

## LS 405: CHEMISTRY OF MACROMOLECULES

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### Course Objectives

**Credit: 02**

Biological systems are guided by the same rules that govern chemical processes making it important for students of life sciences to develop an appreciation of the chemistry of biological macromolecules. This course is designed to introduce perspectives of chemistry in the study of biomolecules for students of Life Sciences at the Masters-level. Elementary knowledge of chemistry (up to the higher secondary school level) is presumed for students starting this course.

| <i>Chemistry for Biology</i>                                    |                                                                                                                                                                                                                                                                                                                                                                                                              | <b>Total lectures<br/>28 hours</b> |
|-----------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------|
| <i>Equilibrium Thermodynamics:</i>                              |                                                                                                                                                                                                                                                                                                                                                                                                              | <b>7 hours</b>                     |
| Revisiting basic concepts of thermodynamics:                    | Energy and its importance for all processes. The relevance of thermodynamics in the study of biological processes. Some basic concepts: defining a system, universe, state functions, and path functions and their significance for understanding biological processes. The first law of thermodynamics. Work done and the concept of enthalpy in chemical reactions. Specific heats and their significance. | <b>1 (KK)</b>                      |
| Application of thermodynamic principles to biological reactions | Application of Hess' law to biologically relevant chemical reactions. Predicting which way is downhill and the 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.                                                                         | <b>1 (KK)</b>                      |
|                                                                 | 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.                                                                                                                                                                                          | <b>1 (KK)</b>                      |
|                                                                 | Understanding different types of biochemical equilibria. Ligand binding to biological macromolecules. The association/ dissociation constant. Different ways of analyzing binding data.                                                                                                                                                                                                                      | <b>1 (KK)</b>                      |
|                                                                 | Ionic product of water. Acid-base equilibria and the Henderson-Hasselbach equation. Buffers and their importance for biochemistry. $pK_a$ of amino acids and their relevance. $pI$ and optimum $pH$ for enzyme activity.                                                                                                                                                                                     | <b>2 (KK)</b>                      |
|                                                                 | Chemical potential and ionic equilibria. Donnan membrane equilibrium and its significance. Nernst Equation and biochemical equilibrium.                                                                                                                                                                                                                                                                      | <b>1 (KK)</b>                      |
|                                                                 |                                                                                                                                                                                                                                                                                                                                                                                                              |                                    |
| <i>Kinetics</i>                                                 |                                                                                                                                                                                                                                                                                                                                                                                                              | <b>4 hours</b>                     |
| Revisiting 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.                                                                                                                              | <b>1 (KK)</b>                      |

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|                                                                        | Half-life of first- and second-order reactions and their significance. Examples. The principle of microscopic reversibility and its relevance.                                                                                     | <b>1 (KK)</b>  |
| Application of Kinetics to the study of biological reactions           | Writing rate equations for reversible biochemical reactions. Equilibrium versus the steady state approximation in enzyme catalyzed reactions.                                                                                      | <b>2 (SSK)</b> |
| <b><i>Quantum mechanics and spectroscopy</i></b>                       |                                                                                                                                                                                                                                    | <b>8 hours</b> |
| A historical introduction to the field                                 | Understanding the break between classical and quantum physics.                                                                                                                                                                     | <b>1 (SSK)</b> |
| Basic concepts of quantum mechanics                                    | Introduction to the idea of the wave-particle duality and the time-independent Schrödinger's equation.                                                                                                                             | <b>1 (SSK)</b> |
|                                                                        | Significance of boundary conditions for the concept of quantization. Wavefunctions and orbitals.                                                                                                                                   | <b>1 (SSK)</b> |
| Applications of quantum theory                                         | A particle in one, two and three-dimensional boxes and its implications for the understanding of the H-atom. Predicting absorption spectra of conjugated systems (porphyrins/ $\beta$ -carotene) using such simple approximations. | <b>2 (SSK)</b> |
|                                                                        | Energy and wavefunctions of the H-like atoms. Radial distribution functions and shapes of orbitals. Ionic potential and electronegativity.                                                                                         | <b>2 (SSK)</b> |
|                                                                        | Molecular orbital theory and orbital hybridization. The interaction of light with matter.                                                                                                                                          | <b>1 (SSK)</b> |
| <b><i>Organic chemistry</i></b>                                        |                                                                                                                                                                                                                                    | <b>5 hours</b> |
| Revisiting concepts of physical organic chemistry                      | Conjugation, aromaticity and resonance. Inductive effects. Hydrogen bonding. Hydrophobicity.                                                                                                                                       | <b>1 (KK)</b>  |
| Application of organic chemistry to biology                            | $S_N1$ , $S_N2$ , E1, E2, electrophilic addition reactions; Free radical reactions                                                                                                                                                 | <b>1 (KK)</b>  |
|                                                                        | Understanding reaction mechanisms of some biological reactions.                                                                                                                                                                    | <b>3 (KK)</b>  |
| <b><i>Coordination chemistry</i></b>                                   |                                                                                                                                                                                                                                    | <b>4 hours</b> |
| Revisiting concepts of coordination chemistry                          | Coordination bonds and metal-ligand interactions; Hard-soft acid-base (HSAB) theory                                                                                                                                                | <b>1 (SSK)</b> |
| Application of coordination chemistry to understand biological systems | Coordination geometries; Jahn Teller Distortion; porphyrins as ligands for metals in biology                                                                                                                                       | <b>1 (SSK)</b> |
|                                                                        | Role of the central metal ion in metalloproteins and metalloenzymes                                                                                                                                                                | <b>2 (SSK)</b> |

Suggested Readings:

- 1) Atkins' Physical Chemistry
- 2) A guidebook to mechanism in organic chemistry by Peter Sykes
- 3) Advanced Inorganic Chemistry by Cotton and Wilkinson

Other standard reading material as per requirement will be suggested during classroom discussions.