LS 405A	**Chemistry of Macromolecules**	**2 Credits**
Name of the Faculty: Prof. Sneha Sudha Komath*, Dr. Karunakar Kar		

Sr.No.	**Topic**	**Faculty Name/ Contact Hours**
A.	***Equilibrium Thermodynamics***	
1.	**Basic concepts of thermodynamics:** Energy and its importance for all processes. The relevance of thermodynamics in the study of biological processes. Basic concepts: defining a system, universe, state functions, and path functions; and their significance for understanding the biological processes. Laws of thermodynamics. Concept of enthalpy in chemical reactions. Specific heats and their significance.	KK/01
2.	**Application of thermodynamic principles to biological reactions:** Application of Hess' law to biologically relevant chemical reactions. Predicting which way is down hill, concept of entropy of a system. Understanding what is free about free energy. Gibbs energy and its relationship with enthalpy and entropy of a system. The biochemical standard state. Coupled biochemical reactions.	KK/01
	Reversible biochemical reactions at equilibrium. The equilibrium constant (K_{eq}). Relationship between standard state Gibbs energy and K_{eq}. Temperature dependence of K_{eq} and Van't Hoff equation.	KK/01
	Types of biochemical equilibria. Ligand binding to biological macromolecules. The association/dissociation constant. Analysis of binding data.	KK/01
	Ionic product of water. Acid-base equilibria and the Henderson-Hasselbach equation. Buffers and their importance for biochemistry. pKa of amino acids and their relevance. pI and optimum pH for enzyme activity.	KK/02
	Chemical potential and ionic equilibria. Donnan membrane equilibrium and its significance. Nernst Equation and biochemical equilibrium.	KK/01
B.	***Kinetics***	
3.	**Basic concepts of kinetics:** Path dependence of kinetics of chemical processes. Activation energy, transition states and intermediates. Rates and rate constants for first order, second order and pseudo first order reactions. Writing rate equations- the differential method and the integration method.	KK/01
	Half-life of first-and second- order reactions and their significance with examples. Principle of microscopic reversibility and its relevance.	KK/01
4.	**Application of kinetics to the study of biological reactions:** Writing rate equations for reversible biochemical reactions. Equilibrium versus steady state approximation in enzyme catalyzed reactions.	SSK/02
C.	***Quantum mechanics and spectroscopy***	
5.	**A historical introduction to the field:** Understanding the break between classical and quantum physics.	SSK/01
6.	**Basic concepts of quantum mechanics:** Introduction to wave-particle duality and the time-independent Schrödinger's equation.	SSK/01

	Significance of boundary conditions for the concept of quantization. Wave functions and orbitals.	SSK/01
7.	**Applicationsof quantum theory:** A particle in one, two and three-dimensional boxes and its implications for the understanding of H-atom. Predicting absorption spectra of conjugated systems (porphyrins/β-carotene) using such simple approximations.	SSK/02
	Energy and wave functions of the H-like atoms. Radial distribution functions and shapes of orbitals. Ionic potential and electronegativity.	SSK/02
	Molecular orbital theory and orbital hybridization. The interaction of light with matter.	SSK/01
D.	***Organic chemistry***	
8.	**Revisiting concepts of physical organic chemistry:** Conjugation, aromaticity and resonance. Inductive effects. Hydrogen bonding. Hydrophobicity.	KK/01
9.	**Application of organic chemistry to biology:** SN1, SN2, E1, E2, electrophilic addition reactions; Free radical reactions	KK/01
	Understanding reaction mechanisms of some biological reactions.	KK/03
E.	***Coordination chemistry***	
10.	**Concepts of coordination chemistry:** Coordination bonds and metal-ligand interactions; Hard-soft acid-base (HSAB) theory	SSK/01
11.	**Application of coordination chemistry to understand biological systems** Coordination geometries; Jahn Teller Distortion; porphyrins as ligands for metals in biology	SSK/01
	Role of the central metal ion in metalloproteins and metalloenzymes	SSK/02

References:

1. Atkins' Physical Chemistry
2. A guide book to mechanism inorganic chemistry by Peter Sykes
3. Advanced Inorganic Chemistry by Cotton and Wilkinson
4. Other standard reading material as per requirement will be suggested during classroom discussions.