Semester	**3**
Programme	**CHEMISTRY**
Course	**MAJOR (PHYSICAL CHEMISTRY 2)**
Paper Code	**C2CH230312T/ C2CH230312P**
Credits	**4 (3 THEORY+1 PRACTICAL)**
Hours/week	**7 (THEORY 3 + PRACTICAL 3)**
Category: Core/MDC/SEC/VEC	**CORE**
Theory/Practical/Composite	**COMPOSITE**
Number of Modules	**03**
Syllabus	**Module 1. Chemical Thermodynamics II (12 Lectures)** 1. Need for the Second Law: reversibility and spontaneity of a process 2. Caratheodory's principle 3. Principle of increase in entropy of the universe in natural processes 4. Clausius inequality 5. heat engine and refrigerator 6. Entropy change of the universe and maximum work for reversibility 7. Carnot cycle, efficiency 8. Kelvin-Plank and Clausius Statements of the second law; their equivalence: impossibility of attaining absolute zero of temperature 9. Carnot theorem 10. Combined first and second law 11. Thermodynamic equations of states 12. Auxiliary state functions – Gibbs and Helmholtz free energies, calculation in their change in different types of processes 13. Maxwell relations 14. Revisiting Joule-Thomson experiment: isenthalpic lines and T-P diagram 15. Temperature dependence of Gibbs free energy: Gibbs-Helmholtz equations 16. Gibbs free energy of real gases and fugacity 17. Chemical potential of pure substances 18. Partial molar quantities 19. Gibbs-Duhem equation **Module 2: Quantum Mechanics II (12 Lectures)** 1. Operators, Linear operators 2. Hermitian operators: definition and properties

	3. Postulates of Quantum Mechanics 4. Schrödinger equation 5. Solution of Schrödinger equation as wave function and energy (eigenvalues and eigenfunctions) 6. Commutators and their implication with respect to x, px. 7. Expectation values 8. Properties of eigenfunctions 9. Energy quantization 10. Simple systems: 1-D, 2-D, 3-D box (eigenvalues, eigenfunctions, expectation values, quantum numbers, degeneracy, probability density) 11. Simple Harmonic Oscillator: Setting the Schrödinger equation, derivation, eigenvalues and eigenfunctions, zero-point energy 12. Tunneling- Basic concepts **Module 3: Electrochemistry I (12 Lectures)** 1. Flow of charge through conductor: metallic and electrolytic conduction 2. Week and strong electrolytes: Arrhenius classification 3. Forces on an ion and its dynamics in an ideal solution across an applied potential difference 4. Validity of Ohm’s law and resistance equation in electrolytic solution 5. Conductance, specific conductance, equivalent conductance and their inter-relation 6. Mobility of ions in ideal solution: inter-relation to conductance, specific conductance and equivalent conductance 7. Reason for choosing conductance instead of resistance 8. Variation in conductance, specific conductance and equivalent conductance with concentration variation in ideal solution of strong and weak electrolytes 9. Effect of dilution, dielectric constant of solvent, viscosity of solvent and temperature on conductance of strong and weak electrolytes 10. Origin of non-ideality in electrolytic solution: activity and mean ionic activity of an electrolyte 11. Electrophoretic effect: effect of non-ideality on viscous force acting on an ion in electrolytic solution 12. Asymmetric effect: effect of local electric field due to asymmetric ionic atmosphere 13. Debye-Huckel limiting law: expression of mean ionic activity coefficient in ideally dilute solution 14. Determination of acidity constant of a weak acid: Ostwald dilution law, ionic product of water, determination of ionic radii 15. Infinitely dilute solution and withdrawal of ion-ion interaction in electrolytic solution: Kohlrausch’s law 16. Transport number and its determination: Hittorf and moving boundary method

	17. Effect of concentration and temperature variation on transport number 18. Abnormal transport number 19. True and apparent transport number 20. Conductometric acid-base and precipitation titrations **Practicals:** 1. Study of first order kinetics of decomposition of H_2O_2 by clock method 2. Study of kinetics of hydrolysis of esters by titrimetric method 3. Kinetics of base catalysed ester hydrolysis by conductometric method 4. Determination of thermodynamic solubility product of KHTa 5. pH-metric estimation of monobasic and dibasic acid and determination of pK_a or pK_2, wherever applicable 6. Determination of solubility product of a sparingly soluble salt (AgCl) by conductometric method.
Course Overview	Theory: 1. They will also develop the concepts of classical thermodynamics at the macroscopic level and learn through problem solving at different levels of complexity. 2. The Schrodinger equation will be introduced with the ground work of operators. Some examples with zero and non-zero potentials will be discussed. Solution of the corresponding Schrodinger equation, leading to the eigenstates and corresponding eigenvalues will be analysed. 3. The focus here is on molecular motion. The concept of flux and the relation between flux and force will be introduced. Expressions will be derived that govern the migration of properties through matter. One of the most useful consequences of this general approach is the formulation of the diffusion equation. Practicals: 1. Study of kinetics titrimetrically and conductometrically Study of solubility product of sparingly soluble salts titrimetrically and conductometrically.
Course Outcomes	Upon successful completion of this course, students will be able to: **CO1:** Evaluate the Second Law of Thermodynamics through the lens of entropy, reversibility, and the Carnot cycle. **CO2:** Derive and apply thermodynamic equations of state, the Joule-Thomson effect, and Maxwell relations to determine changes in state functions. **CO3:** Calculate Gibbs and Helmholtz free energy changes for various processes, evaluate the fugacity of real gases, and analyze the temperature dependence of free energy via the Gibbs-Helmholtz equation. **CO4:** Utilize the concept of chemical potential, partial molar quantities, and the Gibbs-Duhem equation to explain phase stability and equilibrium in multi-component systems. **CO5:** Define and apply linear and Hermitian operators, evaluate commutators (e.g., $[x, p_x]$) and expectation values, and apply the postulates of quantum mechanics to interpret the properties of eigenfunctions.

	CO6: Solve the time-independent Schrödinger equation for simple model systems (1-D, 2-D, and 3-D particle-in-a-box, and the simple harmonic oscillator) to obtain eigenvalues, eigenfunctions, quantum numbers, degeneracy, and probability densities. **CO7:** Explain the basic concept of quantum mechanical tunneling through a potential barrier as a non-classical phenomenon arising from the wave nature of matter. **CO8:** Interrelate conductance, specific conductance, and equivalent conductance, and explain their variation with concentration, dilution, dielectric constant, viscosity, and temperature for strong and weak electrolytes. **CO9:** Explain the origin of non-ideal behaviour in electrolytic solutions (electrophoretic and asymmetric effects) and apply the Debye-Hückel limiting law to evaluate the mean ionic activity coefficient of an electrolyte. **CO10:** Apply Kohlrausch's law of independent migration of ions and Ostwald's dilution law to determine the degree of dissociation, acidity constant of a weak acid, and the ionic product of water. **CO11:** Determine ionic transport numbers by the Hittorf and moving-boundary methods (distinguishing true and apparent values), and apply conductometric methods to acid-base and precipitation titrations. **CO12:** Integrate experimental data obtained via pH-metric, conductometric, and titrimetric methods to determine rate constants of reaction kinetics and solubility products of sparingly soluble salts. **CO13:** Synthesize theoretical knowledge of thermodynamics, quantum mechanics, and electrochemistry to model real-world molecular and ionic phenomena.
Program Outcomes	**PO1: Fundamental Knowledge:** Demonstrate a comprehensive understanding of core concepts in chemistry, including organic, inorganic, physical, analytical, and biochemistry. **PO2: Laboratory Skills:** Acquire hands-on experience in laboratory techniques and instrumentation, applying safety protocols and proper methodologies to conduct experiments and analyse results. **PO3: Problem Solving:** Develop critical thinking and problem-solving skills by applying chemical principles to real-world scenarios, including the ability to design experiments and interpret data. **PO4: Research Competency:** Engage in independent and collaborative research projects, employing scientific methods to formulate hypotheses, conduct experiments, and communicate findings effectively. **PO5: Interdisciplinary Applications:** Understand the interdisciplinary nature of chemistry, exploring its applications in fields such as medicine, environmental science, materials science, and nanotechnology. **PO6: Communication Skills:** Effectively communicate scientific information, both verbally and in written form, to diverse audiences, demonstrating the ability to present complex ideas clearly and concisely. **PO7: Ethics and Sustainability:** Recognize the ethical implications and responsibilities of scientific research and practice in chemistry, emphasizing the importance of sustainability and environmental stewardship in chemical practices.

CO #	Course Outcome Statement	Bloom's Taxonomy	Mapped POs
CO 1	Evaluate the Second Law of Thermodynamics through the lens of entropy, reversibility, and the Carnot cycle.	**K4 (Analyze)**	PO1, PO3
CO 2	Derive and apply thermodynamic equations of state, the Joule-Thomson effect, and Maxwell relations to determine changes in state functions.	**K4 (Analyze)**	PO1, PO3
CO 3	Calculate Gibbs and Helmholtz free energy changes for various processes, evaluate the fugacity of real gases, and analyze the temperature dependence of free energy via the Gibbs-Helmholtz equation.	**K3 (Apply), K4 (Analyze)**	PO1, PO3
CO 4	Utilize the concept of chemical potential, partial molar quantities, and the Gibbs-Duhem equation to explain phase stability and equilibrium in multi-component systems.	**K4 (Analyze)**	PO1, PO3
CO 5	Define and apply linear and Hermitian operators, evaluate commutators (e.g., $[x, p_x]$) and expectation values, and apply the postulates of quantum mechanics to interpret the properties of eigenfunctions.	**K3 (Apply)**	PO1, PO3
CO 6	Solve the time-independent Schrödinger equation for simple model systems (1-D, 2-D, and 3-D particle-in-a-box, and the simple harmonic oscillator) to obtain eigenvalues, eigenfunctions, quantum numbers, degeneracy, and probability densities.	**K4 (Analyze)**	PO1, PO3
CO 7	Explain the basic concept of quantum mechanical tunneling through a potential barrier as a non-classical phenomenon arising from the wave nature of matter.	**K2 (Understand)**	PO1, PO5
CO 8	Interrelate conductance, specific conductance, and equivalent conductance, and explain their variation with concentration, dilution, dielectric constant, viscosity, and temperature for strong and weak electrolytes.	**K4 (Analyze)**	PO1, PO3
CO 9	Explain the origin of non-ideal behaviour in electrolytic solutions (electrophoretic and asymmetric effects) and apply the Debye-Hückel limiting law to evaluate the mean ionic activity coefficient of an electrolyte.	**K3 (Apply), K4 (Analyze)**	PO1, PO3
CO 10	Apply Kohlrausch's law of independent migration of ions and Ostwald's dilution law to determine the degree of dissociation, acidity constant of a weak acid, and the ionic product of water.	**K3 (Apply)**	PO1, PO3

CO 11	Determine ionic transport numbers by the Hittorf and moving-boundary methods (distinguishing true and apparent values), and apply conductometric methods to acid-base and precipitation titrations.	**K3 (Apply), K5 (Evaluate)**	PO1, PO4
CO 12	Integrate experimental data obtained via pH-metric, conductometric, and titrimetric methods to determine rate constants of reaction kinetics and solubility products of sparingly soluble salts.	**K3 (Apply), K4 (Analyze)**	PO2, PO6
CO 13	Synthesize theoretical knowledge of thermodynamics, quantum mechanics, and electrochemistry to model real-world molecular and ionic phenomena.	**K6 (Create)**	PO1, PO5

Reading/Reference Lists	1. Glasstone, S, Thermodynamics for Chemists, EWP. 2. Zemansky, M. W. & Dittman, R.H. Heat and Thermodynamics, TataMcGraw-Hill. 3. Denbigh, K. The Principles of Chemical Equilibrium Cambridge University Press. 4 Nag, A. K, Physical Chemistry Vol. 1, 2, Mcgraw Hill. 5. Klotz, I.M., Rosenberg, R. M. Chemical Thermodynamics: Basic Concepts and Methods, Wiley. 6. Sears, F. W., Salinger, G. L., Thermodynamics, Kinetic Theory, and Statistical Thermodynamics (Addison-Wesley Principles of Physics Series), Pearson; 3rd edition 7. Metiu, H., Physical Chemistry: Thermodynamics, Taylor and Francis. 8. Kaufman, M., Principles of Thermodynamics, Taylor and Francis. 9. Honig, J. M., Thermodynamics, Academic Press. 10. Glasstone, S. An Introduction to Electrochemistry, East-West Press. 11. Levine, I. N. Quantum Chemistry, PHI. 12. Atkins, P. W. and Friedman, Molecular Quantum Mechanics, Oxford. 13. Eisberg, R., Resnick, R, Quantum Physics of Atoms, Molecules, Solids, Nuclei and Particles, 2ed, Wiley. 14. Griffiths, D. J., Introduction to Quantum Mechanics, Cambridge India. 15. Heimz, P. C., Rajagopalan, R., Principles of Colloid and Surface Chemistry, Marcel Dekker. Practicals: 1. Mukherjee, G. N., University Hand Book of Undergraduate Chemistry Experiments	
Evaluation	Theory: 60 Internal: 15 (CIA: 10; Other form of Assessment: 2; Attendance: 3) Semester Exam: 45	Practical: 40 CA: 30 ; Attendance:2 Semester Exam: 8
Paper Structure for Theory Semester Exam	Answer SEVEN out of NINE questions, of 10 marks each.	