II. Undergraduate Degree courses

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

(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_3, H_2F 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