CHEM4054: CHEMICAL BONDING AND MOLECULAR SPECTROSCOPY

Effective Term
Semester A 2022/23

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

This course aims to present the basic theories of chemical bonding and applications of some important spectroscopic techniques which are essential in all branches of chemistry.

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	Understand 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	Comprehend 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.

Teaching and Learning Activities (TLAs)

	TLAs	Brief Description	CILO No.	Hours/week (if applicable)
1	Lectures	Students will learn the origin of quantum mechanics through literature searches (lectures)	1	
2	Lectures	Large group interactive activities will enable students to understand light-matter interactions (lectures)	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	Tutorials	Student-centered learning and student oral presentation to provide students opportunities in rationalizing the relationship between chemical bonding and spectroscopic data (tutorials)	4	
5	Tutorials	Problem-based learning activities to provide opportunities for students to design appropriate spectroscopic methods for chemical analysis (tutorials)	5	
6	Hands-on demonstration	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 (e.g. Parameter for GenAI use)
1	Homework Assignments	1, 2, 3, 4, 5	12	
2	Tests	1, 2, 3, 4, 5	18	

Continuous Assessment (%)

30

Examination (%)

70

Examination Duration (Hours)

2

Additional Information for ATs

Starting from Semester A, 2015-16, students must satisfy the following minimum passing requirement for courses offered by CHEM:
"A minimum of 40% in both coursework and examination components."

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 Syllabus

Quantum 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. Molecular Orbital Theory. Molecular H2+ ion and H2. 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 Spectroscopyby Daniel C. Harris and Michael D. Bertolucci, Dover, 1989