Course Specifications

Course Title:	**Quantum Chemistry and Its Applications**
Course Code:	**532CHEM-2**
Program:	**Master of Science in Chemistry**
Department:	**Chemistry**
College:	**Science**
Institution:	**King Khalid University**

Table of Contents

A. Course Identification

1. Credit hours:	**2**
2. Course type	
a.	University ☐ College ☐ Department ■ Others ☐
b.	Required ■ Elective ☐
3. Level/year at which this course is offered:	**Level 2 – year 1**
4. Pre-requisites for this course (if any)**:**	**No prerequisite**
5. Co-requisites for this course (if any)**:**	**No co-requisite**

6. Mode of Instruction (mark all that apply)

No	Mode of Instruction	Contact Hours	Percentage
1	Traditional classroom	2	100%
2	Blended	0	0%
3	E-learning	0	0%
4	Correspondence	0	0%
5	Other	0	0%

7. Actual Learning Hours (based on academic semester)

No	Activity	Learning Hours
Contact Hours		
1	Lecture	30
2	Laboratory/Studio	0
3	Tutorial	0
4	Others (specify)	0
	Total	30
Other Learning Hours*		
1	Study	30
2	Assignments	20
3	Library	15
4	Projects/Research Essays/Theses	15
5	Others (specify)	0
	Total	80

* The length of time that a learner takes to complete learning activities that lead to achievement of course learning outcomes, such as study time, homework assignments, projects, preparing presentations, library times

B. Course Objectives and Learning Outcomes

1. Course Description

The course of "Quantum Chemistry and Its Applications" introduces the basic principles of quantum chemistry and its applications to the description of atoms and molecules and their interactions with other molecular systems and electromagnetic radiation. In addition, this

course describes the electronic structure of an atom and the arrangement of electrons around a nucleus, as well as the electronic structure of molecules and chemical bonding among atoms in a molecule.

2. Course Main Objective

- Describe, analyze, and apply the postulates of quantum mechanics to for simple chemical systems that model the translational, vibrational, and rotational motions.
- Write and solve the Schrödinger equation in 1, 2, or 3 dimensions for typical model systems, and interpret the meaning and significance of the solutions.
- Describe the structure of hydrogenic and many-electron atoms including atomic orbitals and their energies and illustrate how quantum mechanics prescribes the periodic table.
- Demonstrate how to use Slater determinants of spin and spatial eigenfunctions to build antisymmetric atomic wavefunctions.
- Analyze and interpret the spectra of hydrogenic and complex atoms.

3. Course Learning Outcomes

	CLOs	Aligned PLOs
1	**Knowledge:**	
1.1	Describe the postulates of quantum mechanics for simple chemical systems that model the translational, vibrational, and rotational motions.	K4 and K5
1.2	Describe the structure of hydrogenic and many-electron atoms including atomic orbitals and their energies.	K4 and K5
2	**Skills :**	
2.1	Illustrate how quantum mechanics prescribes the periodic table.	S4
2.2	Analyze the postulates of quantum mechanics for simple chemical systems that model the translational, vibrational, and rotational motions.	S4
2.3	Analyze and interpret the spectra of hydrogenic and complex atoms.	S4
2.4	Write and solve the Schrödinger equation in 1, 2, or 3 dimensions for typical model systems, and interpret the meaning and significance of the solutions.	S4
2.5	Demonstrate how to use Slater determinants of spin and spatial eigenfunctions to build antisymmetric atomic wavefunctions.	S4
3	**Competence:**	
3.1	Apply the postulates of quantum mechanics to simple chemical systems that model the translational, vibrational, and rotational motions.	C2 and C3
3.2	Analyze and interpret the spectra of hydrogenic and complex atoms.	C2 and C3

C. Course Content

No	List of Topics	Contact Hours

1	Introduction to Quantum Theory	2
2	Course Introduction	2
3	The Quantum Theory of Motion	4
4	Translational motion	4
5	Vibrational motion	2
6	Rotational motion	2
7	Atomic structure and spectra	4
8	Hydrogenic atoms	4
9	Many-electron atoms	4
10	Atomic spectra	2
Total		30

D. Teaching and Assessment

1. Alignment of Course Learning Outcomes with Teaching Strategies and Assessment Methods

Code	Course Learning Outcomes	Teaching Strategies	Assessment Methods
1.0	**Knowledge**		
1.1	Describe the postulates of quantum mechanics for simple chemical systems that model the translational, vibrational, and rotational motions.	Lectures and dialogue and discussion.	Homework and exams
1.2	Describe the structure of hydrogenic and many-electron atoms including atomic orbitals and their energies.		
2.0	**Skills**		
2.1	Illustrate how quantum mechanics prescribes the periodic table.	Lectures and dialogue and discussion.	Homework and exams
2.2	Analyze the postulates of quantum mechanics for simple chemical systems that model the translational, vibrational, and rotational motions.		
2.3	Analyze and interpret the spectra of hydrogenic and complex atoms.		
2.4	Write and solve the Schrödinger equation in 1, 2, or 3 dimensions for typical model systems, and interpret the meaning and significance of the solutions.		
2.5	Demonstrate how to use Slater determinants of spin and spatial eigenfunctions to build antisymmetric atomic wavefunctions.		
3.0	**Competence**		
3.1	Apply the postulates of quantum mechanics to simple chemical systems that model the translational, vibrational, and rotational motions.	Lectures and dialogue and discussion.	Homework and exams

3.2	Analyze and interpret the spectra of hydrogenic and complex atoms.		

2. Assessment Tasks for Students

#	*Assessment task	Week Due	Percentage of Total Assessment Score
1	Homework Assignments	Every two weeks	15
2	Oral discussion	Every week	5
3	First Mid-Exam	6	15
4	Second Mid-Exam	12	15
5	Final Exam	16	50

***Assessment task** (i.e., written test, oral test, oral presentation, group project, essay, etc.)

E. Student Academic Counseling and Support

Arrangements for availability of faculty and teaching staff for individual student consultations and academic advice :

10 office hours are offered for students for individual consultations. Communications are available on-site, or through the blackboard system

F. Learning Resources and Facilities

1.Learning Resources

Required Textbooks	Atkins' Physical Chemistry. Peter Atkins and Julio dePaula. 2014, 10th ed. Oxford University Press.
Essential References Materials	Quantum Chemistry and Spectroscopy. Thomas Engel. 2012. 3rd ed. Prentice Hall. Molecular Quantum Mechanics. Peter W Atkins and Ronald S Friedman. 2010. 5th ed. Oxford University Press.
Electronic Materials	E-Learning Deanship (http://elc.kku.edu.sa/) Atkins & de Paula: Physical Chemistry 10e (http://global.oup.com/uk/orc/chemistry/pchem10e/) Applicable software for molecular modeling such as Spartan
Other Learning Materials	None

2. Facilities Required

Item	Resources
Accommodation Classrooms, laboratories, demonstration) (.rooms/labs, etc	One classroom with at least 20 seats and equipped with projector and Internet access One demonstration room with at least 20 seats and equipped with projector and Internet access.

Technology Resources AV, data show, Smart Board, software,) (.etc	Data show
Other Resources Specify, e.g. if specific laboratory) equipment is required, list requirements or (attach a list	

G. Course Quality Evaluation

Evaluation Areas/Issues	Evaluators	Evaluation Methods
Course delivering	Student	Questionnaire
Course contents (update)	Plan and curriculum committee	Report
Teaching materials	Faculty	Meeting
Learning materials	Student	Discussion
Assignment	Program instructor and Faculty	Report
Exams	Program instructor and Faculty	Report

Evaluation areas (e.g., Effectiveness of teaching and assessment, Extent of achievement of course learning outcomes, Quality of learning resources, etc.)
Evaluators (Students, Faculty, Program Leaders, Peer Reviewer, Others (specify)
Assessment Methods (Direct, Indirect)

H. Specification Approval Data

Council / Committee	**Chemistry Department Council**
Reference No.	**Session number 22**
Date	**27/04/2021M / 15/09/1442H**