

## Semester I

CH103	Chemistry	L-T-P-CR-CH: 3-0-1-4-5
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### Course Objectives

- CO1. To explain the basic principles of Physical, Inorganic and Organic Chemistry
- CO2. To explain the basic principles of different spectroscopic techniques and demonstrate their practical applications
- CO3. To demonstrate the role of chemistry in everyday life using some simple examples in theory classes as well as with hands-on experiments

### Learning Outcomes

Upon the completion of the course, the students will be able to:

- LO1. Solve problems of chemistry with the knowledge of fundamental principles.
- LO2. Connect the basic chemistry knowledge with the daily experiences.
- LO3. Utilize the knowledge of chemistry in their future studies.

### SYLLABUS

#### Theory:

**Unit 1:** Atomic and molecular structure (11 lectures)

Schrödinger 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 multicentre orbitals. Equations for atomic and molecular orbitals. Energy level diagrams of diatomics. 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 (6 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 characterization techniques. Diffraction and scattering.

**Unit 3:** 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>3</sub>, H<sub>2</sub>F and HCN and trajectories on these surfaces.

**Unit 4:** Use of free energy in chemical equilibria (5 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.

**Unit 5:** Nuclear Chemistry (4 lectures)

Isotopes, isotones, isobars,  $\alpha$ ,  $\beta$  and  $\gamma$  rays, nuclear transformations, fission and fusion, cosmic rays, binding energy, packing fraction, radioactive hazards, nuclear power plants.

**Unit 6:** 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

**Unit 7:** 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.

### **Practical:**

**Experiment 1:** Standardization of sodium thiosulphate solution with standard potassium dichromate solution and application for estimation of copper in a solution.

**Experiment 2:** Determination of the dissociation constant of a weak acid using pH meter.

**Experiment 3:** Determination of the strength of a strong acid by conductometric titration with a strong base.

**Experiment 4:** Determination of the strength of a weak acid by conductometric titration with a strong base.

**Experiment 5:** Determination of the total hardness of water by complexometric titration.

**Experiment 6:** Preparation of Mohr's salt.

**Experiment 7:** Determination of the wavelength of maximum absorption ( $\lambda_{\max}$ ) of a colored solution using spectrophotometer.

**Experiment 8:** Preparation of buffer solution and determination of pH.

**Total** (46 lectures)

**Books:**

1. University Chemistry; B. H. Mahan and Rollie J. Myers; Pearson Publication, Fourth Edition. 2017.
2. Chemistry: Principles and Applications; M. J. Sienko and R. A. Plane
3. Fundamentals of Molecular Spectroscopy; C. N. Banwell; Tata McGraw-Hill Education, Fourth Edition 2001.
4. Physical Chemistry; P. W. Atkins, Julio De Paula; Oxford University Press, Ninth Edition, 2009.
5. Organic Chemistry: Structure and Function; K. P. C. Vollhardt and N. E. Schore; W.H. Freeman and Company, 7th Edition, 2014.  
<http://bcs.whfreeman.com/vollhardtschore5e/default.asp>
6. Engineering Chemistry (NPTEL Web-book), by B. L. Tembe, Kamaluddin and M. S.

Krishnan