

Undergraduate Degree courses

Course code	BSC102(Th)/BSC105(Lab)				
Category	Basic Science Course				
Course title	Chemistry (Theory & Lab.) <u>Contents</u> (i) Chemistry-I (Concepts in chemistry for engineering) (ii) Chemistry Laboratory				
Scheme and Credits	L	T	P	Credits	Semester –I/II
	3	1	3	5.5	
Pre-requisites (if any)	-				

(i) Chemistry (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 H₃, H₂F 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

1. University chemistry, by B. H. Mahan
2. Chemistry: Principles and Applications, by M. J. Sienko and A. Plane
3. Fundamentals of Molecular Spectroscopy, by C. N. Banwell
4. Engineering Chemistry (NPTEL Web-book), by B. L. Tembe, Kamaluddin and M. S. Krishnan
5. Physical Chemistry, by P. W. Atkins
6. 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, electronegativity, oxidation states and electronegativity.