

CHEM4054: CHEMICAL BONDING AND MOLECULAR SPECTROSCOPY

Effective Term

Semester A 2025/26

Part I Course Overview

Course Title

Chemical Bonding and Molecular Spectroscopy

Subject Code

CHEM - Chemistry

Course Number

4054

Academic Unit

Chemistry (CHEM)

College/School

College of Science (SI)

Course Duration

One Semester

Credit Units

3

Level

B1, B2, B3, B4 - Bachelor's Degree

Medium of Instruction

English

Medium of Assessment

English

Prerequisites

Nil

Precursors

CHEM2008/BCH2008 Principles of Physical Chemistry

CHEM3016/BCH3016 Physical Chemistry

Equivalent Courses

BCH4054 Chemical Bonding and Molecular Spectroscopy

Exclusive Courses

Nil

Part II Course Details

Abstract

The aim of this course is to enable students to:

- (i) comprehend the fundamental theories of chemical bonding
- (ii) learn about various spectroscopic phenomena and principles
- (iii) apply spectroscopic techniques to different branches of chemistry

By the end of the course, students will have a strong grasp of the basic theories governing chemical bonding. They will also gain knowledge of diverse spectroscopic techniques and their underlying principles. Students will develop crucial ability to utilize spectroscopic methods to investigate and analyze chemical systems across various subdisciplines of chemistry, such as organic, inorganic, analytical, and physical chemistry. The course will provide students with the conceptual foundation and practical skills to effectively leverage spectroscopic tools in their future studies and research endeavors.

Course Intended Learning Outcomes (CILOs)

CILOs		Weighting (if app.)	DEC-A1	DEC-A2	DEC-A3
1	Use molecular orbital theory and valence bond theory to describe chemical bonding in molecules.	20	x	x	
2	Identify the origin of electronic, vibrational and rotational spectra and relate the spectroscopic phenomenon with the quantized energy levels and atomic/molecular properties.	25	x	x	
3	Discover the spectra for simple organic and inorganic compounds qualitatively and extract useful chemical information such as bonding and reactivity from spectroscopic data.	20	x	x	x
4	Describe gas-phase collision dynamics of molecules and reaction mechanisms on potential energy surfaces.	20		x	x
5	Apply the concept in group and symmetry theory in the chemical bonding, reactivity and spectroscopy.	15		x	x

A1: Attitude

Develop an attitude of discovery/innovation/creativity, as demonstrated by students possessing a strong sense of curiosity, asking questions actively, challenging assumptions or engaging in inquiry together with teachers.

A2: Ability

Develop the ability/skill needed to discover/innovate/create, as demonstrated by students possessing critical thinking skills to assess ideas, acquiring research skills, synthesizing knowledge across disciplines or applying academic knowledge to real-life problems.

A3: Accomplishments

Demonstrate accomplishment of discovery/innovation/creativity through producing /constructing creative works/new artefacts, effective solutions to real-life problems or new processes.

Learning and Teaching Activities (LTAs)

LTAs		Brief Description	CILO No.	Hours/week (if applicable)
1	Lectures	Students will be given lectures to learn the origin of quantum mechanics through literature searches	1	
2	Lectures	Students will be given lectures to understand light-matter interactions.	2	
3	Lectures and tutorials	Through a number of case studies the students will discover the techniques of assigning spectra (lectures and tutorials).	3	
4	Lectures and tutorials	Student-centered learning and tutorial exercises provide students opportunities in rationalizing the relationship between chemical bonding and spectroscopic data.	4	
5	Lectures and tutorials	Students will be given lectures about the working principles of spectroscopic methods and guided to apply appropriate spectroscopic methods for chemical analysis through problem-based learning activities.	5	
6	Hands-on demonstration and homework assignments	Students will conduct computational simulations to predict IR, UV/VIS and NMR spectra for chemical molecules and learn to construct potential energy surfaces.	2, 3	

Assessment Tasks / Activities (ATs)

ATs		CILO No.	Weighting (%)	Remarks ("- for nil entry)	Allow Use of GenAI?
1	Homework Assignments	1, 2, 3, 4, 5	12	-	Yes
2	Tests	1, 2, 3, 4, 5	18	The tests are in a closed-book format.	No

Continuous Assessment (%)

Examination (%)

70

Examination Duration (Hours)

2

Minimum Continuous Assessment Passing Requirement (%)

40

Minimum Examination Passing Requirement (%)

40

Assessment Rubrics (AR)**Excellent (A+, A, A-)**

Student completes all the assessment tasks/activities (quizzes, laboratory reports, group presentations, and exams) and demonstrates excellent grasp of the important concepts to various aspects of the topic covered in this course, and can apply these concepts to solve problems with clear and logical explanations. Strong evidence of superior writing and presentation skills.

Good (B+, B, B-)

Student completes all assessment tasks/activities and can describe and explain the important concepts to several aspects of the topic covered in this course. Shows, to some extent, the ability to use concepts for rationalization and to solve problems. Displays effective writing and presentation skills.

Fair (C+, C, C-)

Student completes most of the assessment tasks/activities and can describe some key elements on the topics covered in the course. Shows limited ability to apply concepts, and competent writing and presentation skills.

Marginal (D)

Student has little participation and interest, and demonstrates limited ability in analysis.

Failure (F)

Student has no participation, interest or original thought.

Part III Other Information

Keyword SyllabusQuantum Mechanics

Schrödinger Equation. Wavefunction and Probability. Born-Oppenheimer Approximation. Postulates of Quantum Mechanics. Hydrogen Atom. Many-electron Atom. Spin-Orbit Coupling. Zeeman Effect. Term Symbols.

Chemical Bonding

Particle in a Box. Particle in a Ring. Molecular Orbital Theory. Molecular H_2^+ ion and H_2 . Valence-Bond Theory. Hybridization. Hückel Theory. Antisymmetric Wavefunction.

Symmetry and Group Theory

Irreducible Representations. Direct Products. Symmetry Operations. Projection Operators.

Electronic Absorption Spectroscopy

Franck-Condon Principle. Ground and Excited Electronic States. Vibronic Coupling. Configuration Interaction. Oscillator Strength.

Vibrational Spectroscopy

Infrared and Raman Spectroscopies. Harmonic Oscillator Approximation. Normal Mode of Vibration. Vibrations of Polyatomics. Anharmonicity and Vibrational Coupling. Birge-Sponer Plot. Symmetry Selection Rules. Transition Probability and Dipole Moment Operator. Zero-point Energy.

Rotational Spectroscopy

Microwave Spectroscopy. Rigid Rotor Model. Rotational Transitions. Maxwell-Boltzmann Distribution. Centrifugal Distortion. Ro-vibrational Transitions. P-, Q- and R- branches. Selection Rules. Density of States.

Gas-Phase Reaction Dynamics

Hard-Sphere Collision Theory. Potential Energy Surfaces. Collisional Activation. Impact Parameter. Reaction Cross Section. Internal Energy, Velocity and Angular Distribution.

Spectral Simulation

Predictions of IR, UV/VIS and NMR spectra. Construction of potential energy surfaces.

Reading List

Compulsory Readings

Title	
1	Physical Chemistry: Quantum Chemistry and Spectroscopy, Thomas Engel and Philip Reid, Pearson, 4th Ed., 2018.

Additional Readings

Title	
1	Symmetry and Spectroscopy: An Introduction to Vibrational and Electronic Spectroscopy by Daniel C. Harris and Michael D. Bertolucci, Dover, 1989