Department of Chemical Sciences

Course Structure and Syllabus of M. Sc. in Chemistry

Minimum Credit requirement: 81 Credit
Minimum duration: 2 years (4 semesters)
Maximum duration: 3 years (6 semesters)

Course Structure

Semester I

Course Code	Course Name	L-T-P	CH	Credit	Remarks
CH-401	Principles of Inorganic Chemistry	3-0-0	3	3	
CH-402	Principles of Organic Chemistry	3-0-0	3	3	
CH-403	Chemical and Statistical Thermodynamics	3-0-0	3	3	
CH-404	Quantum Chemistry and Chemical Bonding	3-0-0	3	3	
CH-405	Laboratory Course in Organic Chemistry	0-0-6	12	6	
CBCT		3-0-0	3	3	
		Total	**27**	**21**	

Semester II

Course Code	Course Name	L-T-P	CH	Credit	Remarks
CH-408	Chemistry of Transition Elements	3-0-0	3	3	
CH-409	Organic Reactions and Mechanism	3-0-0	3	3	
CH-410	Chemical Dynamics and Electrochemistry	3-0-0	3	3	
CH-411	Principles and Applications of Spectroscopy	3-0-0	3	3	
CH-412	Laboratory Course in Inorganic Chemistry	0-0-6	12	6	
CBCT		3-0-0	3	3	
		Total	**27**	**21**	

Semester III

Course Code	Course Name	L-T-P	CH	Credit	Remarks
CH-501	Bio-Organic Chemistry	3-0-0	3	3	
CH-502	Physical Chemistry of Surface and Condensed Systems	3-0-0	3	3	
CH-503	Special Topics in Inorganic Chemistry	3-0-0	3	3	
CH-504	Analytical Techniques	3-0-0	3	3	
CH-505	Laboratory Course in Physical Chemistry	0-0-6	12	6	
CBCT		3-0-0	3	3	
		Total	**27**	**21**	

Semester IV

Course Code	Course Name	L-T-P	CH	Credit	Remarks
CH-506/507/508	Elective I	3-0-0	3	3	
CH-509/510/511	Elective II	3-0-0	3	3	
CH-512/513/514/515/516	Elective III	3-0-0	3	3	
CH-517	Project Work	0-0-9	18	9	
		Total	**27**	**18**	

Elective I: Any one from the following group
CH-506 Catalysis (Physical)
CH-507 Bio-inorganic Chemistry (Inorganic)
CH-508 Methods in Organic Synthesis (Organic)

Elective II: Any one from the following group
CH-509 Polymer Chemistry (Physical)
CH-510 Organometallic Chemistry (Inorganic)
CH-511 Heterocyclic Compounds and Medicinal Applications (Organic)

Elective III: Any one from the following group
CH-512 Chemistry of Materials
CH-513 Organic Solid States Chemistry
CH-514 Biomolecular Chemistry
CH-515 Environmental and Green Chemistry
CH-516 Computational Chemistry and Numerical Analysis

CBCT
CH-406 Chemistry in Everyday Life
CH-407 Introduction to Polymer Science
CH-413 Chemistry and Biology of Selected Natural Products
CH-414: Introductory Environmental and Green Chemistry

Detailed Syllabi

CH-401 Principles of Inorganic Chemistry (L 3-T 0-P 0-CH 3- Credit 3)

Unit 1

Brief review of the following: Periodic properties, ionic bonding, valence bond theory and LCAO-MO theory, orbital symmetry and overlap, bond energy and covalent radii, Metallic bonding, band theory, hydrogen bonding, clathrates, VSEPR model and Walsh diagram, bonding in alloys, intermetallic compounds.

Unit 2

Stereochemistry and bonding in non-transition element compounds, Cages, clusters, rings – boranes, carboranes, metalloboranes and metallocarboranes, siloxanes, hetero-atomic rings, phosphonitrilic compounds.

Unit 3

Oxidation and reduction: Use of redox potential data, analysis of redox cycles, redox stability in water, disproportionation, Frost, Latimer and Pourbaix diagrams.
Acids and bases: Generalized acid base concept including hardness and softness.

Unit 4

Group theory: Symmetry elements and symmetry operations, symmetry groups, molecular dissymmetry and optical activity, symmetry point groups for compounds having co-ordination number 2 to 9, matrix representation of groups, reducible and irreducible representation, the Great orthogonality theorem.

Unit 5

Bioinorganic chemistry: Scope, inorganic elements in biological systems, basic bioenergetics, Active transport of cations across membranes, Na^+/K^+ pump, heme-protiens – hemoglobin, and myoglobin: structure, thermodynamics and kinetics of oxygenation.

Text Book(s)

1. Cotton, F.A., Wilkinson, G. *Advanced Inorganic Chemistry, 5th edn.,* (John Wiley, 1988).
2. Huheey, J. E., Keiter, E. A., Keiter, R. L, Medhi, O. K., *Principles of Structure and Reactivity, 1st edn.*, (Pearson Education, 2006).

Reference Book(s)

1. Cotton, F.A., *Chemical Application of Group Theory, 3rd edn.,* (John Wiley & Sons, 1999).
2. Atkins, P., Overton, T., Rourke, J., Weller, M., Armstrong, F., *Inorganic Chemistry,* (Oxford University Press, 2006).

CH-402 Principles of Organic Chemistry (L 3-T0-P 0-CH 3- Credit 3)

Unit 1

Structure and Bonding: Reactivity of organic molecules, aromaticity, n-annulenes and hetero-annulenes, fullerenes (C_{60}), Graphene, Cryptans, bonds weaker than covalent: addition compounds, inclusion compounds and rotaxenes.

Unit 2

Thermodynamics and Kinetics: Acids and bases, Concept of Hard and soft acids and bases, symbiosis, labeling and kinetic isotope effects, Hammett equation, σ–ρ relationship, non-classical

carbenuim ion (or carbocation), kinetic and thermodynamic control. Hammand principle, Curtin-Hammett principle, transition state and intermediates.

Unit 3
Stereochemistry: Chirality and isomerism in organic system, conformational analysis of simple cyclic and acyclic systems, interconversion of Fischer, Newman and Sawhorse formula, E-Z isomerism, R-S nomenclature, diastereomerism in acyclic and cyclic systems, newer methods of asymmetric synthesis (including enzymatic and catalytic nexus), enantio-, and diastereo selective synthesis, stereospecific synthesis, effect of conformation on reactivity. Methods of resolution, optical purity, optical activity in absence of chiral atom, Neighbouring group participation

Unit 3
General reaction mechanism, aliphatic substitution reaction, S_N1, S_N2, mixed S_N1 and S_N2 and S_Ni reaction, Set reaction, Classical and nonclassical carbocations. Electrophilic sunstitution reaction, S_E1, S_E2, S_Ei mechanism, Aromatic substitution reaction, SNAr, Benzyne, SRN^1 mechanism, Reactivity, effect of substrate, leaving group and attacking nucleophile. Elimination reaction, E^1 E^2 and E^1cB.

Unit 4
Addition Reaction: Mechanism and stereochemical aspects of addition reaction in carbon-carbon multiple bonds, region and chemoselectivity, orientation and reactivity, mechanism of condensation reactions involving enolates- Aldol, cross Aldol, Knoevenagel, Claisen, Perkin and Stobbe reactions.

Unit 5
Heterocyclic Chemistry: Synthesis, reactions and reactivity of heterocycles, e.g. furan, thiophene, pyrrole, pyridine, quinoline, isoquinoline and indole, Skraup synthesis, Fischer-Indole synthesis, π-excessive and π -deficient heterocycles.

Text Book(s)
1. Smith M. B., March, J. *Advanced Organic Chemistry, Reaction Mechanism and Structure*, (John Wiley, 2001).
2. Kalsi, P. S. *Stereochemistry, Conformation and Mechanism*, (New Age international Publishers, 2009).

Reference Book(s)
1. Sykes, P. *A Guide Book to Mechanism in Organic Chemistry, 6th edn.*, (Longman, 1986).
2. Carey, F. A., Sundberg, R. J. *Advanced Organic Chemistry, 4th edn*., (Plenum Publishers, 2001).

CH-403 Chemical and Statistical Thermodynamics (L 0-T 0-P 3- CH 3-Credit 3)

Unit 1
Brief review of thermodynamic functions and laws of thermodynamics: Temperature dependence of thermodynamic functions; Experimental determination of thermodynamic functions; Thermodynamic description of mixtures, Gibbs-Duhem equation; Chemical equilibrium; Thermodynamic description of phase transitions, Clapeyron-Claussius equation, Phase diagrams; Thermodynamics of nonideal systems – fugacity and activity concepts, excess properties.

Unit 2
Concepts of statistical thermodynamics, entropy and probability, ensembles, distribution laws of MB, FD and BE, partition functions and statistical formulation of macroscopic variables. Use of

statistical thermodynamics including calculation of electrical and magnetic properties, and heat capacity of solids, application of BE statistics to helium

Unit 3

Non-equilibrium thermodynamics, thermodynamic criteria for non-equilibrium states; Assumptions of non-equilibrium thermodynamics; Uncompensated heat, entropy production and entropy flow, entropy balance. Onsager formalism, relation between forces and fluxes, transformations of generalised fluxes and forces, microscopic reversibility and Onsager's reciprocity relations. Electrokinetic phenomena, diffusion, electric conduction, irreversible thermodynamics for biological systems, coupled reactions.

Text Book(s)

1. Engel, T. and Reid, P. *Thermodynamics, Statistical Thermodynamics and Kinetics 2nd edn.,* (Pearson, New delhi, 2011).
2. Kalidas, C. and Sangaranarayanan, M.V. *Non-equilibrium Thermodynamics, Principles and applications,* (Mamillan, New Delhi, 2002).

Reference Book(s)

1. Atkins, P. and Paula, J. de. *Atkins' Physical Chemistry, 9th edn.,* (Oxford University Press, New Delhi, 2010).
2. Berry, R. Rice S.A. and Ross, J. *Physical Chemistry, 2nd edn.,* (Oxford, London, 2010).

CH-404 Quantum Chemistry and Chemical Bonding (L 3-T 0-P 0-CH 3 Credit 3)

Unit 1

Mathematical Review: Basic vector algebra, matrix, determinant, Eigen value equations, quantum mechanical operators, orthogonal functions, Schmidt's orthogonalization technique.

Unit 2

Planck's quantum theory, wave-particle duality, uncertainty principle, postulates of quantum mechanics, Schrödinger equation, free particle, particle in a box, degeneracy, harmonic oscillator, rigid rotator, the hydrogen atom, angular momentum, electron spin, spin-orbit coupling.

Unit 3

Approximate methods in quantum mechanics: The variation theorem, linear variation principle and perturbation theory (first order and non-degenerate), application of variation method and perturbation theory to the Helium atom, antisymmetry, Slater determinant, term symbols and spectroscopic states.

Unit 4

Born-Oppenheimer approximation, Hartree-Fock method, Brillouin theorem, Koopman's theorem, Roothan's equations, models of chemical bonding- Molecular orbital (MO) and Valence bond (VB) theories, application to diatomic molecules such as, H_2, H_2^+, N_2, O_2, and CO. Hybridisation and MOs of H_2O, NH_3 and CH_4, Introduction to the SCF method.

Unit 5

Quantitative MO theory - Huckel π-electron theory and its application to ethylene, butadiene and benzene, energy levels of di- and tri- atomic molecules, Walsh diagrams and molecular geometry, extended Huckel MO theory and calculation on some simple molecules.

Text Book(s)

1. Atkins, P. W., Friedman, R. S., *Molecular Quantum Mechanics*, (Oxford University Press, 1997).
2. McQuarrie, D. A. *Quantum Chemistry* (Viva Books Private Limited, 2003).

Reference Book (s)

1. Levine, I. N *Quantum Chemistry*, (Pearson Education, Inc. 2004).
2. Prasad, R. K. *Quantum Chemistry,* (Wiley Eastern Limited, 2006).

CH-405 Laboratory Course in Organic Chemistry (L 0-T 0-P 6-CH 12-Credit 6)

Unit 1

Separation techniques of organic compounds and their spectroscopic identification

Experiments involving the separation and purification of organic compounds from a mixture, using chromatographic techniques, steam distillation, fractional crystallization and sublimation

Unit 2

Synthesis of organic compounds using common reagents: At least eight preparation (involving two or more than two steps) involving the following representative reactions: (a) Oxidation of alcohol (b) Reduction of carbonyl group (c) Nucleophilic substitution; (d) Cycloaddition reaction; (e) Condensation reaction; (f) Aromatic electrophilic substitution; (g) Preparation of dyes, (h) Heterocyclic synthesis, (i) Solid phase synthesis etc.

Unit 3

Natural product extraction: Caffeine, Nicotine, Carotenoides etc.

Unit 4

Estimation of Glucose, acetic acid in vinegar, -OH groups etc.

Unit 5

Determination of acid value and saponification value of fat/ oil

Unit 6

Green experiments

Text Book(s)

1. Pasto, D., Johnson, Miller, M. *Experiments and Techniques in Organic Chemistry*, (Prentice Hall, 1992).
2. Williamson, K. L. *Macroscale and Microscale Organic Experiments*, (D. C. Heath & Company, 1999).

Reference Book (s)

1. Furniss, B. S., Ford, A. J. H., Smith, P. W. H., Tatchell, A. R. *Vogel's Textbook of Practical Organic Chemistry, 5th edn.*, (Wiley, 1989).

CH-408 Chemistry of Transition Elements (L 3-T 0-P 0-CH 3- Credit 3)

Unit 1

Aspects of d- and f-block elements: Elements of first transition series and their comparison with the second and third series, general periodic trends, chemistry of various oxidation states of first

row transition metals and their comparison with the second and third row transition metals based on electronic configuration. The splitting of d-orbitals in various fields and splitting of f-orbitals in octahedral field, lanthanide contraction, oxidation states, complexes of lanthanides and actinides, qualitative angular overlap model.

Unit 2

Electronic structure and spectra of transition metal complexes: Spectroscopic states, Crystal Field Theory, Orgel and Tanabe-Sugano diagrams, selection rules, band intensities and band width, Adjusted Crystal Field Theory, Spectrochemical and Nephelauxetic series, molecular orbital theory of complexes (including complexes with and without π bonding), MO diagrams for octahedral and tetrahedral complexes, Jahn-Teller effect, Charge-transfer spectra, optical properties of lanthanides and actinides.

Unit 3

Magnetic properties of transition metal complexes: Types of magnetic behaviour: dia-, para-, ferro- and anti-ferromagnetic compounds, spin-orbit coupling, temperature independent paramagnetism, application of Crystal Field Theory to explain magnetic properties, spin-crossover. Thermodynamic effects-hydration, ligation, lattice energy, magnetic properties of lanthanides and actinides.

Unit 4

Reaction Mechanism of inorganic complexes: Stepwise and overall formation constants. Factors affecting the stability of metal complexes, chelate effect, determination of binary formation constants, Energy profile of a reaction, inert and labile complexes, kinetics of substitution in octahedral complexes, acid hydrolysis and base hydrolysis. Dissociative, associative and interchange mechanism, trans-effect, isomerisation and racemisation in tris-chelate complexes, electron-transfer reactions, stereo-chemical non-rigidity and fluxional molecules.

Text Book(s)

1. Huheey, J. E., Keiter, E. A., Keiter, R. L, Medhi, O. K. *Principles of Structure and Reactivity, 1st edn.*, (Pearson Education, 2006).
2. Cotton, F. A., Wilkinson, G., Murillo, C. A., Bochmann, M. *Advanced Inorganic Chemistry, 6th edn.*, (John Wiley, 1999).

Reference Book(s)

1. Greenwood, N. N., Earnshaw, A. *Chemistry of the Elements*, (Pergamon Press, 1984).
2. Carlin, R.L. *Magnetochemistry*, (Springer Verlag, 1986.)

CH-409 Organic Reactions and Mechanism (L 3-T 0-P 0-CH 3- Credit 3)

Unit 1

Reduction: Catalytic hydrogenation and dehydrogenation, dissolving metal reduction, hydride reduction of functional groups, Meerwein-Pondrof Verley reduction, hydroboration and related reaction, reaction of alkyl borane and tributyltin hydride, Wolff-Kishner reduction, non metallic reducing agents such as diimide.

Unit 2

Oxidation: Oxidation by Cr and Mn compounds; oxidation of alcohol, aldehyde, C=C, C-H bonds, PCC, Oxidation with per acids and peroxides: C=C, Sharpless epoxidation, Baeyer-Villiger oxidation. Other types: Prevost and Woodward hydroxylation, cis- and trans-hydroxylation, glycol cleavage reagents; $KMnO_4$, OsO_4, HIO_4, $Pb(OAc)_4$, mercuric acetate; SeO_2 oxidation of allylic C-H bond.

Unit 3
Rearrangement reactions: Formation and stability of carbenium ions, carbanions, carbenes, nitrenes, radicals, ylides and arynes. Rearrangement reactions involving carbocation (Wagner-Meerwein, Pinacol-Pinacolone rearrangement), carbenes (Wolff & Arndt- Eistert synthesis), nitrenes (Hoffman, Curtius, Schmidt, Lossen, Beckman), acyl cation, PPA cyclization and Fries rearrangement

Unit 4
Photochemistry: Cis-trans isomerisation, Paterno-Buchi reaction, Norrish type I & II reaction, photoreduction of Ketones, dipimethane rearrangement, photochemistry of arenes, Barton reaction.

Unit 5
Pericyclic reactions: Orbital symmetry, selection rules and stereochemistry of electrocyclic reaction, cycloaddition and sigmatropic shift, Sommelet, Hause, Cope and Claisen rearrangement.

Unit 6
Free radical reactions: Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, reactivity of the attacking radicals, the effect of solvents on reactivity, allylic halogenation by NBS, oxidation of aldehydes to carboxylic acids, auto-oxidation.

Unit 7
Selected organic reaction and reagents: Favörski, Hofmann-Loffler-Freytag, ene, Stork-enamine, Michael addition, Robinson annulation, Mannich, Shapiro, Chichibabin and Witting reaction, Gilman's reagent, DCC, LDA, 1,3–dithiane (reactivity umpolung), trimethyl silyl iodide, Baker's Yeast, Phase-transfer catalysts.

Text Book(s)
1. Smith, M. B., March, J. *Advanced Organic Chemistry: Reaction Mechanism and Structure*, (John Wiley, 2009).
2. House, H. O. *Modern Synthetic Reaction*, (W. A. Benjamin Inc. 1972).

Reference Book(s)
1. Norman, R. O. C., Coxon, J. M. *Principles of Organic Synthesis*, (Blackie Academic and Professional, 1993).
2. Caruthers, W., Coldham, I. *Modern Methods of Organic synthesis, 4th edn.,* (Cambridge University Press, 2004).

CH-410 Chemical Dynamics and Electrochemistry (L 3-T 0-P 0-CH 3-Credit 3)

Unit 1
Brief review of chemical kinetics: Determinations of reaction rates; Kinetics and mechanism; Steady state kinetics; Kinetic and thermodynamic control of reactions; Composite reactions, chain reactions; Oscillatory reactions;
Photophysical and photochemical processes; Fast reactions; study of fast reactions by flow method, relaxation method, flash photolysis, T and P jump and nuclear magnetic resonance method; Femto-chemistry.
Reactions in solutions; Ionic reactions, kinetic salt effect; Electron transfer and proton transfer reactions; Kinetics of enzyme catalysis and micellar catalysis; Phase transfer catalysis; Kinetics and techniques of polymerization; Polymer molecular weight control.

Unit 2
Theories of reaction rates: Arrhenius theory; Collision theory, Activated complex theory; Treatment of unimolecular reactions; Lindemann-Hinshelwood and RRKM theory.

Unit 3
Equilibrium electrochemistry of ions, hydration number, activity coefficient, Debye-Huckel theory, Debye-Huckel-Onsager treatment and its extension, ion-solvent interactions, Debye-Huckel-Jerum model, electro-capillarity. Ion transport, Ion channels; Diffusion of ions and molecules in solutions; Electrocatalysis – influence of various parameters

Unit 4
Electrodes and electrochemical cells, hydrogen electrode, cell reactions, Nernst equation; Electrode kinetics, electrode/electrolyte interface, electrical double layer, various models. Exchange current density, Butler-Volmer equation, over potential, Tafel plot; Voltammetry, polarography, half-wave potential, batteries, solid state battery, fuel cells, corrosion and its prevention.

Text Book(s)
1. Atkins, P. and Paula, J. de. *Atkins' Physical Chemistry*, *9th edn*., (Oxford University Press, New Delhi, 2010).
2. Engel, T. and Reid, P. *Thermodynamics, Statistical Thermodynamics and Kinetics*, *2nd edn*., (Pearson, New Delhi, 2011).

Reference Book(s)
1. Laidler, K. J. *Chemical Kinetics*, *4th edn*., (McGraw Hill, New Delhi, 2007).
2. Bokris, J.O.M. and Reddy, A.K.N. *Modern Electrochemistry*, *Vol. I & II*, (Plenum, 2001).

CH-411 Principles and Application of Spectroscopy (L 3-T 0-P 0-CH 3-Credit 3)

Unit 1
Rotational and Vibrational spectra: Basic principles, selection rule, fundamental vibrations, Raman Effect. Identification of some representative organic and inorganic compounds.

Unit 2
Electronic spectra: Frank-Condon principle, Fluorescence, Phosphorescence, electronic spectra of diatomic molecules, chromophores , auxochromes, absorption and intensity shifts, solvent effects, Woodward Fieser rules.

Unit 3
Nuclear Magnetic Resonance Spectroscopy: Basic principles, origin of chemical shifts, factors affecting the chemical shifts and their interpretation, spin-spin coupling, relaxation processes, coupling constants. Nuclear Overhouser effect (NOE) 2D-NMR, DEPT, HMQC, HMBC, ^{1}H, ^{13}C, ^{31}P, ^{15}N and ^{19}F NMR spectra of selected compounds. Shift reagents, spin tickling.

Unit 4
Mass spectrometry: Basic principles and instrumentation, mass spectral fragmentation of organic compounds, applications to organometallic compounds.

Unit 5
EPR spectroscopy: Basic principles, origin of g-shifts , hyperfine and super hyperfine coupling, spin orbit coupling, line shape, zero field splitting, Kramer degeneracy, ESR analysis of organic compounds, transition metal complexes of.vanadium, copper, cobalt and iron.

Unit 6
Mö ssbauer spectroscopy: Nuclear resonance absorption, recoil energy, Doppler effect, Mö ssbauer effect, Isomer shift, quadruple interactions, effect of magnetic field, determination of oxidation states of iron (including bioinorganic systems, ferredoxins) tin and cobalt compounds.

Text Book(s)
1. Banwell, C. N., Mc.Cash, E. M. *Fundamentals of Molecular Spectroscopy*, (Tata McGraw Hill, 1994).
2. Drago, R. S. *Physical Methods for Chemistry*, (Saunders Company, 1992).

Reference Book(s)
1. Nakamoto, K. *Infrared and Raman Spectra: Inorganic and Coordination Compounds, 6th edn.*, (John Wiley, 2009).
2. Pavia, D.L., G.M. Lampman, G.S. Kriz, J. R. Vyvyan, *Spectroscopy*, (Cengage India, 2008)

CH-412 Laboratory Course in Inorganic Chemistry (L 0-T0-P 6-CH 12-Credit 6)

Unit 1
Quantitative estimation involving volumetric (redox and complexometry), gravimetric and spectrophotometric methods of analysis of constituents in three component mixtures, alloys and minerals

Unit 2
Synthesis and characterization of inorganic compounds, including those involving green synthetic methodology: Characterization includes elemental analysis, studies by IR, electronic spectra, magnetic susceptibility, conductance measurements, cyclic voltammetry. TG, DSC.

Text Book(s)

1. Marr, G., Rockett, B. W. *Practical Inorganic Chemistry*, (Van Nostrand, 1972).
2. Jolly, W. L. *Synthesis and Characterization of Inorganic Compounds*, (Prentice Hall, 1970).

Reference Book(s):
1. Wollins, J. D. *Inorganic Experiments*, (VCH, 1994).
2. Parshall, G. W. (Ed. in Chief). *Inorganic Synthesis, Vol. 15*, (McGraw Hill, 1974).

CH-501 Bio-Organic Chemistry (L3-T 0-P 0-CH 3- Credit 3)

Unit 1
Bio-organic chemistry :Structure of amino acids and physical and chemical properties, method of synthesis (including Merrifield synthesis) of peptides and polypeptides, naming of polypeptides chain, amino acid sequence determination (N-terminal and C-terminal), structure of protein (Helical and pleated structure), denaturation of protein, biosynthesis of proteins, therapeutic and diagnostic applications

Unit 2

Structure of purines and pyrimidine bases and their biosynthesis, nucleosides and nucleotides and their nomenclature, structure of RNA and DNA, replication of DNA and mutagenesis, codon, anticodon, t-RNA, structure and genetic code, transcription and translation,

Unit 3

Enzymes: Mechanism of enzyme action and models, kinds of reactions catalyzed by enzymes, nomenclature, stereochemical aspects, cofactors, co-enzyme chemistry. structure and function of NADH,
FAD, ADP and ATP..

Unit 4

Terpenoids: Classification, structure, chemistry and biosynthesis of some important mono, sesqui, di and tri-terpenes. e.g. limonene, carvone or carveol etc.

Unit 5

Alkaloids: Characteristic reaction, general methods of degradation, structure and chemistry of some well known alkaloids, e.g. quinine, cocaine, morphine, heroin.

Unit 6

Biosynthetic pathway for Shikimic acid, polyketide derived natural products.

Unit 7

Prostaglandins: General structure, classification, biosynthetic pathway, stereoselective synthesis of Prostaglandins E_2 and F_2.

Text Book(s)

1. Lehninger, A. L. *Principles of Biochemistry*, (Worth Publishers, 1993).
2. Blackburn, G. M., Gait, M. J., Loakes, D., Williams, D. M. ed., *Nucleic Acids in Chemistry and Biology*, *3rd edn.*, (RSC publishing, 2006).

Reference Book(s)

1. Salerini, O. L. *Natural and synthetic organic medicinal compounds*, (C. V. Mosby Co. 1976).
2. Mann, J.; Davidson, R. S.; Hobbs, J. B.; Banthrope, D. V., Harborne, J. B. *Natural Products, their chemistry and biological significance*, (Longmann, Essex., 1994).
3. Norman, R., Coxon, J. M. *Principles of Organic Synthesis*, (Blackie, Academic and Professional, 1997).

CH-502 Physical Chemistry of Surface and Condensed Systems (L 3-T 0-P 0-CH 3-Credit 3)

Unit 1

Thermodynamic description of surface; Surface tension, capillary action, pressure across curved surface, vapor pressure of droplet; Gibbs adsorption isotherm; BET equation, estimation of surface area; Surface film of liquids.Various adsorption isotherms: Freundlich isotherm, Langmuir isotherm, Dubinin-Radushkevich isotherm, Temkin isotherm,

Unit 2

Colloids; Surfactants, micelle, thermodynamics of micellization, microemulsion; Interfacial phenomenon, micellar catalysis; Host-guest chemistry. Lipids and biological membranes, functions of cell membrane, ion transport through cell membrane, nerve conduction, biological cell and its constituents, biomolecules, bioenergetics.

Unit 3
Polymer molecular weight determination of polymers and bipolymers; Thermodynamics of polymerization; Thermodynamics of polymer and biopolymer solution, phase separation of polymer solutions; Polymer solution properties; Stereochemistry of polymer.

Unit 4
Structures of solids and liquids, liquid crystals; Nanoparticles and nanotechnology; Defects in solids, thermodynamics of Schottky and Frenkel defect formation; Thin films; Langmuir-Blodget film. Electrical properties of solids, intrinsic and extrinsic semiconductors, doping of semiconductors, p-n junction, super conductors, conducting polymers, organic conductors, molecular electronic devices, nonlinear optical materials, optical reflectance, photoconduction, ionic conductors.

Unit 5
Reactions on solid surfaces; Diffusion in solids, Solid state batteries.
Zeolites: Synthesis, structure, surface area and catalytic properties; glasses, ceramics and composites.

Text Book(s)

1. Atkins, P. and Paula, J. de. *Atkins' Physical Chemistry, 9th edn.,* (Oxford University Press, New Delhi, 2010).
2. Chakrabarty, D.K. *Solid State Chemistry, 1st edn.,* (New Age Publishers, 2005).

Reference Book(s)
1. West, A.R. *Solid State Chemistry and its Applications, 4th edn.,* (Plenum, 2007).
2. Billmeyer, F.W. *Textbook of Polymer Science, 2nd edn.,* (Wiley, 2007).

CH-503 Special Topics in Inorganic Chemistry (L 3-T 0-P 0-CH 3-Credit 3)

Unit 1
π- Acid complexes: Preparation, properties, structures and bonding of metal complexes with CO, N_2, NO, PR_3, AsR_3 as ligands, metal carbonyl hydrides and metal carbonyl clusters. LNCC and HNCC, Compounds with metal-metal multiple bonds

Unit 2
Organometallics: Structure, bonding, synthesis and reactions of metal complexes with alkyls, aryls, alkenes, alkynes and allyls, double and multidecker sandwich complexes.

Unit 3
Homogeneous and heterogeneous catalysis: Oxidative addition and reductive elimination reactions, insertion and extrusion reactions, reactions involving co-ordinated ligands, cyclometallation reactions. Catalytic reactions of alkenes – isomerisation, hydrogenation, carbonylation, hydroformylation and polymerization, Fischer-Tropsch process

Unit 4
Introduction to Supramolecular Chemistry, supramolecular synthesis of organic, metal-organic and inorganic compounds, host-guest chemistry

Unit 5

Inorganic Photochemistry: Excited states, ligand field states, Adamson's rules ,charge-transfer states and Thexi states; Phosphoresence and fluorescence; Photochemical reactions: substitution and redox reactions of Cr (III), Ru(II) and Ru(III) complexes

Text Book(s)

1. Elschenbroich, C., Salzer, A. *Organometallics – A Concise Introduction, 2nd edn.*, (VCH Publication 1992).
2. Ramamurthy, V., Schanze, K. S. *Multimetallic and Macromolecular Inorganic Photochemistry molecular and Supramolecular Photochemistry, 4th edn.*, (Marcel Dekker, 1999).

Reference Book(s)

1. Crabtree, R. H. *The Organometallic Chemistry of the Transition Metals, 4th edn.*, (John Wiley, 2005).
2. Hammer, F. *Inorganic Photochemistry*, (Sarup Book Publishers, 2009).

CH-504 Analytical Techniques (L 3-T 0-P 0-CH 3- Credit 3)

Unit 1

X-ray methods: X-ray diffraction, X-ray fluorescence and X-ray absorption and X-ray emission spectroscopy.

Unit 2

Thermoanalytical methods: Thermo gravimetric analysis, differential thermal analysis and differential scanning calorimetry.

Unit 3

Electrochemical methods: Coulometry, Polarography, anode-stripping voltammetry, pulse techniques, cyclic voltammetry, electrogravimetry, spectroelectrochemistry.

Unit 4

Chromatographic methods: Adsorption, liquid-liquid partition, ion–exchange, paper and thin-layer chromatography, HPLC, gel permeation chromatography and gas chromatography, HPTLC, Flash chromatography.

Unit 5

Radiochemical methods: Tracers in chemical analysis, isotopic exchange, isotopic dilution technique, labeling experiments in studying reaction mechanism.

Unit 6

Optical microscopy: Optical Rotatory Dispersion and Circular Dichroism: Definition, Deduction of absolute configuration, octane rule for ketones.
Transmission electron microscopy (TEM) and scanning electron microscopy (SEM).

Unit 7

Atomic absorption spectroscopy: Inductively coupled Plasma- mass spectroscopy (ICP-MS), ICP-AES (Atomic Emission Spectroscopy),

Text Book(s)

1. Drago, R. S. *Physical Methods in Chemistry*, (Saunders College Publishing, 1992).
2. Hollas, J. M. *Modern Spectroscopy*, (John Wiley, 1996).

Reference Book (s)

1. Willard, H. H. *Instrumental Methods of Analysis*, (East West Press, 1998).
2. Bard, A. J., Faulkner, L. R. *Electrochemical Methods, Fundamentals and Applications,* (John Wiley, 2000).

CH-505 Laboratory Course in Physical Chemistry (L 0-T 0-P 6-CH 12-Credit 6)

Unit 1

Purification of chemicals and calibration of analytical instruments; Error analysis- primary and secondary data, accuracy and precision, averaging of data, types of experimental error, significant figures, estimation and representation of error, and minimization of errors; Handling of basic instruments, e.g., potentiometer, conductivity meter, spectrophotometer, etc., through three basic experiments.

Unit 2

Four minor experiments chosen from: Kinetics by spectrophotometry, polarimetry and conductometry; Relative strength of two acids by conductance; Interfacial tension between two liquids by Tensiometer; Determination of a weak acid and a strong acid in mixture by potentiometry; Study of liquid-liquid phase diagram; Determination of fluoride by ion selective electrode, nitrate spectrophotometry; Determination of average molecular weight of a polymer by viscometry, etc.

Unit 3

Four major experiments chosen from: Study of non-Newtonian polymer solutions by Brookfield viscometer; Study of excess adiabatic compressibility of binary system by ultrasonic interferometry; Simultaneous determination of CMC and partition equilibrium constant by spectroscopic method; Kinetics of the catalytic decomposition of H_2O_2 by manganese (IV) oxide; Determination of CMC by Du Nouy Tensiometry; Micellar catalysis by spectroscopy; Determination of pK_a by spectroscopy; Determination of stoichiometry and the stability constant of the complex formation; Study of pseudo-ternary phase diagram of oil-water-(surfactant-cosurfactant) system; Determination of activation energy of reaction by polarometry; Preparation and characterization of nanoparticles; etc.

Text Book(s)

1. Practical Physical Chemistry, B. Viswanathan & P. S. Raghavan, (Viva Books Pvt. Ltd., 2005).
2. Practical Physical Chemistry, A. M. James & F. E. Prichard, *3rd edn.*, (Longman, 1974).

Reference Book(s)

1. Advanced Practical Physical Chemistry, J.B. Jadav, *7th edn*., (Goel, 2008).
2. Experiments in Physical Chemistry, GW Garland, JW Nibler, DP Shoemaker, *7th edn*., (McGraw- Hill, 2003).

CH-506 Catalysis (L 3-T 0-P 0- CH 3- Credit 3)

Unit 1

Introduction: Definition, role of catalysts, classification of catalysts. Homogeneous catalysts: Mechanism of homogeneous catalysis, acid-base catalysis, enzyme catalysis, micellar catalysis, phase transfer catalysts, homogeneous catalysis in industry, Zigler-Natta catalysts, olefin and acetylene polymerization, isomerization, hydrogenation and HY addition, carbonylation reactions, hydroformylation, oxidation of olefins, metallocene catalysts.

Unit 2
Theory and mechanism of heterogeneous catalysts: Adsorption and catalysis, mechanism of heterogeneous catalysis, kinetics of heterogeneous catalytic reactions, volcano principle, shape and size selectivity of catalysts.

Unit 3
Characterization of catalysts and their surfaces: Methods of surface analysis, surface area, pore size, void fraction, particle size, mechanical strength, surface chemical composition, surface acidity and reactivity.

Unit 4
Examples of heterogeneous catalysts: Clays, zeolites, bimetallic, semiconductor and oxide catalysts, supported catalysts, polymer catalysts. Production and design of industrial catalysts: Materials and methods, precipitated catalysts, impregnated catalysts, skeletal catalysts, fused and molten catalysts, calcination, reduction, shape formation of catalyst particles, optimal shape and size of catalysts particle

Unit 5
Reactors: Definition, classification, reactor design, choosing reactors in laboratory and plant.

Unit 6
Catalyst promotion and deactivation: Promotion and promoters, causes and mechanism of deactivation, poisoning, sintering, prevention of catalyst decay, regeneration of catalysts

Unit 7
Examples of heterogeneous catalytic reactions: Catalytic processes in petroleum industry-reforming, cracking and hydrotreating; hydrogenation, hydrodesulphurization, Fischer-Tropsch process, etc.

Future Trends: Environmental aspect.

Text Book(s)
1. Bartholomew, C. H., Furrauto, R. J. *Fundamentals of Industrial Catalytic Processes 2nd edn.*, (Wiley Interscience, 2006).
2. Chakrabarty, D. K., Viswanathan, B. *Heterogeneous Catalysis* (New Age Int., 2008).

Reference Book(s)
1. Gates, B. C. *Catalytic Chemistry*, (John Wiley & Sons, 1992).
2. Augustine, R.L. *Heterogeneous Catalysts for Synthetic Chemists*, (Marcel-Dekker, 1996).

CH-507 Bioinorganic Chemistry (L 3-T 0-P 0-CH 3 Credit 3)

Unit 1
Calcium in biology: Calcium in living cells, transport and regulation, molecular aspects of intramolecular processes, extracellular binding protiens. Role in muscle contraction, blood clotting mechanism and biological calcification

Unit 2
Protiens and enzymes of Fe, Co, Cu, Mo and Zn: Hemerythrin, ferritin and transferrins, peroxidase, catalase, cytochrome P-450. Iron – sulphur proteins: rubredoxin and ferredoxins. Cytochrome C oxidase and superoxide dismutase, ceruloplasmin, Vitamin B12, B12 co-enzymes and cobalamines, carbonic anhydrase, carboxy peptidase, metallothionins, interchangeability of Zn and Co in enzymes. Structural and functional models

Unit 3
Biological nitrogen fixation, photosynthesis, Photosystem I and II in cleavage of water

Unit 4
Metals in medicine: Toxicity of mercury, cadmium, lead, chromium, beryllium, selenium and arsenic, biological defence mechanisms, chelation therapy, metals used for diagnosis and chemotherapy, platinum complexes as anticancer drugs, complexes of gold, copper, zinc, mercury, arsenic and antimony as drugs.

Text Book(s)
1. Cowan, J. A. *Inorganic Biochemistry- An Introduction*, (Wiley- VCH, 1997).
2. Hanzlik, R. P. *Inorganic Aspects of Biological and Organic Chemistry*, (Academic Press, 1976).

Reference Book(s)
1. Lippard, S. J., Berg, J. M. *Principles of Bioinorganic Chemistry*, (University Science Book, Mill Valley, 1994).
2. Hay, R. W. *Bioinorganic Chemistry*, (Ellis Hollwood, 1984).

CH-508 Methods in Organic Synthesis (L 3-T 0-P 0-CH 3-Credit 3)

Unit 1
Alkylation of carbon via enolates and enolate equivalents: Generation of carbon nucleophiles by proton abstraction, kinetic vs thermodynamic control in formation of enolates, alkylation of enolates, generation and alkylation of dianions, solvent effect in enolate alkylations, oxygen vs carbon as the site of alkylation, alkylation of aldehydes, esters, lactones and nitro compounds, use of enol derivatives (enamines, vinyl acetates, vinyl-silyl-ethers, C- or O-Sn- derivatives, boron aluminium enolates). Michael addition: (a) of Cu-derivatives (Gilman reagents), (b) improvements of the Robinson annulation –with alpha –silyl methylvinyl ketone use of vinyl pyridine, (c) of vinyl-silyl-ethers and allylsilanes.

Unit 2
Reaction of nucleophilic carbon species with carbonyl groups: Aldol and related condensation reaction, Mannich reaction, acylation of nucleophilic carbon, carbonyl olefination (Wittig types reaction and methylenation, recent improvements of the use of phosphorous compounds, ylides, Peterson olefination with alpha-silyl carbanions, olefination with carboxylic acid dianions through betalactones), Tebbe reagent.

Unit 3
Umpolung of reactivity in carbonyl chemistry: Addition of electrophiles to carbonyl carbons, enolate cations (use of ketene thioacetates etc.), homoenolate anions (metalated allyl ethers amines, thio-ethers, silanes), bis-homoenolate cations. Addition reactions of C-C multiple bonds (oxymercuration, hydroboration etc.) and organoboranes.

Unit 4
Organometallic compounds in organic synthesis, protective groups (hydroxyl, amine, carbonyl and carboxylic and C-C double bond protecting groups) in organic synthesis. New techniques to carry out polar reaction (crown ethers and cryptates, phase transfer catalysed reaction, micellar catalysis and solid phase synthesis),

Unit 5
Retrosynthetic analysis of multistep synthesis.

Text Book(s)
1. Mundy, B. P., Ellerd, M. G. *Name reaction and reagent in organic synthesis*, (John Wiley and Sons. 1998).
2. Smith, M. B. *Organic Synthesis, 2nd edn.*, (McGraw Hill, 2002).

Reference Book(s)
1. Carruthers, W. *Some modern methods of organic synthesis, 3rd edn.*, (Cambridge University Press, 1987).
2. March, J. *Advanced organic chemistry, 4th edn.*, (John Wiley and Sons, 1992).
3. Clayden, J., Greeves, N., Warren, S., Wothers, P. *Organic Chemistry*, (Oxford University Press, 2008).

CH-509 Polymer Chemistry (L 3-T 0-P 0-CH 3-Credit 3)

Unit 1
Introduction: Historical background, basic nature, classification, raw materials for polymers, gas cracker, naphtha cracker.

Unit 2
Kinetics and mechanism of polymerization: Degree of polymerization and molecular weight of polymer, kinetics of various types of polymerization, co-polymerization, reactivity ratio, molecular weight distribution, control of molecular weight

Unit 3
Polymerization techniques: Special features of polymerization, various polymerization techniques, polymerization reactors

Unit 4
Polymer characterization: Determination of molecular weight and molecular weight distribution, GPC, light scattering, end group analysis method, Zimm plot, viscosity of polymer solutions, thermal, mechanical, rheological and electrical properties of polymers, polyelectrolytes, ion-exchange resins.

Unit 5
Thermodynamics of polymer solutions: Chain conformation, molecular dimensions in solution, solubility of polymers, solubility parameters, lattice theory, ΔH, ΔS and ΔG of mixing in polymer solution, dilute polymer solutions, χ_1 and θ-temperature, phase separation, fractionation

Unit 6
Structure-property relationship: Stereochemistry of polymers, cross-linking, polymer architecture, elasticity, viscoelasticity, crystallinity

Unit 7
Natural polymers: rubber, natural fibers, silk fibers, Synthetic polymers: HDPE, LDPE, PP, PS, Nylon; synthetic polymeric resins and rubbers, moulding, Applications and Future trends: Applications, degradation and future trends.

Text Book(s)
1. Misra, G.S. *Introductory Polymer Chemistry* (Wiley Eastern Limited, 1993)
2. Billemeyer, F. *Textbook of Polymer Science* (Wiley, 1984)

Reference Book(s)
1. Odian, G. *Principles of Polymerization* (Wiley, 2004)
2. Sun, S.F. *Physical Chemistry of Macromolecules, 2nd edn.,* (Wiley, 2004)

CH-510 Organometallic Chemistry (L 2-T 0-P 2-CH 3-Credit 3)

Unit 1
Main Group Organometallics: Structure and bonding involving main group (Li, Be, Zn, Hg, Tl, Si, Sn and related systems) and transition elements (Cu, Ag, Au), metal organyls, isolobal analogy.

Unit 2
Transition Metal-Carbon Bond: Transition metal vinylidene and allenylidene compounds, cyclopropenyl cation ($C_3R_3^+$) and C_4R_4 as a ligand.

Unit 3
Organometallics in catalysis and synthesis: Heck reaction, Suzuki reaction, Stille reaction, hydrozirconation of alkenes and alkynes, hydroboration, hydrosilation, C-C cross coupling and related reactions, reactions of conjugated dienes. Insertion reactions involving molecules other than CO

Unit 4
Theoretical study of the electronic structure of some organometallic compounds

Textbook(s)
1. Elschenbroich, C., Salzer, A. *Organometallics – A Concise Introduction, 2nd edn.,* (VCH Publication 1992).
2. Cotton, F. A., Wilkinson, G., Murillo, C. A., Bochmann, M. *Advanced Inorganic Chemistry, 6th edn.,* (John Wiley, 1999).

Reference Book(s)
1. Crabtree, R. H. *The Organometallic Chemistry of the Transition Metals, 4th edn*., (John Wiley, 2005).
2. Powell, P. *Principles of Organometallic Chemistry, 2nd edn*., (Chapman, London, 1988).

CH-511 Heterocyclic Compounds and Medicinal Applications (L3-T0-P0-CH3-Credit3)

Unit 1
History of medicinal chemistry, interaction between drug molecule and receptor sites, drug action mechanism, drug metabolism, approaches to drug design; pharmacokinetics-pharmacodynamics, xenobiotics. Drug development, screening, lead optimisation, phase I, II and III trails.

Unit 2
Introduction to heterocyclic compounds: Nomenclature, classification, heterocycles and aromaticity, importance of heterocycles in medicinal chemistry.

Unit 3
Non-aromatic heterocycles: Syntheses and reactivities of small ring non-aromatic strained heterocycles like epoxides, aziridines, azetidines, oxetanes, thietanes. Syntheses, conformations and medicinal importance of six-membered non-aromatic heterocycles like piperdines, piperzines, morpholines, tetrahydropyrans.

Unit 4
Benzo-fused heterocycles containing one heteroatom: Syntheses and reactions of benzo-fused heterocycles containing one heteroatom *e.g*., benzofurans, 2,3-dihydrobenzofurans, benzothiophenes, benzopyrans, 1,2,3,4-tetrahydroquinolines etc. Examples and selected syntheses of some important drugs containing this class of benzo-fused heterocycles.

Unit 5
Aromatic heterocyclic compounds containing one hetero atom: Preparation and properties of furan, thiophene, pyrrole, indole, quinoline and isoquinoline derivatives.

Unit 6
Heterocyclic compounds containing two or more hetero atoms:Synthetic methods of preparation, properties and applications in medicinal chemistry *e.g*., azoles (pyrazole, imidazole, oxazole and thiazole derivatives), diazines (pyrazine, pyrimidine and pyridazine derivatives), benzo-diazines, heterocyclic compounds containing one nitrogen atom and an oxygen or sulphur atom (oxazine, phenoxazine and thiazine derivatives), triazines and tetrazines.

Text Book(s)
1. Abraham, D. J. ed., *Burger's Medicinal Chemistry and Drug Discovery (6 volume set), 6th edn.,* (Wiley Interscience, 2003).
2. Thomas, G. *Medicinal Chemistry, An Introduction,* (Wiley, 2000, Single Edition).

Reference Books
1. Bansal, R. K., *Heterocyclic chemistry*
2. Finar I. L., *Organic Chemistry,* Vol. I and II, John Wiley & Sons
3. Patrick, G. L. *An Introduction to Medicinal Chemistry, 2nd edn.,* (Oxford University Press, 2001).

CH-512 Chemistry of Materials (L 3-T 0-P 0-CH 3- Credit 3)

Unit 1
Solid state ionic conductors: Structure, physico-chemical principles, applications.

Ferrous alloys, Fe-C phase transformations in ferrous alloys; non-ferrous alloys - properties and applications of ferrous and non-ferrous alloys, magnetic alloy. Metallic glass, ceramics, Nano-materials and optical materials

Unit 2
Polymeric materials: Molecular shape, structure and configuration, crystallinity, stress-strain behaviour, thermal behaviour, polymer types and their applications, conducting and ferro-electric properties.

Unit 3
Inorganic Polymers: Polysiloxanes, polysilanes, polyphosphazenes, polymeric sulphur –synthesis, structure, properties and applications. co-ordination polymers and organometallic polymers.

Unit 4
Liquid crystals: Nomatic, smectic, cholesteric – properties and applications. High Tc materials: Defect Perovskites- high Tc superconductivity in cuprates, 1-2-3 and 2-1-4 materials; anisotropy, temperature dependence of electrical resistance, optical phonon modes, superconducting state, heat capacity, coherence length, elastic constants, position lifetimes, micro-wave absorption pairing and multigap structure in high Tc materials, applications of high Tc materials.

Unit 5
Organic solids: Conducting organics, organic superconductors, Magnetism in organic materials.
Fullerenes: doped fullerenes as superconductors.
Molecular devices: molecular rectifiers and transistors, artificial photosynthetic devices, sensors.
Clay-polymer and carbon composites, phosphor and laser materials.

Text Book(s)

1. Keer, H.V. *Principles of the Solid State* (Wiley Eastern, 1993)
2. Ashcroft, N.W.; Mermin, N.D. *Solid State Physics* (Saunders College, 1993)

Reference Book(s)

1. Callister, W.D. *Material Science and Engineering- An Introduction* (Wiley, New York, 1985)
2. Lever, K.D.; Alexender, J.M.; Rawlings, R.D. *Materials Science* (J.C. Senderson, ELBS)
3. Marck, J.E.; Allcock, H.R.; West, R. *Inorganic Polymers* (Prentice Hall, 1992)

CH-513 Organic Solid States Chemistry (L 3-T 0-P 0-CH 3-Credit 3)

Unit 1
Intermolecular Interactions: General Properties, van der Waals Interactions, Hydrogen Bonds, Halogen Bonds, Other Interactions

Unit 2
Crystal Engineering: Organic Solid States, Properties, Structure activity Relationship, X-ray Crystallography, Pharmaceutical Developments

Unit 3
Crystal Design Strategies: Synthesis in Chemistry, Supramolecular Chemistry, Synthon in Crystal Engineering

Unit 4

Crystallization of Organic Solids, Nucleation, Thermodynamics and Kinetics of Crystallization, Crystal Growth Mechanism, Crystal Morphology and Habit, Crystal Morphology Engineering

Unit 5

Polymorphism: Definition and Occurrence, Thermodynamic and Kinetic relationships of the Formation of Polymorphs, Methods of Polymorph Characterization, Properties of Polymorphs, Case Studies from the Pharmaceutical Industry, Polymorphism Today

Unit 6

Multi-component Crystals: Classification, Definition and Nomenclature, Solid Solutions, Host-Guest Compounds, Solvates and Hydrates, Donor-Acceptor Complexes, Co-crystals of pharmaceutical importance

Unit 7

Coordination Polymers: Definition, Classification and Design Strategies, Network Topologies, Supramolecular Isomerism, Interpenetration, Porous Coordination Polymers, Properties and Applications

Text Book(s)

1. Desiraju, G. R.; Vittal, J. J.; Ramanan, A. *Crystal Engineering: A Textbook*, © World Scientific Publishing Company, 2011.
2. Bernstein, J. *Polymorphism in Molecular Crystals*, Monographs on Crystallography, No. 14, Clarendon Press/International Union of Crystallography, 2002.

Reference Book(s)

1. Desiraju, G. R. *Crystal Design: Structure and Function*, © John Wiley & Sons, 2003.
2. Steed, J. W.; Atwood, J. L. *Supramolecular Chemistry*, John Wiley & Sons, 2009

CH-514 Biomolecular Chemistry (L 3-T 0-P 0- CH 3-Credit 3)

Unit 1

Interface of Chemistry and Biology, interaction between drug molecule and receptor sites

Unit2

The molecular design of life, biochemical reactions, Chemical and physical foundations of biomolecules : water, acid, base and buffers; the biosynthesis, structure and functions of key biomolecules (nucleic acids, amino acids, peptides and proteins, lipids and carbohydrate); synthesis and oxidations of fatty acids; biological membranes; membrane structure and transport mechanisms, membrane channels and pumps, molecular motors, cell signaling and signal transduction pathways, Principle of thermodynamics; bioenergetics and energy metabolism in cells, carbohydrate and glycobiology, glycolysis and gluconeogenesis, citric acid cycle, oxidative phosphorylation; light reaction of photosynthesis, Calvin cycle.

Unit 3

Detection and isolation of natural biomolecules, synthetic and semi-synthetic ways to different biomolecules, stereochemical consequences, protein and DNA X-ray crystallography, biomolecular spectroscopy (absorption and emission spectroscopy, polarization in light scattering, NMR, fluorescence spectroscopy, mass spectrometry for protein identification, vibrational spectroscopy)

Unit 4
Biodiversity of natural products

Text Book(s)

1. Blackburn, G. M., Gait, M. J., Loakes, D., Williams, D. M. ed., *Nucleic Acids in Chemistry and Biology, 3rd edn.,* (RSC publishing, 2006).
2. Patrick, G.L. *An Introduction to Medicinal Chemistry, 2nd edn.,* (Oxford University Press, 2001

Reference Book(s)

1. Nogradi, M. *Stereoselective synthesis, A Practical approach, 2nd edn.*, (VCH, Weinheim, 1995).
2. Lehninger, A. L. *Principles of Biochemistry,* (Worth Publishers, 1993).
3. Thomas, G. *Medicinal Chemistry, An Introduction,* (Wiley, 2000, Single Edition).

CH-515 Environmental and Green Chemistry (L 3-T 0-P 0-CH 3-Credit 3)

Unit 1
Environment and chemistry; Matter and cycles of matter; The atmosphere and atmospheric chemistry: The geosphere and geochemistry; Aquatic chemistry, CO_2 distribution, acid-base and redox equilibrium in water, pE-pH curves, water quality parameters

Unit 2
Chemistry and environmental pollution: Chemical hazards, chemical disasters, Water pollution, air pollution and soil pollution; Industrial pollution, vehicular pollutions, agricultural pollution, pollution by plastics; environmental biochemistry, toxicological chemistry

Unit 3
Environmental analysis: Analysis of water and wastewater, solid-wastes and air pollution.

Unit 4
Environmental protection: pollution prevention, green chemistry, biodegradation, water and wastewater purification – removal of arsenic, iron, fluoride, etc.; air purification, waste minimization, industrial and municipal waste treatment and soil remediation

Unit 5
Green chemistry principles: Principles of green chemistry, atom economy, less hazardous chemical syntheses, designing safer chemicals, safer solvents and auxiliaries, design for energy efficiency, renewable feedstock, catalysis, design for degradation, real time analysis for pollution prevention, and inherently safer chemistry for accident prevention.

Unit 6
Design of green synthesis: Ideal synthesis, clean routes, supercritical solvents, ionic liquids, green catalyst, auto-exhaust catalyst and clean technology.
Real world examples

Text Book(s)

1. Manahan, S. E. *Environmental Chemistry, 9th edn* (CRC Press, Boca Raton, 2010).

2. Anastas, P. T. and Warner, J. C. *Green Chemistry: Theory and Practice*, (Oxford University Press, 1998).

Reference Book(s)

1. Hutzinger, O. *Handbook of Environmental Chemistry*, Springer-Verlag, 1991.
2. Cann, M. C. & Connelly, M. E. *Real World Cases in Green Chemistry,* ACS, , 2000.

CH-516 Computational Chemistry and Numerical Analysis (L 3-T 0-P 0-CH 3-Credit 3)

Unit 1

Data analysis, mean and standard deviation, absolute and relative errors, linear regression, covariance and correlation coefficient. Curve fitting, solution of polynomial equation, numerical integration (Trapezoidal Rule, Simpson's Rule, Gaussian Quadrature), solution of ordinary differential equations (Euler's Method, Runge-Kutta methods, predictor-corrector method), matrix multiplication, inversion and diagonalisation.

Unit 2

Molecular Mechanics: Basic geometrical description of molecules; force-field development, intermolecular interactions, origin and modeling of dispersion forces & hydrogen bonds, strengths, weaknesses and applicability of currently available force-fields.

Unit 3

Static properties of complex systems: Introduction to Monte Carlo as a way of averaging. Metropolis Monte Carlo algorithm: introduction and applications.
Dynamical properties of complex systems: Molecular Dynamics as a way of averaging. Integration of the Newton's equations: initial conditions, numerical algorithms (Verlet and leap-frog), and thermostats.

Unit 4

Quantum Chemistry: Many electron systems, Hartree-Fock method, basis sets, electron correlation and its treatment, basics of density functional theory, DFT based reactivity descriptors. Introduction to popular softwares (like Gaussian, DMol, GAMESS). Applications to simple molecular systems.

Unit 5

Combined QM/MM methods: Implications of the choice of QM and MM methods; Application of QM/MM methods in organic, inorganic and organometallic systems including bio-organic and bio-inorganic molecules.
Quantitative structure activity relation (QSAR): Early approaches, topological indices, fragmental models; quantum mechanical descriptors

Text Book(s)

1. Lewars, E. *Computational Chemistry*, (Springer, 2003).
2. Balagurusamy, E. *Numerical Methods,* (Tata McGraw-Hill Publishing Company Limited, 2002

Reference Book(s)

1. Leach, A. R. *Molecular Modeling: Principles and Applications, 2nd edn.* (Pearson Prentice Hall, 2001).
2. Cramer, C. J. *Essentials of Computational Chemistry* (Wiley 2002).
3. Jensen, F. *Introduction to Computational Chemistry* (Wiley 1999).

CH-517 M. Sc. Project Work (L 0-T 0-P 9-CH 18- Credit 9)

In the final semester, students have to carry out project work at Tezpur University. The area of the work is to be decided by the advisor. On completion of the project work, students have to submit the work in the form of a dissertation followed by oral presentation in the presence of faculty members and external expert(s).

CH-406 Chemistry in Everyday Life (L 2-T 0-P 2-CH 3-Credit 3)

Unit 1

Materials we depend on – metals, polymers, paper, cement, ceramics and glass, chemical products- petroleum products, petrochemicals and their use in day to day life, LPG; semiconductors, plastics, dyes, paints, fabric and clothing; medicines, soap and detergents, cosmetics and personal care products, fertilizer, pesticides, herbicides: their uses and toxicity.

Unit 2

Basic chemistry of medicine, food, nutrition, preservatives, drinking water, beverages,
Negative aspects of chemistry and green chemistry: environmental pollution, carbon emission, industrial and vehicular pollution, water pollution, chemical mischief and adulteration, hazardous chemicals and chemical hazards, explosives, fireworks, disaster, green chemistry.

Unit 3

Chemistry in social life: green way of life at home, workplace; chemistry of love, esthetics, theatre and the arts, style and fashion, food habit.

Text Book(s)

1. Rao, C.N.R.; *Understanding Chemistry*, University Press (India) Ltd., Hyderabad,1999.
2. Seager S.L. and Slabaugh, M.R. *Chemistry for Today – General, Organic and Biochemistry*, *4th edn.*, (Brooks/Cole, 2000).

Reference Book(s)

1. Kurukstis K.K. and Van Hecke, G.R. *Chemistry Connections*, Academic Press,2000.

CH-407 Introduction to Polymer Science (L 3-T 0-P 0-CH 3-Credit 3)

Unit 1

Introduction: Historical background, basic nature and classification, importance of polymers as a class of material, polymer raw materials

Unit 2

Polymerization techniques: Special features of polymerization, step polymerization, radical chain polymerization, living and non-living chain polymerization, co-ordination polymerization, co-polymerization, ionic polymerization, ring opening polymerization, characterization of polymers, GPC, Spectroscopy of polymer, Rheology.

Unit 3

Structure-property relationship: Stereochemistry of polymers, modification of polymers, cross-linking, polymer architecture, polymer processing and fabrication, polymer composites.

Unit 4
Natural and synthetic polymers: rubber, natural fibers, silk fibers, PS, Nylon, etc.
Applications of polymers: Applications and future prospects

Text Book(s)

1. Gowarikar, V.R; Viswanathan, N.V.; Sreedhar, J. *Polymer Science* (Wiley-Eastern Limited, 1986)
2. Misra, G.S. *Introductory Polymer Chemistry* (Wiley Eastern Limited, 1993)

Reference Book(s)

1. Sperling, L.H. *Introduction to Physical Polymer Science* (Wiley-Interscience, 1986)
2. Odian, G. *Principles of Polymerization* (Wiley, 2004)
3. Sun, S.F. *Physical Chemistry of Macromolecules, 2nd edn.,* (Wiley, 2004)

CH-413 Chemistry and Biology of Selected Natural Products (L 3-T 0-P 0-CH 3-Credit 3)

Unit 1
Study of isolation, structure, stereochemistry, synthesis, biogenesis and biological properties of the following classes of natural products from plant, animal, and microbial sources.

Unit 2
Acetogenins and shikimates: Microbial metabolites: Pencillin G, Cephalosphorins and streptomycin.

Unit 3
Terpenes: Forskolin, taxol and azadirachtin.

Unit 4
Alkaloids: Morphine, Strychnine, Reserpine and vincristine

Unit 5
Vitamins: water and fat soluble vitamins

Text Book(s):

1. Finar, I. L., *Organic Chemistry, Volume 2. Stereochemistry and chemistry of natural products*
2. John Mann, *Chemical Aspects of Biosynthesis,*, Oxford University Press, Oxford.

Reference Book(s)

1.Krishnaswamy N.R. *Chemistry of Natural Products*: A Unified Approach, University Press (India) Ltd., Orient Longman Limited, Hyderabad, 1999.

CH 414: Introductory Environmental and Green Chemistry (L 3-T 0-P 0-CH 3-Credit 3)

Unit 1
Concept and scope of Environmental Chemistry: Definition and explanation for various terms, segments of environment, principles and cycles in the environments.

Unit 2

Chemistry of various organic and inorganic toxic materials and their effects, Introduction to chemical hazards and safety, Hydrocarbons - Chemistry of hydrocarbon decay, environmental effects, effects on macro and microorganisms, Detergents, dyes, synthetic polymers, Industrial wastes-some examples,

Unit 3

Atmospheric pollution: Acid-rain, Smog, industrial and vehicular pollution, ozone layer depletion, global warming and minimization of these problems.

Water pollution: Eutrophication, ground water contamination with arsenic, fluoride, toxic heavy metals and remediation, drinking water contamination and water-borne diseases, sources of germs and prevention.

Unit 4

Soil pollution: Soil pollution due to industrial disposal and use of chemicals including pesticides and synthetic fertilizers, remediation of agricultural lands.

Unit 5

Analysis and monitoring of environmental pollution: Introduction to equipments used for different environmental monitoring and assessments processes for water, air and soil samples.

Unit 6

Green Chemistry: Principles of green chemistry, concept of atom economy, renewable feedstock: natural polymers, natural dyes etc., use of less hazardous chemical syntheses and chemical synthetic methods, designing safer chemicals, use of safer solvents, catalysts and biodegradable polymers, design for green technology- energy efficient techniques, atom economy in syntheses, use of water as solvents and other biodegradable solvents, reusable heterogeneous catalysts.

Text Book(s)

1. Manahan, S.E. *Environmental Chemistry, 9th edn*., (CRC Press 2009).
2. Anastas, P.T. & Williamson,T.C. *Green Chemistry: Designing Chemistry for Environment*, (ACS, 2000).

Reference Book(s):

1. Moore J. W. & Moore. E. A. *Environmental Chemistry, 2nd edn*., (Academic Press, New York 1985).
2. B.K. Sharma, & Kaur, H. *Environmental Chemistry,* (Goel Publishing House, Meerut, India, 1996).
3. Ahuliwala,V.K. *Green Chemistry: Greener Alternatives to Synthetic Organic Transformations, (*Narosa Publishers, Delhi, 2009).

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