Name of the Academic Program: B. Tech. (CSE)

Course Code: BTCSE-101

Title of the Course: Chemistry

L-T-P: 3–1–0

Credits: 4

COURSE OUTCOMES (COs)

CO-1 Analyse microscopic chemistry in terms of atomic and molecular orbitals and intermolecular forces. (Cognitive Level: Analyse)

CO-2 Rationalize bulk properties and processes using thermodynamic considerations. (Cognitive Level: Evaluate)

- **CO-3** Distinguish the ranges of the electromagnetic spectrum used for exciting different molecular energy levels in various spectroscopic techniques (Cognitive Level: Apply)
- **CO-4** Rationalize periodic properties such as ionization potential, electronegativity, oxidation states, and electronegativity. (Cognitive Level: Analyse and Evaluate)
- **CO-5** List major chemical reactions that are used in the synthesis of molecules. (Cognitive Level: Apply and Create)

Mapping of Course Outcomes (COs) with Program Outcomes (POs) and Program Specific Outcomes (PSOs)

| | PO1 | PO2 | PO3 | PO4 | PO5 | PO6 | PO7 | PO8 | PO9 | PO10 | PO11 | PO12 | PSO1 | PSO2 | PSO3 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|
| CO1 | 1 | | 1 | 3 | | 2 | | 2 | 1 | 1 | 2 | 2 | 1 | | 2 |
| CO2 | | 1 | | 3 | 2 | 2 | 1 | 1 | | | 2 | 2 | | 3 | 2 |
| CO3 | 1 | | 2 | 3 | | 2 | | | 2 | 1 | 2 | 2 | 2 | | 2 |
| CO4 | | 1 | | 3 | 1 | 2 | 2 | 1 | | 1 | 2 | 2 | | 3 | 2 |
| CO5 | 2 | | 3 | 3 | | 2 | | | | | 2 | 2 | 3 | | 2 |

Detailed Syllabus

Unit 1: Atomic and molecular structure

(12 Hours)

Schrodinger equation. 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 multicentre 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.

Unit 2: Spectroscopic techniques and applications

(10 Hours)

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.

Unit 3: Use of free energy in chemical equilibria

(10 Hours)

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. Corrosion. Use of free energy considerations in metallurgy through Ellingham diagrams.

Unit 4: Periodic properties

(6 Hours)

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

Unit 5: Stereochemistry

(5 Hours)

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

Unit 6: Organic reactions

(5 Hours)

Introduction to reactions involving substitution, addition, elimination, oxidation, reduction, cyclization and ring openings.

Reference Books:

- 1. University chemistry, by B. H. Mahan
- 2. Chemistry: Principles and Applications, by M. J. Sienko and R. A. Plane
- 3. Fundamentals of Molecular Spectroscopy, by C. N. Banwell
- 4. Physical Chemistry, by P. W. Atkins
- 5. Organic Chemistry: Structure and Function by K. P. C. Volhardt and N. E. Schore,

Teaching-Learning Strategies in brief

- 1. Learning through discussion among the peer group
- 2. Learning through Case Studies
- 3. Open ended questions by teacher
- 4. Open ended questions from student

Assessment Methods and Weightages in Brief

A variety of assessment methods that are appropriate to the subject area and a programme of study have been used to assess progress towards the course learning outcomes. Priority has been accorded to formative assessment. Progress towards achievement of learning outcomes have been assessed using the following:

Time-Constrained Examinations; Problem-Based Assignments Individual Project Report (Case-Study Reports); Oral Presentations, Including Seminar Presentation; Viva Voce Interviews, Etc.