 16 & 17
Vibrations and rotations of diatomic molecules Harmonic oscillator Rigid Rotor (particle on a ring) Spherical harmonics Angular momenta	Chapter 18
Atomic structure and spectra Hydrogen atom Hydrogen like atom Variation principle Helium atom Electron spin & Pauli principle Hartree-Fock, SCF	Chapters 20, 21 & 22

Molecular structure and bonding Chapters 23, 24 & parts of 26
Born-Oppenheimer approximation
Molecular orbital theory, H_2^+
LCAO-MO theory
Qualitative molecular orbital theory
Modern electronic structure theory

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

1. The Uncertainty Principle (2 weeks)

   By performing Young experiment, students will have 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. Introduction to Spartan and use to Construct Models for Molecular Symmetry and Point Groups (1 week)

   Student will get familiar with the modelling software used in this course.

4. Character Tables (2 weeks)

   Student will learn to build a character table and to use it to assess the allowance of spectroscopic transitions.

5. AM1 calculations for selected molecules, assigning symmetry to orbitals and to vibrations. (1 week)

   In this computational laboratory, students will investigate the allowance of spectroscopic transitions for more complex molecules, which cannot be performed manually.

6. Mini research project (1 week)

   Students will critically assess and review a manuscript involving computational methods to investigate the spectroscopic properties of some molecules.

Department Approval: Approved by Department Head Date: September 6, 2017