Course specifications

(Postgraduate Degree)

Course Title:	**Chemical Physics**
Course Code:	**CHEM 631**
Program:	**Doctor of Philosophy in Chemistry (PhD)**
Department:	**Chemistry**
College:	**Science**
Institution:	**King Saud University**

Table of Contents

A. Course Identification

1. Credit hours: 3 (3 +0 +0)
2. Course type ☒ Required ☐ Elective
3. Level/year at which this course is offered: 2nd Level / 1st Year
4. Pre-requisites for this course (if any)**:** MSc in chemistry
5. Co-requisites for this course (if any)**:** None

6. Mode of Instruction (mark all that apply)

No	Mode of Instruction	Contact Hours	Percentage
1	**Traditional classroom**	42	100%
2	**Blended**		
3	**E-learning**		
4	**Correspondence**		
5	**Other**		

7. Actual Learning Hours (based on academic semester)

No	Activity	Learning Hours
Contact Hours		
1	**Lecture**	42
2	**Laboratory/Studio**	
3	**Seminars**	
4	**Others** (specify)	
	Total	42
Other Learning Hours*		
1	**Study**	
2	**Assignments**	30
3	**Library**	
4	**Projects/Research Essays/Theses**	
5	**Others** (specify)	
	Total	30

* 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

A Lengthend discussion covers the topics of statistical thermodynamics and molecular spectroscopy.

2. Course Main Objective

At the end of the course students will ..

1. understand the principal of quantum theory, energy quantization and the terms of Schrödinger equation and wave function.
2. extract all the dynamical information possible about the system from its wave function.
3. realize how thermodynamic properties emerge from the properties of atoms and molecules.
4. calculate the partition function of a system.
5. express all of the usual thermodynamic quantities such as internal energy, entropy, heat capacity, and so on in terms of the partition function.
6. understand how molecules store energy.
7. gain an in-depth knowledge and expertise in the field of molecular spectroscopy.
8. understand the molecular spectroscopy of diatomic and polyatomic molecules.
9. use the principles of quantum theory to calculate the properties of microscopic particles in motion.
10. learn how to use molecular spectra to obtain information about the molecular system such as electronic energy levels, bond lengths, bond angles, and bond strength.

3. Course Learning Outcomes

Course Learning Outcomes (CLOs)		Aligned PLOs*
1	**Knowledge**	
1.1	To describe the fundamental concepts of quantum chemistry.	K1
1.2	To interpret the partition function and how to calculate it in a number of simple cases.	K3
1.3	To recognize the importance of statistical thermodynamics in providing the link between the microscopic properties of matter and its bulk properties.	K2
1.4	To obtain advanced knowledge about the interactions of electromagnetic radiation and matter and their applications in spectroscopy.	K2
1.5	To understand rotational, vibrational, Raman and electronic spectra.	K1
1.6	To select the molecular spectroscopy methods suitable for solving given scientific problem.	K3
2	**Skills**	
2.1	To acquire insight into the molecular origins of chemical properties.	S3
2.2	To explain how molecules or particles of a system are distributed over the available energy levels.	S2
2.3	To derive thermodynamic functions, such as the internal energy, entropy, Helmholtz and Gibbs energy etc. in terms of partition function.	S1
2.4	To relate microscopic properties of atoms and molecules to bulk properties using partition function.	S1
2.5	To explain the interaction between light and matter at the atomic and molecular level.	S2
3	**Competence**	
3.1	To communicate ideas via presentation and group discussion.	C1

* Program Learning Outcomes

C. Course Content

No	List of Topics	Contact Hours
1	The principles of quantum theory	4
2	The quantum theory of motion - Translational motion - Vibrational motion - Rotational motion - Electronic motion	5
3	The Boltzmann distribution - Configurations and weights - The derivation of the Boltzmann distribution	3
4	Molecular partition functions - The significance of the partition function - Contributions to the partition function	2
5	Molecular energies - The basic equations: Mean energy of a two-level system - Contributions of the fundamental modes of motion	2
6	The canonical ensemble - The concept of ensemble - The mean energy of a system - Independent molecules revisited - The variation of energy with volume	3
7	The internal energy and the entropy - The calculation of internal energy - Entropy and the partition function	4
8	Derived functions - Deriving an equation of state, Calculating a standard Gibbs energy of formation from partition functions. - Equilibrium constants	5
9	The basis of absorption and emission of radiation by molecular species - The wave properties of the light - The quantum theory of light - Molecular energies and the Born-Oppenheimer approximation - The types of molecular motion and spectroscopy associated with each	4
10	Vibrational spectroscopy - Diatomic vibration spectra (Harmonic Oscillator model and Morse oscillator Model) - Vibrational Polyatomic Infrared Spectroscopy Local Modes and Group Frequencies	4
11	Rotational spectroscopy - Microwave spectroscopy - Rotational Raman spectroscopy	3
12	Electronic spectroscopy - Electronic spectra of diatomic molecules - Electronic spectra of polyatomic molecules	3
Total		

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	To describe the fundamental concepts of quantum chemistry.	Interactive methods: - *Brainstorming* - *Discussion* Integrating Technology (Visualization): - *Interactive whiteboard to display images and videos).* Lecture	Midterm exams Final exam
1.2	To interpret the partition function and how to calculate it in a number of simple cases.		
1.3	To recognize the importance of statistical thermodynamics in providing the link between the microscopic properties of matter and its bulk properties.		
1.4	To obtain advanced knowledge about the interactions of electromagnetic radiation and matter and their applications in spectroscopy.		
1.5	To understand rotational, vibrational, Raman and electronic spectra.		
1.6	To select the molecular spectroscopy methods suitable for solving given scientific problem.		
2.0	**Skills**		
2.1	To acquire insight into the molecular origins of chemical properties.	Interactive methods: - *problem-solving exercises.*	Midterm exams Final exam
2.2	To explain how molecules or particles of a system are distributed over the available energy levels.		
2.3	To derived thermodynamic functions, such as the internal energy, entropy, Helmholtz and Gibbs energy etc. in terms of partition function.		
2.4	To relate microscopic properties of atoms and molecules to bulk properties using partition function.		
2.5	To explain the interaction between light and matter at the molecular level.		
3.0	**Competence**		
3.1	To communicate ideas via presentation and group discussion.	Presentation and discussion.	Power point presentation

sessment Tasks for Students

#	Assessment task*	Week Due	Percentage of Total Assessment Score
1	Midterm exam 1	7	20 %
2	Midterm exam 2	13	20 %
4	Presentation	14	10 %

#	Assessment task*	Week Due	Percentage of Total Assessment Score
5	Final exam	15	40 %

***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:
Students can reach their course instructor during regular office hours or by arranging an appointment.

F. Learning Resources and Facilities

1. Learning Resources

Required Textbooks	1. Peter Atkins and Julio de Paula, ***Physical Chemistry***, 10th edition, W. H. Freeman and company, New York. 2. D. A. McQuarrie and J. D. Simon, ***Physical Chemistry: A Molecular Approach***. (University Science Books, Sausalito, California, 1997). 3. C. N. Banwell, ***Fundamentals of Molecular Spectroscopy***, 3re edition, McGraw-Hill Book Company, 1983.
Essential Reference Materials	1. A. Cooksy, *Physical chemistry,* ***Quantum Chemistry and Molecular Interactions***, Pearson Education, 2014. 2. A. Cooksy, *Physical chemistry,* ***Thermodynamics, Statistical Mechanics and Kinetics***, Pearson Education, 2014.
Electronic Materials	
Other Learning Materials	

2. Educational and research Facilities and Equipment Required

Item	Resources
Accommodation (Classrooms, laboratories, demonstration rooms/labs, etc.)	Regular classroom.
Technology Resources (AV, data show, Smart Board, software, etc.)	- Smart board - Internet connection
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
Student comprehension	Instructor	Quizzes and Exams
Course content	Faculty	Periodic review of the course content
Student perspective	Students	A paper or electronic questionnaire

Evaluation Areas/Issues (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	
Reference No.	
Date	