

## **CHEMISTRY-1**

**Code: CHEM 1001**

**Contacts: 3L + 1T = 4**

**Credits: 4**

### **MODULE 1**

#### **Atomic structure and Wave Mechanics**

Brief outline of the atomic structure, Dual character of electron, De Broglies's equation, the Heisenberg uncertainty principle, brief introduction of quantum mechanics, the concept of operators, the Schrodinger wave equation, Hermitian operator and its properties, solution of the Schrodinger equation for particle in a one dimensional box, interpretation of the wave function  $\Psi$ , concept of atomic orbital, Brief mention of angular momentum operators, Quantum numbers.

**2L**

**Thermodynamics:** Carnot cycle, 2nd law of thermodynamics, entropy, Clausius inequality, free energy and work function, Clausius Clapeyron Equation, Chemical Potential, Activity and Activity coefficient. Gibbs Duhem Relation

**4L**

#### **Spectroscopic Techniques & Application**

Electromagnetic spectrum: EMR interaction with matter - absorption and emission of radiation. Principle and application of UV- visible and IR spectroscopy  
Principles of NMR Spectroscopy and X-ray diffraction technique

**3L**

### **MODULE 2**

#### **Chemical Bonding**

Covalent bond, VSEPR Theory, hybridization, molecular geometries. Dipole moment. Intermolecular forces, V.B. and M.O. theory and its application in Homo and Heteronuclear diatomic molecules. Band theory of solids. Pi-molecular orbitals of ethylene and butadiene

**5L**

#### **Periodicity**

Effective nuclear charge, electronic configurations, atomic and ionic sizes, ionization energies, electron affinity and electronegativity, inert pair effect.

**3L**

#### **Ionic Equilibria**

Acid Base Equilibria, Salt Hydrolysis and Henderson Equation, Buffer solutions, pH indicator, Common ion Effect, Solubility product, Fractional Precipitation

**2L**

## **MODULE 3**

### **Conductance**

Conductance of electrolytic solutions, Strong and Weak electrolytes, effect of temperature and concentration. Kohlrausch's law of independent migration of ions, transport numbers and hydration of ions. Application of conductance Acid-base and precipitation titration

**3L**

### **Electrochemical Cell**

Thermodynamic derivation of Nernst equation, Electrode potential and its application to predict redox reaction; Standard Hydrogen Electrode, Reference electrode, cell configuration, half cell reactions, evaluation of thermodynamic functions; Reversible and Irreversible cells; Electrochemical corrosion.

Electrochemical Energy Conversion: Primary & Secondary batteries, Fuel Cells

**4L**

### **Reaction dynamics**

Rate Laws, Order & Molecularity; zero, first and second order kinetics.

Pseudo-unimolecular reaction, Arrhenius equation.

Mechanism and theories of reaction rates (Transition state theory, Collision theory).

Catalysis: Homogeneous catalysis (Definition, example, mechanism, kinetics).

**3L**

## **MODULE 4**

### **Stereochemistry (4 lectures)**

Representations of 3 dimensional structures, structural isomers and stereoisomers, configurations and symmetry and chirality, enantiomers, diastereomers, optical activity, absolute configurations and conformational analysis.

**4L**

### **Structure and reactivity of Organic molecule**

Inductive effect, resonance, hyperconjugation, electromeric effect, carbocation, carbanion, free radicals, aromaticity.

**3L**

### **Organic reactions and synthesis of drug molecule (4 lectures)**

Introduction to reaction mechanisms involving substitution, addition, elimination and oxidation-reduction reactions. Synthesis of commonly used drug molecules.

**3L**

**TEXT BOOKS**

1. Physical Chemistry, P.W. Atkins
2. Organic Chemistry, I. L. Finar
3. Engineering Chemistry, Jain & Jain
4. Fundamental Concepts of Inorganic Chemistry, A.K.Das
5. Engineering Chemistry -I, Gour Krishna Das Mahapatra

**REFERENCE BOOKS**

1. General & Inorganic Chemistry, R. P. Sarkar
2. P. C. Rakshit, Physical Chemistry, Sarat Book House (7th Edition)
3. Organic Chemistry, Morrison & Boyd
4. Fundamentals of Molecular Spectroscopy, C.N. Banwell
5. Physical Chemistry , G. W. Castellan
6. A Text book of Engineering Chemistry, Shashi Chawla, Dhanpat Rai & Co Pvt Ltd
7. Basic Stereo chemistry of Organic Molecules, Subrata Sengupta