Chemistry

APCH100	Chemistry	3L: 0 T: 0P	3 Credits

Course Objective:

The objective of the Chemistry I is to acquaint the students with the basic phenomenon/concepts of chemistry, the student faces during course of their study in the industry and Engineering field. The student with the knowledge of the basic chemistry, will understand and explain scientifically the variouschemistry related problems in the industry/engineering field. The student will able to understand the new developments and breakthroughs efficiently in engineering and technology. The introduction of the latest (R&D oriented) topics will make the engineering student upgraded with the new technologies.

Course Content:

Module I: Atomic and Molecular Structure

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 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.

Module II: Spectroscopic techniques and applications

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.

Module III: Intermolecular forces and potential energy surfaces

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.

Module 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.

Module V: Periodic properties

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, electronaffinity and electronegativity, polarizability, oxidation states, coordination numbers and geometries, hard soft acids and bases, molecular geometries.

Module VI: Stereochemistry

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.

Module VII: Organic reactions and synthesis of a drug molecule

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

LABORATORY

Choice of 10-12 experiments from the following:

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

Text/Reference Books:

1. AICTE's Prescribed Textbook: Chemistry – I with Lab Manual, Manisha Agrawal, Khanna Book Publishing, 2023.
2. Engineering Chemistry, by Manisha Agrawal.
3. University chemistry, by B. H. Mahan
4. Chemistry: Principles and Applications, by M. J. Sienko and R. A. Plane
5. Fundamentals of Molecular Spectroscopy, by C. N. Banwell
6. Engineering Chemistry (NPTEL Web-book), by B. L. Tembe, Kamaluddin and M. S. Krishnan
7. Physical Chemistry, by P. W. Atkins
8. Organic Chemistry: Structure and Function by K. P. C. Volhardt and N. E. Schore, 5th Edition http://bcs.whfreeman.com/vollhardtschore5e/default.asp

Alternative NPTEL/SWAYAM Course:

S. No.	NPTEL Course Name	Instructor	Host Institute
1	Chemistry - I	Prof. Mangala Sunder Krishnan	IITM

EXPERIMENTS THAT MAY BE PERFORMED THROUGH VIRTUAL LABS:

S. No.	Experiment Name	Experiment Link(s)
1	Determination of surface tension and viscosity.	http://pcv-au.vlabs.ac.in/physical-chemistry/Determination_of_Viscosity_of_Organic_Solvents/
2	Ion exchange column for removal of hardness of water.	http://icv-au.vlabs.ac.in/inorganic-chemistry/Water_Analysis_Determination_of_Chemical_Parameters/
3	Determination of chloride content of water.	http://vlabs.iitb.ac.in/vlabs-dev/labs/nitk_labs/Environmental_Engineering_1/experiments/determination-of-chloride-nitk/simulation.html
4	Colligative properties using freezing point depression.	http://pcv-au.vlabs.ac.in/physical-chemistry/Cryoscopy/
5	Determination of the rate constant of a reaction.	http://pcv-au.vlabs.ac.in/physical-chemistry/EMF_Measurement/
6	Determination of cell constant and conductance of solutions.	http://icv-au.vlabs.ac.in/inorganic-chemistry/Water_Analysis_Determination_of_Physical_Parameters/
7	Potentiometry - determination of redox potentials and emfs.	http://pcv-au.vlabs.ac.in/physical-chemistry/EMF_Measurement/
8	Saponification/acid value of an oil.	http://biotech01.vlabs.ac.in/bio-chemistry/Estimation_of_Saponification_Value_of_Fats_or_Oils/
9	Lattice structures and packing of spheres.	https://vlab.amrita.edu/?sub=1&brch=282&sim=370&cnt=1

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 nanometre levels, one has to base the description of all chemical processes at molecular levels. The course will enable the students:

- To analyse microscopic chemistry in terms of atomic and molecular orbitals and intermolecular forces.
- To rationalise bulk properties and processes using thermodynamic considerations.
- To distinguish the ranges of the electromagnetic spectrum used for exciting different molecular energy levels in various spectroscopic techniques
- To rationalise periodic properties such as ionization potential, electronegativity, oxidation states and electronegativity.
- To list major chemical reactions that are used in the synthesis of molecules.

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.
- To measure molecular/system properties such as surface tension, viscosity, conductance of solutions, redox potentials, chloride content of water, etc.
- To synthesize a small drug molecule and analyze a salt sample.

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