

Department of Physical Sciences (Chemistry)

CHEM 2160 – 3 Credits
Structure, Bonding and Spectroscopy (3,0,0)
Fall 2023

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Description

This course will provide you with an introduction to quantum chemistry building on topics learned in first year. Concepts such as the wavefunction, operators and eigenvalue equations will be explored as you become familiar with the postulates of Quantum Mechanics. Building on your knowledge of Lewis structures, VSEPR and hybridization theories, Molecular Orbital theory will also be studied, while coupled with elements of photoelectron spectroscopy. Introductory elements of ultraviolet and visible spectroscopy and molecular symmetry (elements, operations, and point groups) will also be discussed.

Prerequisites

CHEM 1500 and CHEM 1510 or 1520 (C- minimum).

Lectures

The official scheduled time for this class is:

Monday, Tuesday, Thursday 10:30 – 11:20 AM OM 2741

Moodle

Electronic course-related materials will be available through Moodle.

Moodle course: CHEM 2160 – Structure, Bonding and Spectroscopy (Mora-Diez)

To access Moodle on the Internet, use the Moodle quick link from the TRU homepage (www.tru.ca).

Assessment

Grades will be assigned on the following basis:

Moodle Quizzes	10%	(One attempt allowed before the closing date)
Test 1	20%	(Thur, Oct 12)
Test 2	20%	(Tue, Nov 7)
Final Exam	50%	(Exam period: Dec 4-16)

Test 1 will evaluate all the topics covered until Oct 6.

Test 2 will evaluate all the topics covered from ca. Oct 2 until Nov 1.

There will be no make-up exams.

If you miss an exam for an approved reason, the value of the Final Exam will be adjusted accordingly.

The Fall semester final exam period is Dec 4-16. Students must be available to write an exam at any time during this period. No special arrangements will be made. No electronic devices, paper dictionaries or translating devices may be used on any closed book Chemistry exam.

A letter grade will be awarded using the TRU Grading System (Policy ED-3-5) on p. 24 of the TRU Calendar. This one-semester course is worth 3 credits.

Reference Texts

I. N. Levine, *Physical Chemistry*, 6th Edition, McGraw-Hill, 2008.

T. Engel, P. Reid, *Physical Chemistry*, 4th Edition, Pearson, 2018.

I. N. Levine, *Quantum Chemistry*, 6th Edition, Prentice Hall, 2009.

Chang: R. Chang, J. Overby, *Chemistry*, 13th Edition, McGraw-Hill, 2019.

Housecroft: C. E. Housecroft, A. G. Sharpe, *Inorganic Chemistry*, 5th Edition, Pearson, 2018.

Academic Policy

It is the responsibility of all students to be aware of TRU Student Academic Policies, Regulations and Procedures found in the TRU Calendar (www.tru.ca/calendar/current/). These include Academic Honesty Policy ED-5-0 (p. 24), Appeals Policy ED-4-0 (p. 25), Students Attendance ED-3-1 (p. 24), and Exams Policy ED-3-9 (p. 24). Forms of Academic Dishonesty are summarized and described on the TRU Calendar, and include cheating, misconduct, fabrication, and plagiarism.

Course Content (may change as the course progresses)**Section 1: Introduction to Quantum Concepts in Chemistry****1.1. Historical background of quantum mechanics**

Wave nature of light; the electromagnetic (EM) spectrum; properties of EM radiation (wavelength, frequency, wavenumber, amplitude); wave-particle properties
The blackbody emission spectra; Planck's theory of quantization
The photoelectric effect; work functions
The atomic line spectra and Bohr's model for an atom
The dual wave-particle behavior of microparticles: de Broglie's equation
The Heisenberg uncertainty principle
Different types of energy levels in molecules; The zero-point energy and the energy at 0 K
Fundamental differences between classical mechanics (CM) and quantum mechanics (QM)

1.2. The wavefunction

Postulate 1: The wavefunction (wf) or state function, Ψ
Characteristics of a well-behaved wf
Complex numbers; complex functions
Physical significance of Ψ
Probability density: Complex conjugates
Normalization condition

1.3. Operators in quantum mechanics

Postulate 2: Observables and QM operators
Operators and some properties (sum, product, commutation)
The Laplacian operator (∇^2)
Evaluation of commutators
Operators in QM: linear momentum operators, the Hamiltonian operator.

1.4. Eigenvalues and eigenvectors

Eigenvalue equations: Eigenvalues and eigenvectors.
Hermitian operators
Postulate 3: Measurement, observable, operator, eigenvalue
Consequence of operators that commute: Simultaneous specification of several exact properties
Operators in QM must be Hermitian and linear
Postulate 4: Expectation (average) value

1.5. The Schrödinger equation

Postulate 5: The Schrödinger equation (time-dependent and time-independent versions)
The Hamiltonian (total energy) operator: expression for several systems (for a particle moving in one and three dimensions, for N particles moving in 3 dimensions)

1.6. The hydrogen atom

The Hamiltonian for the hydrogen and hydrogen-like atoms

Polar coordinates

The solutions to the time-independent Schrödinger equation (wavefunctions and energies)

Radial function and angular component of the wavefunctions

Quantum numbers (n , l , m) and their allowed values

The energy of the system depends on the principal quantum number (n)

Significance of the radial function: graphical interpretation, radial nodes

Probability per unit volume and radial distribution functions (RDF): Interpretation

Significance of the angular component: nodal planes and surfaces

Electron spin and the fourth quantum number

Four quantum numbers and their properties

Section 2: Structure and Bonding Theories

2.1. Lewis structures, VSEPR, hybridization and Valence Bond theories

Self-study from notes and references provided

Rules for constructing Lewis structures

The valence-shell electron-pair repulsion (VSEPR) theory

Molecular geometries predicted by VSEPR

Molecular polarity

Basic aspects of Valence Bond (VB) theory

Hybridization

Types of bonding: σ and π

2.2. Molecular Orbital theory

Basic aspects of Molecular Orbital (MO) theory

Vector spaces: vectors, linear combinations, linearly independent vectors, dimension, basis set/basis functions; the Hilbert space

Pauli exclusion principle, *aufbau* principle and Hund's rule applied to MO theory

Atomic orbital (AO) interactions depend on symmetry and energy

MO diagrams of homonuclear diatomic species: H_2 , X_2 ($X = Li, B, C, N, O, F$) and related ions;

AO mixing and MO ordering implications; electronic configurations

Bond orders and their relationship to bond distances and bond dissociation energies when considering similar chemical systems

MO classification: σ/π , bonding/antibonding/nonbonding, *gerade/ungerade* (for homonuclear diatomic systems)

Frontier orbitals: HOMO (SOMO) and LUMO and their connection with estimates of the ionization energy and the electron affinity of a molecule

MOs and MO expansion coefficients for H_2O

The MO expansion coefficient matrix and its use to understand AO participation in MO formation from calculations

MO diagrams of heteronuclear diatomic species: HF, CO

2.3. Photoelectron spectroscopy

Photoelectron spectroscopy (PES: UPS, XPS) and orbital energies: Koopman's theorem
Ionization or binding energy of an electron: dependence on location
Analysis of PES of atoms and simple molecules: H, He, Li, O, H₂, N₂, HCl, H₂O
Relating MO diagrams to photoelectron spectra
Vertical and adiabatic ionization energy

Section 3: Elements of UV-Visible Spectroscopy

Section 4: Molecular Symmetry

4.1. Introduction to symmetry: Elements and operations

Symmetry in Chemistry: Relevance and Applications
Symmetry elements: planes, axes, points
Symmetry operations: reflection, proper rotation, improper rotation, inversion, identity
Planes of symmetry: horizontal, vertical, dihedral (or diagonal)
Successive operations

4.2. Point groups

Introduction to point groups
Low-symmetry point groups (C_1 , C_s , C_i)
High-symmetry point groups (T_d , O_h , I_h)
Linear point groups ($C_{\infty v}$, $D_{\infty h}$)
 D point groups (D_n , D_{nh} , D_{nd})
 C point groups (C_n , C_{nv} , C_{nh})
 S point groups
Flow diagram for classifying molecular systems into a point group

4.3. Introduction to character tables