

Semester		Course Code	Course Title	Category
Semester –II		BSC102	Chemistry-I (Theory & Lab.)	Basic Science Course
Scheme and Credits				Contents
L	T	P	Credits	(i) Chemistry-I (Concepts in chemistry for engineering)
3	1	3	5.5	
				(ii) Chemistry Laboratory

**(i) Chemistry-I (Concepts in chemistry for engineering) [L : 3; T:1; P : 0 (4 credits)]**

**Detailed contents**

**(i) Atomic and molecular structure (12 lectures)**

Schrodinger equation. Particle in a box solutions and their applications for conjugated molecules and nanoparticles. Forms of the hydrogen atom wave functions and the plots of these functions to explore their spatial variations. Molecular orbitals of diatomic molecules and plots of the multicenter orbitals. Equations for atomic and molecular orbitals. Energy level diagrams of diatomic. Pi-molecular orbitals of butadiene and benzene and aromaticity. Crystal field theory and the energy level diagrams for transition metal ions and their magnetic properties. Band structure of solids and the role of doping on band structures.

**(ii) Spectroscopic techniques and applications (8 lectures)**

Principles of spectroscopy and selection rules. Electronic spectroscopy. Fluorescence and its applications in medicine. Vibrational and rotational spectroscopy of diatomic molecules. Applications. Nuclear magnetic resonance and magnetic resonance imaging, surface characterisation techniques. Diffraction and scattering.

**(iii) Intermolecular forces and potential energy surfaces (4 lectures)**

Ionic, dipolar and van Der Waals interactions. Equations of state of real gases and critical phenomena. Potential energy surfaces of H<sub>2</sub>, H<sub>2</sub>F and HCN and trajectories on these surfaces.

**(iv) Use of free energy in chemical equilibria (6 lectures)**

Thermodynamic functions: energy, entropy and free energy. Estimations of entropy and free energies. Free energy and emf. Cell potentials, the Nernst equation and applications. Acid base, oxidation reduction and solubility equilibria. Water chemistry. Corrosion. Use of free energy considerations in metallurgy through Ellingham diagrams.

**(v) Periodic properties (4 Lectures)**

Effective nuclear charge, penetration of orbitals, variations of s, p, d and f orbital energies of atoms in the periodic table, electronic configurations, atomic and ionic sizes, ionization energies, electron affinity and electronegativity, polarizability, oxidation states, coordination numbers and geometries, hard soft acids and bases, molecular geometries

**(vi) 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. Isomerism in transitional metal compounds

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

Introduction to reactions involving substitution, addition, elimination, oxidation, reduction, cyclization and ring openings. Synthesis of a commonly used drug molecule.

**Suggested Text Books**

- University chemistry, by B. H. Mahan
- Chemistry: Principles and Applications, by M. J. Sienko and R. A. Plane
- Fundamentals of Molecular Spectroscopy, by C. N. Banwell
- Engineering Chemistry (NPTEL Web-book), by B. L. Tembe, Kamaluddin and M. S. Krishnan
- Physical Chemistry, by P. W. Atkins
- Organic Chemistry: Structure and Function by K. P. C. Volhardt and N. E. Schore, 5th Edition

**Course Outcomes**

The concepts developed in this course will aid in quantification of several concepts in chemistry that have been introduced at the 10+2 levels in schools. Technology is being increasingly based on the electronic, atomic and molecular level modifications.

Quantum theory is more than 100 years old and to understand phenomena at nanometer levels, one has to base the description of all chemical processes at molecular levels. The course will enable the student to:

Analyse microscopic chemistry in terms of atomic and molecular orbitals and intermolecular forces.

Rationalise bulk properties and processes using thermodynamic considerations.

Distinguish the ranges of the electromagnetic spectrum used for exciting different molecular energy levels in various spectroscopic techniques

Rationalise periodic properties such as ionization potential, electro negativity, oxidation states and electro negativity.

List major chemical reactions that are used in the synthesis of molecules.

**(ii) Chemistry Laboratory [ L : 0; T:0 ; P : 3 (1.5 credits)]**

**Choice of 10-12 experiments from the following:**

- Determination of surface tension and viscosity
- Thin layer chromatography
- Ion exchange column for removal of hardness of water
- Determination of chloride content of water
- Colligative properties using freezing point depression
- Determination of the rate constant of a reaction
- Determination of cell constant and conductance of solutions
- Potentiometry - determination of redox potentials and emfs
- Synthesis of a polymer/drug
- Saponification/acid value of an oil
- Chemical analysis of a salt
- Lattice structures and packing of spheres
- Models of potential energy surfaces
- Chemical oscillations- Iodine clock reaction
- Determination of the partition coefficient of a substance between two immiscible liquids
- Adsorption of acetic acid by charcoal
- Use of the capillary viscosimeters to demonstrate the isoelectric point as the pH of minimum viscosity for gelatin sols and/or coagulation of the white part of egg .

**Laboratory Outcomes**

The chemistry laboratory course will consist of experiments illustrating the principles of chemistry relevant to the study of science and engineering.

The students will learn to:

Estimate rate constants of reactions from concentration of reactants/products as a function of time

Measure molecular/system properties such as surface tension, viscosity, conductance of solutions, redox potentials, chloride content of water, etc

Synthesize a small drug molecule and analyse a salt sample