香港城市大學
City University of Hong Kong

SYL

Course Syllabus

offered by Department of Chemistry
with effect from Semester A 2021/22

This form is for the completion by the *Course Leader*. The information provided on this form is the official record of the course. It will be used for the City University's database, various City University publications (including websites) and documentation for students and others as required.

Please refer to the Explanatory Notes on the various items of information required.

Prepared / Last Updated by:

Name:	Dr. K C Lau	Academic Unit:	Department of Chemistry
Phone/email:	3442 6849 / kaichung@cityu.edu.hk	Date:	5 July 2021

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Part I Course Overview

Course Title:	Chemical Bonding and Molecular Spectroscopy
Course Code:	CHEM4054
Course Duration:	1 semester
Credit Units:	3 credits
Level:	B4
Proposed Area: *(for GE courses only)*	☐ Arts and Humanities ☐ Study of Societies, Social and Business Organisations ☐ Science and Technology
Medium of Instruction:	English
Medium of Assessment:	English
Prerequisites: *(Course Code and Title)*	
Precursors: *(Course Code and Title)*	CHEM2008/BCH2008 Principles of Physical Chemistry CHEM3016/BCH3016 Physical Chemistry
Equivalent Courses: *(Course Code and Title)*	BCH4054 Chemical Bonding and Molecular Spectroscopy
Exclusive Courses: *(Course Code and Title)*	Nil

Part II Course Details

1. Abstract

(A 150-word description about the course)

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.

2. Course Intended Learning Outcomes (CILOs)

(CILOs state what the student is expected to be able to do at the end of the course according to a given standard of performance.)

No.	CILOs[#]	Weighting* (if applicable)	Discovery-enriched curriculum related learning outcomes (please tick where appropriate)		
			A1	*A2*	*A3*
1.	Use molecular orbital theory and valence bond theory to describe chemical bonding in molecules.	20%	✓	✓	
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%	✓	✓	
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%	✓	✓	✓
4.	Comprehend gas-phase collision dynamics of molecules and reaction mechanisms on potential energy surfaces.	20%		✓	✓
5.	Apply the concept in group and symmetry theory in the chemical bonding, reactivity and spectroscopy.	15%		✓	✓
	** If weighting is assigned to CILOs, they should add up to 100%.*	100%			

[#] Please specify the alignment of CILOs to the Gateway Education Programme Intended Learning outcomes (PILOs) in Section A of Annex.

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 self-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.

3. Teaching and Learning Activities (TLAs)

(TLAs designed to facilitate students' achievement of the CILOs.)

TLA	Brief Description	CILO No.					Hours/week (if applicable)
		1	2	3	4	5	
Lectures	Students will learn the origin of quantum mechanics through literature searches (lectures)	✓					
Lectures	Large group interactive activities will enable students to understand light–matter interactions (lectures)		✓				
Lectures and tutorials	Through a number of case studies the students will discover the techniques of assigning spectra (lectures and tutorials)			✓			
Tutorials	Student-centered learning and student oral presentation to provide students opportunities in rationalizing the relationship between chemical bonding and spectroscopic data (tutorials)				✓		
Tutorials	Problem-based learning activities to provide opportunities for students to design appropriate spectroscopic methods for chemical analysis (tutorials)					✓	
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.		✓	✓			

4. Assessment Tasks/Activities (ATs)

(ATs are designed to assess how well the students achieve the CILOs.)

Assessment Tasks/Activities	CILO No.					Weighting*	Remarks
	1	2	3	4	5		
Continuous Assessment: 30%							
Homework Assignments	✓	✓	✓	✓	✓	12%	
Tests	✓	✓	✓	✓	✓	18%	
Examination: 70% (duration: 2 hours)							
** The weightings should add up to 100%.*						100%	

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."

5. Assessment Rubrics

(Grading of student achievements is based on student performance in assessment tasks/activities with the following rubrics.)

Grade	Grade Definitions	
A+ A A-	Excellent	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.
B+ B B-	Good	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.
C+ C C-	Fair	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.
D	Marginal	Student has little participation and interest, and demonstrates limited ability in analysis.
F	Failure	Student has no participation, interest or original thought.

Part III Other Information (more details can be provided separately in the teaching plan)

1. Keyword Syllabus

(An indication of the key topics of the course.)

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 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.

2. Reading List

2.1 Compulsory Readings

(Compulsory readings can include books, book chapters, or journal/magazine articles. There are also collections of e-books, e-journals available from the CityU Library.)

1.	Physical Chemistry: Quantum Chemistry and Spectroscopy, Thomas Engel and Philip Reid, Pearson, 4th Ed., 2018.
2.	
3.	

2.2 Additional Readings

(Additional references for students to learn to expand their knowledge about the subject.)

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

Annex
(for GE courses only)

A. Please specify the Gateway Education Programme Intended Learning Outcomes (PILOs) that the course is aligned to and relate them to the CILOs stated in Part II, Section 2 of this form:

GE PILO	**Please indicate which CILO(s) is/are related to this PILO, if any** ***(can be more than one CILOs in each PILO)***
PILO 1: Demonstrate the capacity for self-directed learning	
PILO 2: Explain the basic methodologies and techniques of inquiry of the arts and humanities, social sciences, business, and science and technology	
PILO 3: Demonstrate critical thinking skills	
PILO 4: Interpret information and numerical data	
PILO 5: Produce structured, well-organised and fluent text	
PILO 6: Demonstrate effective oral communication skills	
PILO 7: Demonstrate an ability to work effectively in a team	
PILO 8: Recognise important characteristics of their own culture(s) and at least one other culture, and their impact on global issues	
PILO 9: Value ethical and socially responsible actions	
PILO 10: Demonstrate the attitude and/or ability to accomplish discovery and/or innovation	

GE course leaders should cover the mandatory PILOs for the GE area (Area 1: Arts and Humanities; Area 2: Study of Societies, Social and Business Organisations; Area 3: Science and Technology) for which they have classified their course; for quality assurance purposes, they are advised to carefully consider if it is beneficial to claim any coverage of additional PILOs. General advice would be to restrict PILOs to only the essential ones. (Please refer to the curricular mapping of GE programme: http://www.cityu.edu.hk/edge/ge/faculty/curricular_mapping.htm.)

B. Please select an assessment task for collecting evidence of student achievement for quality assurance purposes. Please retain at least one sample of student achievement across a period of three years.

Selected Assessment Task
Group project on a spectroscopic technique.