

Semester	<b>3</b>
Course	<b>Major</b>
Paper Code	C2CH230312T
Paper Title	Physical Chemistry 2
No. of Credits	3 Theory+1 Practical
Theory / Practical / Composite	Composite
Minimum No. of preparatory hours per week a student has to devote	10
Number of Modules	03
Syllabus	<hr/> <p><i>Module 1. Chemical Thermodynamics II (12 Lectures)</i></p> <hr/> <ol style="list-style-type: none"> <li>1. Need for the Second Law: reversibility and spontaneity of a process</li> <li>2. Caratheodory's principle</li> <li>3. Principle of increase in entropy of the universe in natural processes</li> <li>4. Clausius inequality</li> <li>5. heat engine and refrigerator</li> <li>6. Entropy change of the universe and maximum work for reversibility</li> <li>7. Carnot cycle, efficiency</li> <li>8. Kelvin-Plank and Clausius Statements of the second law; their equivalence: impossibility of attaining absolute zero of temperature</li> <li>9. Carnot theorem</li> <li>10. Combined first and second law</li> <li>11. Thermodynamic equations of states</li> <li>12. Auxiliary state functions – Gibbs and Helmholtz free energies, calculation in their change in different types of processes</li> <li>13. Maxwell relations</li> <li>14. Revisiting Joule-Thomson experiment: isenthalpic lines and T-P diagram</li> <li>15. Temperature dependence of Gibbs free energy: Gibbs-Helmholtz equations</li> <li>16. Gibbs free energy of real gases and fugacity</li> <li>17. Chemical potential of pure substances</li> <li>18. Partial molar quantities</li> <li>19. Gibbs-Duhem equation</li> </ol> <hr/> <p><i>Module 2: Quantum Mechanics II (12 Lectures)</i></p> <hr/> <ol style="list-style-type: none"> <li>1. Operators, Linear operators</li> <li>2. Hermitian operators: definition and properties</li> </ol>

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  $x$ ,  $p_x$ .
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

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*Module 3: Electrochemistry I (12 Lectures)*

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1. Flow of charge through conductor: metallic and electrolytic conduction
2. Weak 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

	<p>17. Effect of concentration and temperature variation on transport number</p> <p>18. Abnormal transport number</p> <p>19. True and apparent transport number</p> <p>20. Conductometric acid-base and precipitation titrations</p> <p><b>Practicals:</b></p> <ol style="list-style-type: none"> <li>1. Study of first order kinetics of decomposition of <math>H_2O_2</math> by clock method</li> <li>2. Study of kinetics of hydrolysis of esters by titrimetric method</li> <li>3. Kinetics of base catalysed ester hydrolysis by conductometric method</li> <li>4. Determination of thermodynamic solubility product of KHTa</li> <li>5. pH-metric estimation of monobasic and dibasic acid and determination of <math>pK_a</math> or <math>pK_2</math>, wherever applicable</li> <li>6. Determination of solubility product of a sparingly soluble salt (AgCl) by conductometric method.</li> </ol>
Learning Outcomes	<p>Theory:</p> <ol style="list-style-type: none"> <li>1. They will also develop the concepts of classical thermodynamics at the macroscopic level and learn through problem solving at different levels of complexity.</li> <li>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.</li> <li>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</li> </ol>

	<p>matter. One of the most useful consequences of this general approach is the formulation of the diffusion equation.</p> <p>Practicals:</p> <ol style="list-style-type: none"> <li>1. Study of kinetics titrimetrically and conductometrically</li> <li>2. Study of solubility product of sparingly soluble salts titrimetrically and conductometrically.</li> </ol>	
Reading/Reference Lists	<ol style="list-style-type: none"> <li>1. Glasstone, S, Thermodynamics for Chemists, EWP.</li> <li>2. Zemansky, M. W. &amp; Dittman, R.H. Heat and Thermodynamics, TataMcGraw-Hill.</li> <li>3. Denbigh, K. The Principles of Chemical Equilibrium Cambridge University Press.</li> <li>4 Nag, A. K, Physical Chemistry Vol. 1, 2, Mcgraw Hill.</li> <li>5. Klotz, I.M., Rosenberg, R. M. Chemical Thermodynamics: Basic Concepts and Methods, Wiley.</li> <li>6. Sears, F. W., Salinger, G. L., Thermodynamics, Kinetic Theory, and Statistical Thermodynamics (Addison-Wesley Principles of Physics Series), Pearson; 3rd edition</li> <li>7. Metiu, H., Physical Chemistry: Thermodynamics, Taylor and Francis.</li> <li>8. Kaufman, M., Principles of Thermodynamics, Taylor and Francis.</li> <li>9. Honig, J. M., Thermodynamics, Academic Press.</li> <li>10. Glasstone, S. An Introduction to Electrochemistry, East-West Press.</li> <li>11. Levine, I. N. Quantum Chemistry, PHI.</li> <li>12. Atkins, P. W. and Friedman, Molecular Quantum Mechanics, Oxford.</li> <li>13. Eisberg, R., Resnick, R, Quantum Physics of Atoms, Molecules, Solids, Nuclei and Particles, 2ed, Wiley.</li> <li>14. Griffiths, D. J., Introduction to Quantum Mechanics, Cambridge India.</li> <li>15. Heimz, P. C., Rajagopalan, R., Principles of Colloid and Surface Chemistry, Marcel Dekker.</li> </ol> <p>Practicals:</p> <ol style="list-style-type: none"> <li>1. Mukherjee, G. N., University Hand Book of Undergraduate Chemistry Experiments</li> </ol>	
Evaluation	<p>Theory: 60  Internal: 15 (CIA: 10; Other form of Assessment: 2;  Attendance: 3)  Semester Exam: 45</p>	<p>Practical: 40  CA: 30 ; Attendance:2  Semester Exam: 8</p>
Paper Structure for Theory Semester Exam	<p>Answer SEVEN out of NINE questions, of 10 marks each.</p>	