**Programme: M. Sc. Part-I (Chemistry)**
**Course Code: PCC-401** **Title of the Course: General Physical Chemistry**
**Number of Credits: 03** **Effective from AY: 2018-19**

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| **Prerequisites for the course:** | Should have studied the courses in chemistry at F.Y B.Sc, S.Y B.Sc & T.Y B.Sc levels so as to have basic knowledge of Physical Chemistry and basic principles. | |
| **Course Objectives:** | 6. Introduction of various concepts on thermodynamics.<br>7. Introduction of electro chemistry and kinetics.<br>8. Learning quantum chemistry. | |
| **Course Outcomes:** | 8. Students should be in a position to understand various concepts in physical chemistry.<br>9. Students should be in a position to apply these concepts during the lab course in physical chemistry.<br>10. Students shall be in a position to answer the NET/SET examination questions based on these topics. | |
| **Content:** | 1.**Thermodynamics**<br>1.1 Thermodynamic properties: Gas laws, Real gasses, Boyle temperature, Critical temperature, State and path properties. Intensive and extensive properties. Exact and inexact differentials. Internal energy, enthalpy, entropy, free energy and their relations and significances. Maxwell relations. Thermodynamic equations of state.<br>1.2 Joule-Thomson effect. Joule-Thomson coefficient for van der Waals' gas. Joule-Thomson effect and production of low temperature, adiabatic demagnetization, Joule-Thompson coefficient, inversion temperature.<br>1.3 The third law of thermodynamics. Need for the third law. Apparent exceptions to third law. Application of third law. Use of thermodynamic functions in predicting direction of chemical change. Entropy and third law of thermodynamics.<br>1.4 Phase equilibria: Phase rule, Discussion of two component systems forming solid solutions with and without maximum or minimum in freezing point curve. Systems with partially miscible solid phases.<br>1.5 Three component systems: Graphical representation. Three component liquid systems with one pair of partially miscible liquids. Influence of temperature. Systems with two pairs and three pairs of partially miscible liquids. The role of added salts.<br><br>2.**Electrochemistry**<br>2.1 EMF series, decomposition potential and overvoltage, electronegativity, basic principles, completeness of deposition, Separation with controlled potentials, constant current electrolysis, composition of electrolyte, potential buffers, physical characteristics of metal deposits.<br>2.2 Electroplating and electroless plating, electrosynthesis.<br>2.3 Concepts of acid-base aqueous and non-aqueous solvents, hard and soft acid-base concept and applications. | 10 hrs<br><br>06 hrs |

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| | 3.**Chemical Kinetics**<br>3.1 General introduction to various types of order of reaction including fractional order, Molecularity of the reaction.<br>3.2 Introduction to reversible and irreversible reactions and reactions leading to equilibrium. Van'tHoffs equation and analysis of Gibbs free energy of equilibrium reactions.<br>3.3 Collision Theory and Maxwell Boltzmann distribution of energies of colliding molecules(derivationnotrequired). The concept of collisional cross section and reactive cross section and its significance.<br>3.4 Comparative study of transition state and collision state theory (derivation not required).<br>3.5 Free radical reactions, Complex reactions such as acetaldehyde decomposition and reaction between $H_2$ and $Br_2$, Homogeneous reactions and acid-base catalysis.<br>3.6 Elementary enzyme reactions.<br><br>4. **Quantum Chemistry**<br>4.1 Operators, Functions, Eigen value equations, Postulates.<br>4.2 Schrodinger equation, application to simple system viz. free particle, particle in one dimensional, two dimensional and three dimensional box (quantization, separation of variables, degenerate wave functions).<br>4.3 Hydrogen like atoms, Schrodinger equation and its solutions, atomic orbital wave functions and interpretation.<br>4.4 Hückel MO theory, Secular equations, Secular determinant, delocalization energy, charge density, π-bond order, free valence, applications to $C_2H_4$, $C_3H_5$(radical), $C_4H_6$, $C_4H_4$, $C_6H_6$, $C_6H_8$ | 07 hrs<br><br>13 hrs |
| **Pedagogy:** | Mainly lectures & tutorials. Seminars / term papers /assignments / presentations / self-study or a combination of some of these may be used. Sessions shall be interactive in nature to enable peer group learning. | |
| **References/ Readings** | 1. P. W. Atkins and J. D. Paula, *Physical Chemistry*, Eighth Edition, Oxford University Press, (2007) New Delhi.<br>2. G. M. Barrow, *Physical Chemistry*, Fifth Edition, Tata McGraw Hill, (2016) New Delhi.<br>3. J. E House, *Principles of Chemical Kinetics* (Second edition) Academic Press,2007 Elsevier Burlington, USA<br>4. I. N. Levine, *Quantum Chemistry*, Seventh Edition, Prentice-Hall, (1999) New Delhi. | |