DEPARTMENT OF CHEMISTRY				*CLASS: I M.Sc. Chemistry*				
Sem	**Course Type**	**Course Code**	**Course Title**	**Credits**	**Contact Hours/week**	**CIA**	**Ext**	**Total**
I	Major Core	21P2CMC6	Physical Chemistry – II	4	5	25	75	100

Nature of Course				
Knowledge and skill	✓		Employability oriented	
Skill oriented			Entrepreneurship oriented	

Course Objectives: *The objective of this course is to make the student*

(i) To utilize the principles of quantum mechanics of simple systems in order to gain knowledge on the applications of quantum mechanics.

(ii) To infer knowledge on the quantum mechanical treatment of multi electron atoms.

(iii) To know the various basic theories of adsorption.

(iv) To understand the mode of distribution of energy among gaseous molecules and their dynamic properties

(v) To know colligative properties of solution and application of phase rule for three component system

Unit	Description	Hours	K-Level	CLO
I	**QUANTUM CHEMISTRY-I** Black body radiation-Planck's quantum theory-Wave particle duality-Uncertainty Principle. Operators-linear, commutation, Hermitian and Hamiltonian operators. Eigen functions and Eigen values-Postulates of quantum mechanics. Derivation of Schrodinger's time-independent wave equation and its application to particle in a one-dimensional box, particle in a three-dimensional box, harmonic oscillator, rigid rotor and hydrogen atom.	15	Up to K3	CLO-1
II	**QUANTUM CHEMISTRY-II** Born-Oppenheimer approximation-Hydrogen molecule ion. LCAO-MO and VB treatments of the hydrogen molecule. Anti-symmetry and Pauli's exclusion principle. Slater detrimental wave function. The variation theorem and Perturbation theory. Applications of variation method and perturbation theory to the helium atom. Hybridization-determination of bond angles of sp, sp^2 and sp^3 hybridizations. Huckel pi electron (HMO) theory and its applications to ethylene, butadiene and benzene. A brief idea of Hartree and Hartree-Fock self-consistent field theory.	15	Up to K4	CLO-2
III	**SURFACE CHEMISTRY** Surface Phenomena, Gibbs adsorption isotherm, types of adsorption isotherms BET isotherms and derivation of BET isotherm equation, Adsorption with dissociation – competitive adsorption non-ideal adsorption. Thermodynamics of adsorption surface area determination. Kinetics of surface reactions involving adsorbed species, Langmuir-Hinshelwood mechanism, Langmuir-Rideal mechanism, Rideal-Eley mechanism.	15	Up to K3	CLO-3

IV	**GASEOUS AND LIQUID STATE** Equations of states-Molecular speeds-Max Well distribution of molecular velocities- one, two and three dimensions-Energy distribution-Maxwell-Boltzmann distribution law-Principle of equipartition of energy and heat capacity-Rotation, vibration and Translational degree of freedom-Molecular Collisions-Mean free path-Transport Properties-Thermal conductivity Viscosity and diffusion of gases. Liquid State-Theory of liquids-Internal Pressure-Liquid crystals-Nematic, Cholester.	15	Up to K4	CLO-4
V	**COLLIGATIVE PROPERTIES & PHASE RULE** Colligative properties and Raoult's law definition only - Experimental Determination - Lowering of vapour pressure – Elevations of boiling point – depression of freezing point – Osmosis – Osmotic pressure. Basic terminologies of phase rule: Three component system: three liquid system, one liquid and two solid systems - two liquid and one solid system – three solids system.	15	Up to K2	CLO-5

Books for study:

1. A.K. Chandra, Introduction to Quantum Chemistry, Tata McGraw Hill, **1997**.
2. B.R.Puri, L.R.Sharma and M.S.Pathania, Principles of Physical Chemistry, 47th edition, Vishal Publishing Co, **2016.**
3. P. Atkins and J. de Paula, Physical Chemistry, Ninth Edition, Oxford University Press, New Delhi, **2011.**

Books for reference:

1. R.K. Prasad, Quantum Chemistry, Wiley Eastern, **1993**.
2. P.W. Atkins, Molecular Quantum Mechanics, Oxford University Press, Oxford, **1983.**
3. H. Eyring, J. Walter and G. Kimball, Quantum Chemistry, John Wiley and Sons, New York, **1944**.
4. G.M. Barrow, Physical Chemistry, 6th edn, McGraw-Hill Inc., US, **1996**.
5. N. Kundu and S.K. Jain, Physical Chemistry, S. Chand & Company Ltd. **2000.**
6. K.S. Birdi Surface Chemistry Essentials, CRC Press, **2013**

Web resources:

1. https://en.wikipedia.org/wiki/Quantum_chemistry#:~:text=Quantum%20chemistry%2C%20also%20called%20molecular,central%20topics%20in%20quantum%20chemistry.
2. https://chem.libretexts.org/Courses/Mount_Royal_University/Chem_1201/Unit_1%3A_Quantum_Chemistry.
3. https://byjus.com/jee/surface-chemistry/
4. https://dradchem.wordpress.com/tag/colligative-properties/

Rationale for Nature of the course

The course enable the students to comprehend the fundamental knowledge and facts in quantum chemistry and advanced knowledge of surface chemistry, gaseous state, liquid state and phase rule.

Activities having direct bearing on Skill development/ Employability/Entrepreneurship

The students able to understand and apply set of mathematical principles that attempt to explain the behavior of atoms, sub-atomic particles and properties of molecules in gaseous state. They can also differentiate, analyze classical and quantum mechanics. They could be familiar with properties of liquid state such as crystalline property, colligative properties and able to comprehend the phase rule of three component system.

Pedagogy

- Chalk-Talk class room activities
- Seminar
- Assignment and Quiz through ICT- Mode

Lesson Plan

Unit	Descriptions	Hours	Lecture Mode
	QUANTUM CHEMISTRY-I		
	Black body radiation-Planck's quantum theory-Wave particle duality-Uncertainty Principle	3	
	Operators-linear, commutation, Hermitian and Hamiltonian operators, Eigen functions and Eigen values	3	
	Postulates of quantum mechanics, Derivation of Schrodinger's time-independent wave equation application to particle in a one-dimensional	3	
I	Simple harmonic oscillator	3	Chalk and talk/PPT
	Rigid rotor and hydrogen atom	3	
	QUANTUM CHEMISTRY-II		
	Born-Oppenheimer approximation-Hydrogen molecule ionLCAO-MO and VB treatments of the hydrogen molecule.	3	
	Anti-symmetry and Pauli's exclusion principle Slater detrimental wave function. The variation theorem and Perturbation theory	3	
	Applications of variation method and perturbation theory to the helium atom. Hybridization-determination of bond angles of sp, sp^2 and sp^3	3	Chalk and talk/PPT/ Assignment/Quiz
	Huckel pi electron (HMO) theory and its applications to ethylene, butadiene and benzene	3	
II	A brief idea of Hartree and Hartree-Fockself-consistent field theory.	3	
	SURFACE CHEMISTRY		
	Surface Phenomena, Gibbs adsorption isotherm, types of adsorption isotherms BET isotherms. Derivation of BET isotherm equation	5	Chalk and talk/PPT/ Group discussion
	Adsorption with dissociation – competitive adsorption non-ideal adsorption. Thermodynamics of adsorption surface area determination.	5	
	Kinetics of surface reactions involving adsorbed species, Langmuir-Hinshelwood mechanism Langmuir-Rideal mechanism, Rideal-Eley	5	
	GASEOUS AND LIQUID STATE		
	Equations of states-Molecular speeds-Max Well distribution of molecular velocities one, two and three dimensions-Energy	3	
	Principle of equipartition of energy and heat capacity Rotational, vibrational and Translational degrees of freedom	3	Chalk and talk/PPT/ Assignment/ Quiz
	Collisions number -Mean free path Transport properties-. Thermal conductivity Viscosity diffusion of gases	4	
	Liquid State-Theory of liquids Internal Pressure-Liquid crystals-	5	
V	**COLLIGATIVE PROPERTIES & PHASE RULE**		
	Colligative properties and Raoult's law definition Experimental Determination - Lowering of vapour pressure – Elevations of boiling	5	Chalk and talk/PPT/ Group discussio
	Experimental Determination depression of freezing point – Osmosis –	3	
	Basic terminologies of phase rule: - Three component system: three	3	
	one liquid and two solid systems Two liquid and one solid system	4	

Course Learning Outcomes:

After successful completion of this course, the student will be able to

CLOs	CLO statement	Knowledge level
CLO-1	Organize basic concepts of quantum mechanics and to apply operators to solve simple eigen values problems and approximation methods used in solving	Up to K3
CLO-2	Connect various theories behind quantum mechanics to illustrate multi-electron system and to calculate the energy of simple multi-electron atoms and	Up to K4
CLO-3	Use kinetic behaviour of surface reactions in order to develop various	Up to K3
CLO-4	Categorize Maxwell distribution of molecular velocities and to illustrate liquid crystals and various transport properties of matter.	Up to K4
CLO-5	Describe the phase behaviour of three component systems in terms of molecular properties.	Up to K2

Mapping of CLOs with PLOs

	PLO–1	PLO–2	PLO–3	PLO–4	PLO–5
CLO–1	3		2	1	1
CLO–2	3		2	1	1
CLO–3	3	1	2		1
CLO–4	3	2	2	2	2
CLO–5	3	1	2	1	

3-Advance application; 2-Intermediate level; 1-Basic level

Components of Formative Assessment	Marks	K level
Internal Test	**10**	As per below table
Assignment	**5**	K4
Quiz	**5**	K4
Seminar	**5**	K4
Total	**25**	

Learning Outcome Based Education (LOBE) & Assessment
Formative – Blue Print
Articulation Mapping-K Levels with Courses Learning Outcomes (CLOs)

Units	CLOs	K- Level	Section A		Section B (Either/or Choice)	Section C (Open Choice)
			Short Answers			
			No. of Questions	K- Level		
1	CLO x	Up to K3	2	K2,K3	2 (K3&K3)	2 (K2/K3)
2	CLO y	Up to K4	3	K2, K2, K3	2 (K4&K4)	1 (K3/K4)
No. of Questions to be asked			5		4	3
No. of Questions to be answered			5		2	2
Marks for each question			2		5	10
Total Marks for each section			10		10	20

Learning Outcome Based Education (LOBE) & Assessment

Summative Examination – Blue Print

Articulation Mapping-K Levels with Courses Learning Outcomes (CLOs)

UNITS	CLOs	K- Level	Section A		Section B		Section C (Either/or Choice)	Section D (Open Choice)
			MCQs		Short Answers			
			No. of Questions	K- Level	No. of Questions	K- Level		
1	CLO 1	Up to K3	2	K2 & K3	1	K1	2 (K2&K2)	1 (K3)
2	CLO 2	Up to K4	2	K3& K4	1	K2	2 (K4&K4)	1 (K4)
3	CLO 3	Up to K3	2	K2 & K3	1	K2	2 (K3&K3)	1 (K3)
4	CLO 4	Up to K4	2	K3 & K4	1	K3	2 (K4&K4)	1 (K4)
5	CLO 5	Up to K2	2	K1 & K1	1	K1	2 (K1&K1)	1 (K2)
No. of Questions to be asked			10			5	10	5
No. of Questions to be answered			10			5	5	3
Marks for each question			1			2	5	10
Total Marks for each section			10			10	25	30

K1- Remembering and recalling facts with specific answers

K2- Basic understanding of facts and stating main ideas with general answers

K3- Application oriented- Solving Problems

K4- Examining, analyzing, presentation and make inferences with evidences

Distribution of Section-wise Marks with K Levels

K Levels	Section A& B (No Choice)	Section C (Either / or)	Section D (Open Choice)	Total Marks	% of Marks without choice	Consolidated %
K1	6	10	-	16	13.3	35
K2	6	10	10	26	21.7	
K3	6	10	20	36	30	30
K4	2	20	20	42	35	35
Total marks	**20**	**50**	**50**	**120**	**100**	**100**

Name of the course Designers

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