M Sc Chemistry

2018 Syllabus

18CHY501 QUANTUM CHEMISTRY 3 0 0 3

Unit I: Quantum Chemistry - Introduction

Origin of quantum mechanics, de Broglie relationship, the uncertainty principle (no derivation); Postulates of quantum mechanics:postulate I – wave functions, postulate II- Operators in quantum mechanics, operator algebra, postulate-III – eigen values, eigen value equations, postulate IV – Expectation value, postulate V – time dependent and time independent Schrodinger equation

Unit II: Applying Schrodinger equation to various general systems

Translational motion of a quantum entity (particle in one dimensional box and three dimensional box); vibrational motion (harmonic oscillator); rotational motion (rigid rotator, particle on a ring and particle on a sphere); angular momentum.

Unit III: Atomic structure and chemical bonding

Hydrogen and hydrogen-like atoms; Multi electron systems- variation methods, perturbation methods,application to the ground state of Helium atom, SCF method, the exclusion principle

Chemical bonding: Hydrogen molecule ion and hydrogen molecule - molecular orbital and valence bond theory, homo and hetero nuclear diatomic molecules from VB and MO theory, the concept of directed valences and hybridization; quantum mechanics in band theory of metallic solids

Unit IV: Electronic structure of polyatomic systems: Computational quantum chemistry

Semi empirical and ab-initio methods; QM approximations, Details of HMO and EHMO and its application to chemical bonding in unsaturated molecules(ethylene, 1,3butadiene etc) ; Details of SCF procedure, Hartree and Hartree Fock methods (up to ground and excited states of hydrogen molecule); the basis sets, STOs and GTOs, nomenclature of basis sets, basis set errors, introductory ideas on DFT.

Unit V: Molecular properties: Computational quantum chemistry

Calculations of molecular properties like atomic charges, dipole moments, electronic distributions, vibration frequencies, NMR chemical shift etc using Gaussian program, specification of molecular geometry using Cartesian coordinates and internal coordinates, Z-matrix, Z-matrix of some simple molecules, structure of a Gaussian input file

TEXTBOOKS:

1. *Ira N. Levin, 'Quantum Chemistry', 6th Edition, Prentice-Hall, 2008*

2. *Peter Atkins, Ronald Friedman, 'Molecular Quantum Mechanics', 4th edition, Oxford university press*
3. *R K Prasad, 'Quantum Chemistry', New Age International (P) LTD publishers*

.

REFERENCES:

1. *Andrew R Leech,' Molecular Modeling – Principles and Applications', 2nd Edition, Pearson Education.*
2. *Donald A. McQuarrie, 'Quantum Chemistry', Viva Books 2016.*

18CHY502 Concepts in Inorganic Chemistry 3 1 0 4

Unit 1 Nuclear Chemistry

Nuclear structure, mass and charge, mass defect, binding energy, stability rules, magic numbers, nuclear quantum numbers, nuclear parity and statistics, models of nucleus, shell model, liquid drop model, , semi empirical mass equation, equations of radioactive decay and growth, half-life, average life determination of half-lives, nuclear reactions, energetics of nuclear reactions, types of nuclear reactions, spontaneous and induced fission, neutron capture cross sections-critical size principle and working of nuclear reactor. Numerical problems relevant to each session.

Unit 2 Radiation Chemistry

Radioactive elements, decay kinetics, parent-daughter decay relationships, radioactive equilibrium - transient and secular equilibrium, alpha and beta decay, gamma emission, Radiochemical methods - measurement of radioactivity, measurement of radiations - ionization chamber, proportional counter, the Geiger counter, scintillation counter, semiconductor detectors. Applications of nuclear and radiation chemistry, isotope dilution analysis - activation analysis, radioactive tracers, radiometric titrations, radiation dosimetry, hydrated electron.

Unit 3 Inorganic materials I

Alkali and alkaline earth metals, their compounds, crown ethers and cryptands as complexing agents for alkali metal ions, Be and Mg compounds, boron cage compounds, boron hydrides, structure and bonding, 3-centre-2-electron bonds, styx numbers, the importance of icosahedral frame work of boron atoms in boron chemistry, closo, nido and arachno structure, carboranes, metallocene carboranes, B-N compounds, interstitial compounds, metal carbides, nitrides and hydrides, fullerenes, functionalized fullerenes, C-nanotubes .

Unit 4 Inorganic materials II

Inorganic chains and polymers, rings, cages, and clusters, sulphur-nitrogen compounds, polymeric sulphur nitride, isopoly anions, heteropoly anions, Keggin and Dawson polyoxometallates, borazines, metal clusters, nature of Si-Si bonds, silicates, silicates with zero-, one-, two- and three-dimensional structures, structure of elemental P, phosphonitrilic compounds, polymers with P-N bonds, interhalogen and pseudo halogens, intercalation chemistry, intercalation in layered materials like graphite, xenon fluorides & other xenon compounds.

Unit 5 Chemistry of f-block elements

The lanthanides and actinides, stable oxidation states, the lanthanide and actinide contractions, the f-orbitals, spectral and magnetic properties - comparison with inner transition and transition metals, separation of lanthanides, use of lanthanide compounds as shift reagents, photo-emission of lanthanide compounds, organometallic compounds of lanthanides and actinides and their structural features, reactions of lanthanide and actinide compounds, mineral sands of south west India - Ilmenite, Monazite, etc.

TEXTBOOKS:

1. H J Arnikar, Essentials of Nuclear Chemistry, 4th revised edition, New Age International (P) Limited publishers, 2015.
2. H J Arnikar, Nuclear Chemistry through Problems, New Age International Publishers.
3. J. Huheey, Inorganic Chemistry: Principles of Structure and Reactivity, 4th edition, 2006.
4. F.A. Cotton, Advanced Inorganic Chemistry, Wiley; 6th Edition edition (22 April 1999)
5. J.D. Lee Concise Inorganic Chemistry, Oxford University Press, 5th edition, 2008

REFERENCES:

. 1. Gregory R. Choppin, Jan-Olov Liljenzin and Jan Rydberg, Radiochemistry and Nuclear Chemistry (Third Edition), Elsevier, 2002
2. Walter D. Loveland, David J. Morrissey, Glenn T. Seaborg, Modern nuclear chemistry, A JOHN WILEY & SONS, INC., PUBLICATION, 2017.
3. Shriver and Atkins' Inorganic Chemistry, Oxford; 5 edition, 2009

18CHY503 Principles in Organic Chemistry 3 0 0 3

.

Unit 1 Aromaticity: Review of inductive and field effects – Resonance effects. Criteria for aromaticity – structural and electronic. Types – Huckel and Craig's rule, homo (Five, Six, seven and eight, membered rings), hetero (furan, thiophene and pyrrole) and nonbenzenoid aromatic systems. Aromaticity of fused rings, annulenes, catenanes, rotaxanes, mesoionic compounds, metallocenes, cyclic carbocations and carbanions.

Unit 2 Structure activity relationships – Orientation effects of substituent, Quantitative treatment of structure on reactivity - free energy relationships – Hammet equations, Taft equation.

Reactive Intermediates: Generation, structure and reactivity - reactions and rearrangement involving) of carbocations - non-classical carbocations, carbanions, carbon radicals, radical ions, carbenes, nitrenes, isonitrenes, arynes.

Unit 3 Mechanism and methods to determining them: Thermodynamic and kinetic requirement, Baldwin rules for ring closure – Kinetic and thermodynamic control – Hammond postulates, microscopic reversibility, Marcus theory, methods of determining reaction mechanisms - solvents and their effect on course of a reaction.

Acids and Bases: Bronsted and Lewis acids - HSAB concept and bases, pH and pKa, effect of structure on acidity and basicity, effect of medium.

Unit 4 Stereochemistry

Optical and geometrical isomerism, absolute and relative configuration, Cahn-Ingold-Prelog system, prochirality, prochiral centre, atoms, groups and faces, designations. Atropisomerism, optical isomerism in biphenyls, allenes, spirans and "ansa" compounds, compounds containing chiral nitrogen and sulfur atom, geometrical isomerism of cyclic compounds, cumulenes and oximes. Asymmetric synthesis, stereospecific and stereoselective synthesis, regioselective and regiospecific reactions.

Unit 5 Conformational Analysis

Conformational analysis of cyclic and acyclic systems with special emphasis on six membered rings, conformational effects on the reactivity of acyclic and cyclic systems - elimination, substitution and addition, strain, structure and stability of small, medium, and large rings, anomeric effect - cycloalkenes and cycloalkynes - kinetically and thermodynamically favoured products stereochemistry of SN1, SN2, SNi, E1 and E2

Selectivity in organic reactions: Chemoselectivity, regioselectivity, enantio- and stereo-selectivity. Stereoaspects of the addition of X_2, HX, boranes and hydroxylation to C=C systems. *Cis*- and *trans*- hydroxylation of cycloalkenes.

TEXT BOOKS

1. Michael B Smith, "March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure", 7th edition, Wiley (2015).
2. Francis A.Carey and Richard J. Sundberg, "Advanced Organic Chemistry - Part A: Structure and Mechanisms", 5th Edition, Springer, 2008
3. P. S. Kalsi, "Stereochemistry, Conformation and Mechanism", New Age Publications, 2008.

REFERENCES

1. E. L. Eliel and S. H. Wilen, "Stereochemistry in Organic Compounds", John Wiley, 2008.
2. D. Nasipuri, "Stereochemistry of Organic Compounds - Principles and Applications", 4th Revised Edition, New Academic Science, 2012.
3.Peter Sykes, "A Guidebook to Mechanism in Organic Chemistry", Pearson Education; 6 edition, 2003.

18CHY504 Coordination Chemistry 3 0 0 3

Unit 1 Theories and Concepts on *d*-block Coordination Compounds

Introduction - ligands, nomenclature of coordination compounds, coordination compounds of *d*-block ions with coordination numbers of 2, 3, 4, 5, 6, 7 and 8. Werner's coordination theory, Valence bond theory (VBT), Crystal field theory (CFT), CFSE, effects of CFSE on hydration energies and spinel groups (normal and inverse), types of ligands – spectrochemical series, spectral and magnetic properties (spin-only magnetic moments), nephelauxetic effect. Crystal field splitting patterns in complexes having Oh, Td, square planar, square pyramidal and trigonal pyramid geometries, factors affecting the magnitude of CFSE, various types of isomerism in coordination complexes, Jahn-Teller (JT) distortion, manifestation of JT on spectral properties. Molecular orbital theory (MOT), ligand field theory (LFT), molecular orbital energy level diagram for octahedral complexes without pi-bonding, metal-ligand pi-bonding, metal-metal multiple bonds, *d*-orbital based metal-metal σ, π and δ bonds in compounds like $[Re_2Cl_8]^{2-}$, $[Os_2Cl_8]^{2-}$, $Cr_2(CH_3COO)_4$ and R-Cr(I)-Cr(I)-R. Application of group theory to coordination compounds.

Unit 2 Reaction Mechanism

Complex equilibrium - formation constants, chelate and macrocyclic effects, factors affecting stability of complexes, methods of determination of stability constants, stability of complex ions in solutions, inert and labile complexes, mechanisms of ligand displacement and addition reactions in octahedral complexes and square planar complexes of platinum *cis*- and *trans*-effect, substitution reactions, mechanisms of substitution, kinetic consequences of reaction pathways, dissociation, interchange, association, dissociation, linear free energy relationships, conjugate base mechanism, stereochemistry of reactions (substitution in *trans*-complexes and substitution in *cis*-complexes), isomerisation of chelate rings, sigma-bonding and pi-bonding effects, oxidation-reduction reactions, inner and outer sphere electron transfer reactions, conditions for high and low oxidations numbers, reactions of coordinated ligands, hydrolysis of esters, amides and peptides, template reactions, electrophilic substitution, photochemical reactions of coordination compounds.

Unit 3 Coordination Chemistry of Inner-transition (*f*-block) Elements

f-block metal ions – oxidation states preferences, ligand preferences, coordination numbers and the geometry of the complexes, influence of lanthanide contraction and actinide contraction in their coordination behaviour, shapes of *f*-orbitals (4*f* and 5*f*), nature of bonding of *f*-orbitals with ligands, various types of coordination compounds of lanthanides and actinides, stereochemistry and reaction mechanism of *f*-block metal complexes.

Unit 4 Spectral Properties

Stabilization of unusual oxidation states, electronic spectra of transition metal complexes – color wheel, Russell-Saunders coupling schemes, term symbols for various d^n ions, Orgel diagrams for d^n systems, ligand field parameters, *Dq*, Racah parameter *B* and nephelauxetic constant *b*, Tanabe-Sugano (TS) diagrams, evaluation of *Dq* and other parameters from electronic spectra of transition metal complexes using TS diagrams, charge-transfer transitions, MLCT and LMCT, selection rules and band intensities, Laporte- and spin-selection rules, symmetry, spin-orbit and vibronic coupling effects. Photochemistry of transition metal complexes like $[Ru(bipy)_3]^{2+}$, spectral behaviour of *f*-block coordination complexes, special features of their absorption and emission properties.

Unit 5 Magnetic Properties

Magnetic properties of coordination complexes - magnetic susceptibility, contribution of spin-orbit coupling on μ_{eff}, types of magnetic behavior - para-, ferro, anti-ferro and ferri-magnetic systems, Curie law, Curie-Wise law, Guoy, Faraday and superconducting quantum interference device (SQUID) methods, Kotani plots, giant magnetoresistance (GMR), anisotropic magnetoresistance (AMR) effect, effects of temperature on magnetic behavior, tunnelingmagnetoresistance (TMR). Magnetism of coordination complexes by multinuclear homo- and heterometallic 3*d* systems (also with exclusive 4*d* and 5*d* metal ions), mixed 3*d*-4*f* systems, importance of 4*f*-metal ions for functional applications. Nanoscale magnetic systems based on coordination complexes - Single Molecule Magnets (SMMs), Single Ion Magnets (SIMs), Single Chain Magnets (SCMs), Spin-crossover complexes, magnetic refringents (magnetic coolers), magnetic storage systems - magnetic random access memory (MRAM).

TEXTBOOKS:

1. F. A. Cotton and G. Wilkinson, 'Advanced Inorganic Chemistry', John Wiley & Sons, 2009.
2. James E. Huheey, Ellen A. Keiter and Richard L.Keiter, 'Inorganic Chemistry, Principles of Structure and Reactivity', Pearson education, 5th edition, 2009.
3. J. D. Lee, 'Concise Inorganic Chemistry', 5th edition, John Wiley & Sons, 2009.
4. P Atkins, T. Overton, J. Rourke, M.Weller, F. Armstrong, "Shriver & Atkins Inorganic chemistry", 4th Edition, Oxford University Press, 2008.

REFERENCES:

1. B. Douglas, D. McDaniel and J. Alexander "Concepts and Models in Inorganic Chemistry", 3rd Edition, Wiley, 2006.
2. SushantaDattagupta, 'A Paradigm Called Magnetism', World Scientific Publishing Co. Pte. Ltd., 2008.
3. Helen C. Aspinall, 'Chemistry of the *f*-Block Elements', Volume 5 of Advanced chemistry texts, CRC Press, 2001.
4. N. N. Greenwood and A. Earnshaw, 'Chemistry of Elements', Butterworth and Heinemann, 2nd Edition, 2002
5. J. E. House, "Inorganic Chemistry", Academic Press, 2008.
6. T. Shinjo (Editor), 'Nanomagnetism and Spintronics', Elsevier, USA, 2nd Ed., 2014.
7. R. A. Layfield and M. Murugesu (Editors), 'Lanthanides and Actinides in Molecular Magnetism', Wiley-VCH Verlag& Co., 2015.

18CHY505 GROUP THEORY AND ITS APPLICATIONS 3 0 0 3

Unit I Introduction to molecular point groups

Definition of a mathematical group, Symmetry in molecules, elements of symmetry, , matrix representation of symmetry operations, molecular point groups, , abelian group, cyclic group, symmetry operations as group elements, similarity transformation and classes, group multiplication table, symmetry classification of molecules into pointgroups (Schoenflies symbol)

Unit II Construction and interpretation of character tables

Reducible and irreducible representations, Great Orthogonality Theorem and its consequences, character tables, reduction formula, construction of character tables for point groups with order ≤6, interpretation of character tables.

Unit III Applications of Group theory - I (vibrational and electronic spectroscopy)

Infrared and Raman activity of molecular vibrations in H_2O, N_2F_2, BF_3, AB_4type molecules (Td and D_4h) and AB_6 type (Oh) of molecules; selection rules; Electronic structure of free atoms and ions, splitting of terms in a chemical environment, construction of energy level diagrams, estimations of orbital energies, selection rules and polarizations, double groups, a brief idea on electronic spectra of transition metal complexes – selection rules, Orgel diagrams, Tanabe Sugano diagrams.

Unit IV: Applications of Group theory (Chemical bonding - Hybridization and molecular orbital formation)

Group theory to explain hybridization - wave functions as bases for irreducible representations, construction of hybrid orbitals for AB_3 (planar), AB_4 (Td), AB_5 (D_{3h}) and AB_6 (O_h) type of molecules, symmetry adapted linear combinations, projection operators, application of projection operators to pi-bonding in ethylene, cyclopropenyl systems and benzene, application of symmetry to predict polar and chiral compounds;

Unit V: Symmetry in solid state

Symmetry elements and operations in solid state – proper axis of rotation, mirror planes of symmetry, roto-reflection and roto-inversion axes of symmetry, screw axes of symmetry, glide planes; a brief introduction to the crystallographic point groups and space groups

TEXTBOOKS:

1. *F.Albert Cotton, 'Chemical Applications of Group Theory', 3rd Edition, John Wiley, 1990.*
2. *A Salahuddin Kunju, G Krishnan ; 'Group theory and its application in chemistry', second edition, PHI Learning private limited-2015*

REFERENCES:

1. *Robert L Carter, 'Molecular symmetry and Group theory', John Wiley & Sons, Inc.*
2. *V.Ramakrishnan and M.S.Gopinathan, 'Group Theory in Chemistry', 2nd reprint edition, Vishal Publications, 1996.*
3. *P.H.Walton, "Beginning Group Theory for Chemistry", Oxford University Press Inc., New York, 1998.*

18CHY511 CHEMICAL THERMODYNAMICS AND EQUILIBRIA 3 1 0 4

Unit 1 Chemical Thermodynamics

First and second laws of thermodynamics, thermodynamic functions, heat capacity, thermo chemistry, need for second law of thermodynamics, entropy and free energy functions, calculation of changes in thermodynamic function for ideal and non-ideal gases in isothermal and adiabatic process, relation between thermo dynamic functions - Maxwell relations, Joule Thomson effect, coefficient of thermal expansion and compressibility factor, applications of free energy function to physical and chemical changes, equilibrium in chemical reactions, third law of thermodynamics - need for third law, calculation of absolute entropy, unattainability of absolute zero, thermodynamic systems of variable composition - fugacity functions, partial molar quantities, thermodynamics of ideal solutions, real solutions and regular solutions, dilute solutions of nonelectrolytes, Henry's law, Raoult's law, Gibbs-Duhem equations, Gibbs-Duhem-Margules equations, and activity and standard states of non electrolytes.

Unit 2 Irreversible Thermodynamics

Examples for irreversible process, entropy production, non-equilibrium, steady state and near equilibrium conditions, linear relation, phenomenological coefficients, Onsagar reciprocal relations, one component systems with heat and matter transport, application of irreversible thermodynamics to thermal diffusion, thermal osmosis etc., electro kinetic effects, the Glansdorf-Pregogine equation.

Unit 3 Statistical Thermodynamics

Statistical concept, probability and thermodynamic states, entropy and probability, canonical ensemble, Maxwell-Boltzmann, Fermi-Dirac and Bose-Einstein Statistics, electron gas concept, Bose-Einstein condensation, relation among MB, FD & BE Statistics, partition function, partition function for free linear motion, free mo-

tion in a shared space, linear harmonic vibration, translational, rotational and vibrational partition function, molecular partition functions, partition functions and thermodynamic properties, calculation of equilibrium constant, heat capacity of gases, mono atomic solids, Einstein's and Deby's theory.

Unit 4 Equilibrium

Gibb's free energy, direction of spontaneous change of a reaction, chemical potential, chemical potential and equilibrium, ΔG in terms of K, equilibrium constants – real gases and real reactions, equilibrium respond to catalyst, temperature, pressure and $_{P}H$, application of ΔG and K – extraction of metals from their oxides, Ellingham diagram, and thermodynamics of ATP & respiration, biological energy conversion.

Unit 5 Phase Equilibrium

Gibb's Phase rule, one component system, two component systems, vapour pressure diagrams and their interpretation, lever rule, temperature-composition diagrams, liquid-liquid phase diagrams, distillation of partially miscible liquids, azeotropes, liquid-solid phase diagrams, phase diagram for the system Na/K/Na_2K, phase diagram - steel, alloys, Fe-C system, zone refining, three component system, triangular coordinates, three component system – partially miscible liquids - $H_2O/CHCl_3/CH_3COOH$, phase diagram - $NH_4Cl/(NH_4)_2SO_4/H_2O$

TEXTBOOKS:

1. Robert J. Silbey, Robert A. Alberty, Moungi G. Bawendi, Physical Chemistry 4th Edition, Wiley, 2004
2. Samuel H. Maron, Carl F. PruttonPrinciples of Physical Chemistry, The Macmillan Company; 4th edition (1970)
3. *Samuel Glasstone, 'Thermodynamics for Chemists', Lightning Source Incorporated, 2007.*

REFERENCES:

1. Francis Weston Sears and Gerhard L.Salinger, 'Thermodynamics, kinetic theory and statistical thermodynamics' 3rd edition, Addison-Wesley Publications, 1975.
2. Prigogine, 'Introduction to Thermodynamic Irreversible Processes', Interscience Publishers, 3rd edition, 1968.
3. R.P.Rastogi and R.R.Misra, 'An Introduction to Chemical Thermodynamics', 6th Revised edition, Vikas Publishing House Pvt. Ltd., 2006.
4. F.W.Sears, 'Introductions to Thermodynamics, Kinetic Theory of Gases and Statistical Mechanics', Addison Wesley Pub., Cambridge, 1972.

18CHY512 MOLECULAR SPECTROSCOPY 3 1 0 4

Unit 1 Rotational and Vibrational Spectroscopy

Introduction to spectroscopy, rotation spectra - diatomic and polyatomic molecules, selection rules, intensities of spectral lines, stark effect, instrumentation of micro wave spectroscopy, applications and structural determinations, vibration spectra of diatomic molecules, harmonic and anharmonic vibrations, diatomic vibrating rotor, selection rule, breakdown of Born Oppenheimer approximation, rotational character of vibration spectra, different modes of vibrations, vibration-rotation spectra, Fermi resonance, vibration spectra of polyatomic molecules, IR spectra of organic and inorganic compounds, phase, temperature and solvent dependence, FTIR technique, instrumentation, Raman spectra (including the use of laser) - theory, relation with IR spectroscopy, mutual exclusion principle, resonance Raman, stimulated hyper and inverse Raman effects, instrumentation and applications of Raman spectroscopy.

Unit 2 UV-Visible and Fluorescence Spectroscopy

Electronic spectra of atoms - single and multi electron systems, j-j and L-S coupling, electronic spectra of diatomic and polyatomic molecules, its relation to electronic arrangement and symmetry of molecules, application of group theory in electronic spectra, selection rules, nature of electronic excitation, principles of absorption spectroscopy, Beer-Lambert law, presentation of spectra, chromophores, forbidden transition, different types of electronic transitions, p-p*, n-p* etc transitions, nature of transitions in carbonyl compounds, the effect of conjugation, effect of conjugation on alkenes, HOMOs and LUMOs, Woodward-Fieser rules for dienes, spectra of carbonyl compounds, enones, Woodward rule for enones, spectra of aromatic compounds, effect of substituents, structural information from electronic spectra, excited states of molecules, fluorescence and phosphorescence, Jablonski diagram in detail, lifetime of excited states, quantum yields, photosensitization, application of UV-Visible and Fluorescence Spectroscopy for structural elucidation of organic compounds, diffuse reflectance spectra.

Unit 3 NMR Spectroscopy

Nuclear magnetic resonance phenomenon - theory, relaxation effects, NMR uses active nuclei, Fourier Transformation in NMR, measurement of relaxation time, chemical shift, magnetic anisotropic effect, multiplets in NMR, spin-spin splitting, n + 1 rule, Pascal's triangle, tree-diagram, spin-spin splitting constant, J, ^{2}J and ^{3}J and long-range coupling, measurement of J, Karplus relationship, first and second order spectra, AX, AB, AX_2, AX_3, A_2X_3, AMX type spectra, double resonance and spin tickling, chemical shift reagents, spectra in higher fields, spectra of conformational isomers, homotopic, enantiotopic and diastereotopic systems, C^{13} spectra, factors related to ^{13}C spectra, ^{1}H coupled ^{13}C spectra, ^{1}H decoupled ^{13}C spectra, chemical shift values, nuclear Overhauser effect (NOE), cross-polarization, off-resonance resonance decoupling, application of ^{1}H and ^{13}C NMR spectroscopy for the structural elucidation of organic compounds, ^{11}B, ^{15}N, ^{19}F and ^{31}P NMR spectra, spectra of paramagnetic complexes, magnetic susceptibility, contact shift, fluxional molecules and their studies using NMR, solid state NMR.

Unit 4 ESR, NQR and Mossbauer Spectroscopy

ESR spectroscopy - theory, hyperfine and superfine splitting, ESR active simple organic systems, ESR of inorganic systems like Cu^{2+} and VO^{2+} complexes, 'g' markers like DPPH and TCNE, evaluation of spin Hamiltonian like A, g_{ll}, g-, covalency factor in Cu^{2+} complexes, analysis of ESR spectra of VO^{2+} complexes, NQR spectroscopy - theory, relationship between electric field gradient and molecular structure, quadrupole coupling constant and structural information of compounds, Mossbauer spectroscopy, principle, Doppler effect, isomer shift, Zeeman splitting, quadrupole splitting, application of Mossbauer spectroscopy for studying Fe and Sn compounds and phase transformation, application of ESR spectroscopy.

Unit 5 Mass Spectrometry and PES

Mass spectroscopy, base peak and molecular ion peak, isotope ratio data, fragmentation patterns of alkanes, alkenes, alkynes, aromatic hydrocarbons, alcohols, phenols, aldehydes, ketones, esters, carboxylic acids, amines, methods of desorption and ionization (EI, CI, LD, MALDI, PD, FAB, SIMS), MS/MS and determination of molecular formula, metastable ions and their significance, study of fragmentation pattern, application of MS in structural elucidation and other frontiers of science, application of MS for quantitative analysis, photoelectron spectroscopy (PES), principle, application of PES. Structure determination using IR, UV-visible, NMR, MS and ESR spectral techniques.

TEXTBOOKS:

1. *Colin N. Banwell and Elaine M. McCash, 'Fundamentals of Molecular Spectroscopy', 4th Edition, Tata McGraw Hill, 2007.*
2. *W. Kemp, Organic Spectroscopy, 3rd Edition, McMillan International Higher Education*
3. *D. L. Pavia, G. M. Lampman, G. A. Kriz, and J. R. Vyvyan, Introduction to Spectroscopy, 5th Edition, Brooks-Cole, 2009*
4. *G. M. Barrow, 'Introduction to Molecular Spectroscopy', McGraw Hill, 1962.*
5. *R. M. Silverstein, F. X. Webster, D.J. Kiemle, Spectroscopic identification of organic molecules, 7th Edition, John Wiley*
6. P. S. Kalsi, Spectroscopy of Organic Compounds: New Age International Pvt Ltd 6th edition edition,, 2006

REFERENCE:

1. *Hollas, J.M., Modern Spectroscopy, John Wiley & Sons, Fourth Edition, 2004*
2. *J. Keeler, Understanding NMR spectroscopy, Wiley, 2009*
3. *D. A. Skoog, F. J. Holler and S. R. Crouch, 'Principles of Instrumental Analysis', 6th Edition, Thomson Brooks/Cole, 2007.*
4. *W. Kemp, NMR in Chemistry, McMillan, 1988*
5. *J. E. Wertz and J. R. Bolton Electron Spin Resonance, Springer Science*

18CHY513 Organic Reaction Mechanism 3 1 0 4

Unit 1 Nucleophilic Substitution:SN1, SN2, and Borderline (ion pair), SNi, SET mechanisms, Neighboring group participation, substitution at allylic carbons, substitution at aliphatic trigonal carbon, substitution at vinylic carbon. Effect of substrate structure, nucleophile, leaving group and medium on reactivity. Ambident nucleophiles and substrates. Aromatic nucleophilic substitution: SNAr, SN1, benzyne and SRN1 mechanisms. Effect of substrate structure, leaving group and attacking nucleophile on reactivity.

Unit 2 Electrophilic substitution: SE2 and SEi, SE1, substitution accompanied by double bond shift. Effect of substrate, leaving group, and solvent on reactivity. Aromatic electrophilic substitution: Arenium mechanism, Structure – reactivity relationship, substituent effect, o/p ratio, ipso substitution, orientation and reactivity, quantitative treatment.

Free radical reactions: Radical addition. Effect of substrate (aliphatic, aromatic, bridgehead), nature of the radical and solvent on reactivity.

Unit 3 Addition reactions: Mechanism of Electrophilic, nucleophilic and radical addition. Addition to conjugated systems. Orientation and reactivity. Addition of hydrogen halides, Oxymercuration, halogenation, sulfenylation, selenylation, addition involving epoxides, addition via organoborane. Addition of water, alcohol, sulfides, to aldehydes, ketones, imines, isothiocyanates, nitrocompounds, nitriles. Mannich reaction,

Elimination reactions:Mechanism of elimination reactions E2, E1, E1CB, steric effect. Effect of substrate structure, base, leaving group and medium on reactivity. Mechanism of pyrolytic elimination.

Unit 4 Rearrangement reaction: Mechanism of Nucleophilic, electrophilic and radical rearrangements. Nature of migration, migratory aptitudes, memory effects. Wagner-Meerwein, Pinacol, Demyanov, dienone-phenol, Benzil-Benzilic acid, Favorskii, Wolff, Neber, Hofmann, Curtius, Lossen, Schmidt, Beckmann, Baeyer-Villiger, Stevens, benzidine, Hofmann-Loffler and Chapman rearrangements and their mechanisms.

Unit 5 Photochemistry and pericyclic reactions: General principles – Fate of excited state – Jablonsky diagram - chemical process – Photochemistry of alkenes, dienes and polyenes, Carbonyl compounds, Norrish type 1 and Type 2, Patterno –Buchi reaction.

Pericyclic reactions: Cyclo addition - Diels-Alder reaction, Substituent effect on reactivity, regioselectivity and stereochemistry, Catalysis of Lewis acids, Synthetic applications, Enantio selective Diels alder reactions,

Intramolecular Diels-Alder reactions. 1,3 Dipolar Cycloaddition – reactivity, regio and stereoselectivity, Applications. [2+2] cycloaddition – ketenes and alkenes – photochemical Electrocyclic reactions, Orbital symmetry, charged species. Sigmatropic rearrangements – [1,3], [1,5], and [1,7] sigmatropic shifts – [3,3] sigmatropic rearrangements – Cope, Oxy-Cope and Claisen rearrangement. [2,3] rearrangements – oxides and ylides –Wittig and aza – Wittig rearrangements, Cheletropic reactions.

TEXT BOOKS

1. Michael B Smith, "March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure", 7th edition, Wiley (2015).
2. Francis A.Carey and Richard J. Sundberg, "Advanced Organic Chemistry - Part A: Structure and Mechanisms", 5th Edition, Springer, 2008
3. Francis A.Carey and Richard J. Sundberg, "Advanced Organic Chemistry - Part B: Reactions and Synthesis", 5th Edition, Springer, 2008.
4. Singh S P and SM Mukherji, "Reaction Mechanism in Organic Chemistry", 2014

REFERENCES

1. Reinhard Bruckner, Advanced Organic Chemistry, Reaction Mechanisms, Elsevier, 2002
2. R.O.C. Norman and J.M. Coxon, "Principles of organic synthesis", CRC press, 2014
3. Ian Fleming,Frontier Orbitals and Organic Chemical Reactions 1st Edition, Wiley, 1991

18CHY514 Heterocyclic and Natural Product chemistry 3 0 0 3

Unit 1 Heterocyclic compounds

Nomenclature and general characteristics of heterocyclic compounds, study of three and four-membered ring heterocyles containing one heteroatom, structure and synthesis of penicillin and cephalosporin-C, structure and synthesis of reserpine, heteroaromatic compounds (five and six-membered rings) containing one and two heteroatoms, fused ring compounds - indole, quinoline, isoquinoline, coumarin, flavones, purine and pyrimidine, bases present in nucleosides.

Unit 2 Carbohydrates and nucleic acids

Nomenclature – aldoses, ketoses, furanoses, pyranoses. Classification – monosaccharides, disaccharides and polysaccharides. Structure (Fischer, Haworth and chair projection) of ribose, glucose, fructose, maltose, sucrose, lactose, starch, cellulose and cyclodextrins. Preparation of alditols, glycosides, deoxysugars. Biosynthesis of vitamin C from glucose. Structure and synthesis of nucleic acids, genetic code, recombinant DNA. biosynthesis of shikimic acid

Unit 3 Chemistry of Natural Products

Alkaloids - classification, structure elucidation based on degradative reactions (quinine atropine), Terpenoids - classification, structure elucidation and synthesis of abietic acid, terpenoids. Total synthesis of quinine and papavarine (morphine, heroin)

Unit 4 Steroids

Steroids - classification, structure of cholesterol, conversion of cholesterol to progesterone, androsterone and testosterone, classification, structure and synthesis of prostaglandins, biosynthesis of fatty acids, prostaglandins, and steroids.

Unit 5 Amino acids, Peptides and Enzymes

Synthesis of amino acids - Strecker and azlactone synthesis, reactions of amino acids, structure of proteins, introduction to enzymes and coenzymes with special reference to the function of chymotrypsin, NAD, thiamine, pyridoxal, solid phase synthesis – choice of resin, classification and reactions leading to peptide formation.

TEXT BOOKS

1. I.L. Finar Organic Chemistry vol 2 (3rd.ed.) Longmans Green & Co. 1964
2. Sujata V. Bhat, Bhimsen A. Nagasampagi, Meenakshi Sivakumar, Chemistry of Natural Products, Springer 2005

REFERENCES

1.K. C. Nicolaou, Eric J. Sorensen, Classics in Total synthesis, Wiley, 1996.
2. Ashutosh kar, Chemistry of Natural Products, (Volume I and II), CBS

18CHY515 Organometallic Chemistry 3 0 0 3

Unit 1: Concepts and Metal Carbonyls

History and overview on organometallic compounds. Classification and nomenclature – hapticityof fragments, 18-electron and 16-electron organometallic compounds. Structure prediction based on '18 electron rule'. Metal carbonyls – synthesisand bonding of metal carbonyls (based on MO theory), donor and acceptor properties of CO, different types of binding modes of CO, poly-nuclear carbonyls with and without bridging groups, metal-metal bonding in M-CO clusters, cluster valence electron (CVE) count, CVE based structure prediction. IR spectral features of metal carbonyls, activation of CO by bonding with metal ions.

Unit 2: Types of organometallic compounds

Metal phosphines compounds of transition metals, M-N_2 (metal dioxygen), M-O_2 (metal dioxygen), M-NO (metal nitrosyl) and M-CN (metal cyanide/isocyanide) complexes, bonding and structural features. Organometallic compounds with π-donor ligands like olefins, acetylenes and allyl moieties. Metal derivatives of cyclic π-donors (metallocenes, sandwich/half-sandwich compounds, bent metallocenes), metal-carbon σ-donors (metal carbenes – Fischer carbenes, Schrock carbenes and *N*-heterocyclic carbenes, metal polyenes, metal carbines, metal alkyl/aryl derivatives). Organometallic chemistry of lithium and magnesium, aluminum alkyls and all other main-group organometallics. Structural features and nature of bonding in above compounds.

Unit 3: Structure and Bonding

Fragment molecular orbitals (FMO) of various organic and inorganic moietieslike CH_3, CH_2, CH, BH_2, BH, NH_2, NH. FMO's (π-orbitals) of C_3H_5, C_4H_4, C_4H_6, C_5H_5, C_6H_6, C_8H_8. Inorganic fragments MLn with varying number of L's. Symmetry and shape of their FMO's. Isolobal concept, iso-electronic and isolobal relationships between various organic and inorganic (ML_n) fragments. Structure and bonding between various organic and inorganic fragments based on MO level diagrams – metal-olefins, ML_n-cyclobutadiene, ML_n-carbene, ML_n-carbyne, ML_n-cyclopentadienyl systems, compounds with metal-metal multiple bonds (metal-metal σ, π and δ bonds).

Unit 4: Stereochemistry and reactions

Stereochemically non-rigid molecules, fluxional nature of organometallic compounds (including Li-C, Mg-C), characterization of non-rigidity of organometallic compounds by NMR spectroscopy. Difference in NMR spectra of fluxional organometallic compounds at high and low temperatures. Characterization techniques of organometallic compounds (by NMR – ^{1}H, ^{13}C and ^{31}P NMR spectroscopy, Dynamic NMR, Mass spectrometry). Reactions involving various organometallic compounds - oxidative addition reactions, reductive elimination reactions, migratory insertion reactions, 1,1-type and 1,2-type insertion reactions, elimination reactions, β-hydride elimination reactions. Conditions for organometallic compounds to exhibit above reactions, cyclo-metalation and ortho-metalation reactions, agostic interactions.

Unit 5: Organometallic Catalysis

Alkene hydrogenation using Wilkinson's catalyst, water-gas shift reaction, Mosanto process, Cativa Process. Reaction steps in the above catalytic processes. Hydro-formylation reactions, catalytic addition of molecular oxygen to alkenes (Wacker process), Ziegler-Natta polymerization of alkenes, Fischer-Tropsch process, ole-

fin-metathesis (types of Grubbs catalysts and Hoveyda–Grubbs catalysts), oligomerization of alkynes, aluminum alkyls in polymerization of olefins. Palladium based reactions such as Heck, Stille, Suzuki, Sonogashira, Buchwald-Hartwig couplings; Tsuji-Trost C-C bond formations. Homogeneous vs. heterogeneous organometallic catalysis (principles, mechanism and their applications). Organometallics - in industry, in medicine, in agriculture and in environmental science.

TEXTBOOKS:

1. J.E. Huheey, R.A. Keiter, R.L. Keiter, 'Inorganic Chemistry-Principles of Structure and Reactivity', 4th Edn., Prentice Hall, 1997.
2. P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong,' Shriver and Atkins Inorganic Chemistry', 4th Edn., Oxford University Press, 2006.
3. F.A. Cotton, G. Wilkinson, C.A. Murillo, M. Bochmann, 'Advanced Inorganic Chemistry', 6th Edn.,Wiley-Interscience, 1999.
4. Anil Elias, Gupta B.D., "Basic Organometallic Chemistry", Universities Press; 2nd Edition 2013
5. J.D. Atwood, 'Inorganic and Organometallic Reaction Mechanism', 2nd Edn., Wiley-

REFERENCES:

1. R. H. Crabtree, 'Organometallic Chemistry of the Transition Metals', John Wiley & Sons, 6th Ed.
2. VCH, 1997.
3. J. Tsuji, 'Transition metal reagents and catalyst innovations in organic synthesis', John-Wiley- & Sons, Ltd, New York, 2000
4. B.E. Douglas, D.H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007.
5. M. Bochmann, Orgaonometallics: Complexes with Transition Metal-Carbon Sigma Bonds, Oxford University Press, 1994.
6. J. P. Collman, R G Finke and and J R Norton "Principles and Applications of Organo-transition metal Chemistry" University Science Books, 1987.
7. W.K. Li, G.D. Zhou, T. Mak, Advanced Structural Inorganic Chemistry, Oxford University Press, 2008.
8. K. C. Nicolaou, 'Classics in Total Synthesis', Vols I-III, Wiley-VCH, 1996; 2003; 2011

18CHY581 INORGANIC SEMI-MICRO QUALITATIVE ANALYSIS LAB. 0 0 6 2

Semi micro analysis of mixtures

The mixture will include 4 cations including two common (eg. Cations of metals like Cu, Mn, Zn, Ni, Ca, Ba, Mg etc) and two less common cations (eg. Cations of metals like Ti, Zr, V, W, Li, Ce, Th etc).

(The student has to successfully analyze a minimum of 10 mixtures).

TEXTBOOKS:

1. A.I.Vogel, 'A text book of Qualitative Analyses', 4th edition, Longmans publications, 1985.

2. V.V. Ramanujam, 'Inorganic Semi-Micro Qualitative Analysis', 3rd edition, The National Publishing Company, 1974.

REFERENCES:

1. *G.H.Jeffery, J.Bassett, J.Mendham and R. C. Denney, 'Vogel's Text Book of Qualitative Chemical Analysis', 5th edition, John Wiley & Sons Inc, 1989.*
2. *G.W. Parshall, 'Inorganic Synthesis', Vol. 15, Tata McGraw-Hill Education, 1974.*

18CHY582 ORGANIC QUANTITATIVE ANALYSIS LAB. 0 0 6 2

A. Estimations:

Estimation of equivalent weight of an acid
Estimation of glucose
Estimation of phenol
Estimation of acetone
Estimation of acid value of an oil
Estimation of iodine value and sap value of an oil
Estimation of Nitrogen – Kjeldahl method
Estimation of formaldehyde
Estimation of aniline
Estimation of ester

B. Preparations of Organic Compounds

Double stage preparations

(a) m-nitro benzoic acid from ethyl benzoate
(b) p-bromobenzanilide from aniline
(c) p-nitro acetanilide from aniline

Single stage preparations

(a) Benzimidazole
(b) Benzophenone oxime
(c) Dibenzilidene acetone (chalcone)
(d) Benzalacetophenone
(e) Benzanilide
(f) Acetanilide
(g) Acetyl salicylic acid (aspirin)

Name Reactions

(a) Benzil-Benzilic acid rearrangement
(b) Cannizaro reaction
(c) Claisen condensation

For all preparations

1. TLC to be done and Rf values of each compound to be reported
2. Melting point of pure compounds to be found
3. A small portion should be recrystallised from suitable solvent
4. Purified products to be displayed
5. Mechanisms for each preparation should be suggested

REFERENCES:

1. P.W.G. Smith, A.J.Hannaford, B.S.Furnis and A.R. Tatchell, "Vogel's Textbook of Practical Organic Chemistry", ELBS/Logman, 1989.
2. Ralph L. Shriner, Christine K. F. Hermann, Terence C. Morrill, David Y. Curtin, Reynold C. Fuson, 'Systematic Identification of Organic Compounds', John Wiley & Sons, 2003.
3. Mann and Saunders, 'Practical Organic Chemistry', Pearson edition, 2009

18CHY583 ADVANCED PHYSICAL CHEMISTRY LAB. 0 0 5 2

1. Construction of phase diagram for three component system.
2. Determination of equivalent conductance at infinite dilution of weak electrolytes.
3. Determination of order of reaction for ion exchange reaction.
4. Extraction efficiency of solute from a solution by immiscible solvent method.
5. Determination of calorific value using Bomb calorimeter.
6. Kinematic viscosity of lubricants using Bomb calorimeter.
7. Determination of the formation constant of silver-ammonia complex and stoichiometry of the complex potentiometerically.
8. Determination of flash point, fire point of a lubricant.
9. Determination of cloud point and pour point of a lubricant.

TEXTBOOKS:

1. Alexander Findly, 'Practical physical chemistry', 9th edition, Wiley, 1972.

2. R.C.Das and B.Behera, 'Experimental Physical Chemistry', Tata McGraw-Hill, 1983.

REFERENCE BOOKS:

1. J.B.Yadav, 'Advanced Practical Physical Chemistry', Krishna Prakashan Media, 29th edition, 2010.

2. Francis William Gray, 'A Manual of Practical Physical Chemistry' Macmillan and Co., Limited, 1914.

18CHY584 INORGANIC QUANTITATIVE ANALYSIS LAB. 0 0 6 2

1. Estimation of Calcium (Permanganometry)
2. Estimation of Barium (Iodometry)
3. Estimation of Calcium as Calcium Carbonate (Gravimetry)
4. Estimation of Zinc using oxine (Gravimetry)
5. Estimation of Iron as Ferric Oxide (Gravimetry)
6. Analysis of Brass
7. Estimation of Copper and Nickel in a Mixture
8. Estimation of Copper and Iron in a Mixture
9. Preparation and Determination of Ferrous Oxalate
10. Estimation of Different Types of Hardness in the Given Water Sample
11. Estimation of Different Types of Alkalinities in the Given Water Sample
12. Estimation of Dissolved Oxygen in the Given Water Sample
13. Complexometric Estimations

TEXTBOOKS:

1. G. Svehla, 'Vogel's Qualitative Inorganic Analysis', 7th Edition', Prentice Hall, 1996.

2. D.A.Skoog and D.M.West ,'Analytical Chemistry - An Introduction', 4th Edition, CBS Publishing Japan Ltd., 1986.

REFERENCES

1. E.J.Meehan, S.Bruckenstein and I.M.Kolthoff and E.B.Sandell, 'Quantitative Chemical Analysis', 4th Edition, The Macmillan Company, 1969.
2. R.A.Day (Jr) and A.L.Underwood, 'Quantitative Analysis', 6th Edition, Prentice Hall of India, 1991.

18CHY601 ELECTROCHEMISTRY KINETICS AND SURFACE CHEMISTRY 3 1 0 4

Unit 1 Surface Chemistry

Different types of interfaces, molecular and atomic surface structure, surface chemical reactions, surface tension of solutions, surface excess, thermodynamics of surfaces, Gibbs equation and its derivation, surface films, surface potential.

Adsorption by solids, Langmuir isotherm - its kinetic and statistical derivation, Freundlich equation, multilayer adsorption, BET isotherm - its kinetic derivation, measurement of surface area.

Colloids - their preparation, purification, stability & electro kinetic phenomena, Donnan membrane equilibrium, micro and nano emulsions.

Surface analysis using photoelectron spectroscopy, surface imaging techniques like SEM, TEM, AFM etc., sputter coating, ion beam principles, design of surfaces with novel properties.

Unit 2 Electrochemistry I

Review of Faraday's laws, conductivity of electrolytes, ionic mobility, transference number, Kohlrausch law , pH of acids, bases and buffers, solubility product and salt hydrolysis and Ostwald dilution law. Deviations from the Ostwald law , activity and activity coefficients in electrolytic solution, Modern theory of conductance of strong electrolytes and its tests and improvements, Debye-Huckel-Onsager equation – theory of mean activity coefficients of strong electrolyte – Debye-Huckel Limiting Law and its testing and improvement.

Unit 3 Electrochemistry II

Electrochemical cells, standard electrode potentials, reversible cell, concentration cells with and without Electrochemical cells, standard electrode potentials, reversible cell, cell notation and calculation of emf – variation of potential with concentration, pressure and temperature – concentration cells with and without transference, Liquid Junction Potential – its calculation and elimination - Thermodynamics of cell reactions and equilibrium constant - applications of e.m.f. measurements, potentiometric measurement of pH –reference electrodes - glass and quin-hydrone electrodes and their performance and limitations, – ion selective electrodes – biomembranes, Interfacial region – electrical double layers and their structure – Helmholtz-Perrin, Gouy-Chapman and Stern models - charge transfer across interfaces, mass transport – diffusion and convection controlled transport – irreversible electrode processes - activation, concentration and IR polarisation, decomposition potential, Butler-Vohmer equation - over potential (hydrogen, oxygen and metal decomposition over voltage), theories of over voltage, Tafel equation, and Tafel plots – corrosion and its rate from Tafel equation.

Unit 4 Chemical Kinetics I

Reaction rates and order of reactions, determination of order of reactions, complex reactions, reversible, consecutive and concurrent reactions, reactions of variable order, steady state treatment, reaction mechanism and molecularity, theories of unimolecular reactions and termolecular reactions, Arrhenius equation, collision theory and transition state theory, comparative study of the theories of reaction rates, free energy of activation, effect of solvent on rate of reactions, ionic reactions and effect of ionic strength - salt effect, effect of pressure on velocity of gas reactions.

Unit 5Chemical Kinetics II

Reaction dynamics, fast reactions, flash photolysis and relaxation methods, catalysis and inhibition, homogeneous catalysis, acid, base and enzyme catalysis, kinetics of enzyme catalyzed reaction - the Michaelis-

Menten equation. Photochemical kinetics, steady state treatment of photochemical reactions, Semenov-Hinshelwood theory of chain reactions and explosions, free radical reactions - the Rice-Herzfeld mechanism.

TEXTBOOKS:

1. *Gilbert W. Castellan, "Physical Chemistry", 3rd Edition, Narosa Publishing House, 2004.*
2. *K. J. Laiddler, 'Chemical-Kinetics', 3rd Edition, McGraw Hill, New York, 2004.*
3. *An introduction to Electrochemistry, Samuel Glassstone (*2007)

REFERENCES:

1. *W. J. Moore and R. G. Pearson, 'Kinetics and Mechanism', 2nd edition, Wiley, 1981.*
2. *Physical Chemsitry, Peter Atkins, Julio D Paula, OUP Oxford; 9 edition (19 November (2009)*
3. *Textbook of Physical Chemistry, Samuel Glassstone,* D. Van Nostrand company, inc; 2nd edition (1946)
4. John O'M. Bockris, Amulya K.N .Reddy,Modern Electrochemistry 1: Ionics, 2nd Edition, Springer, 1998
5. John O'M. Bockris, Amulya K.N .Reddy, Maria E. Gamboa-Aldeco, Modern Electrochemistry 2A: Fundamentals of Electrodics 2nd Edition, Springer, 2001

18CHY602 Synthetic Strategies and Reagents 3 1 0 4

Unit 1 Synthetic Strategies

Synthetic strategies: Functional group inter-conversion – conversion of one functional group to other. Nitrogen, oxygen, sulphur protection and deprotection – utilization of protection groups in organic synthesis. Retro synthetic analysis, functional group equivalents, use of retrosynthesis in organic synthesis. Reversal of reactivity (Umpolung), Introduction to combinatorial chemistry. Application of phase transfer catalysts.

Unit 2 Oxidation and reduction:

PCC, DDQ, DMSO, Dess-Martin Reagent, TEMPO, osmium tetroxide, ruthenium tetroxide, selenium dioxide, peracids, hydrogen peroxide, singlet oxygen, aluminum isopropoxide, periodic acid, lead tetraacetate. Swern, Jones, Oppeneur oxidation, Woodward and Prevost hydroxylation, Sharpless asymmetric epoxidation, catalytic hydrogenations (heterogeneous and homogeneous), Clemmenson, Wolff Kishner, Rosenmund and MPV reductions, metal hydrides as reagents (aluminium/boron hydrides and hydroboration reaction), Birch reduction, Borche Reduction, hydrazine and diimide reduction.

Unit 3 Organometallic reagents: Preparation, properties and reactions of organo lithium, organosilicon, organozinc (Reformatsky reaction) and organomagnesium reagents (Barbier and Grignard), organocadmium, organo mercury reagents based organometallic reactions involving C-C bond formation. Selected functional group transformations in organic synthesis. Preparation and reactions of Organo copper, organopalladium,- Wacker process – Heck reaction, cross coupling, carbonylation reaction, organonickel, organo cobalt and organo rhodium reagents – Olefin metathesis reaction. Reactions and applications of Organoboron, organo silicon and organotin compounds.

Unit 4 C-C, bond formation

C-C bond formation – aldol, Arndt-Eistert, Bardhan-Sengupta, Baker-Venkataraman,Barbier, Baylis-Hillman, Benzoin, Heck, Fukuyama, Dieckmann, Friedel–Crafts, Michael, Perkin, Claisen, Robinson annulations, Vilsmeier, Wittig, Knoevnagel, Michael additions.

Unit 5C-N, C-O bond formations

C-O bond formation – barton, Fischer esterification, Prins, Darzen, Baeyer-Villiger, Mitsunobu, Williamson's ether synthesis, Ullman Coupling with Boronic Acids.

C-N bond formation – Mannich, Fukuyama, Mitsunobu, Ritter, Gabriel Synthesis, Ugi, Doebner Reaction, Buchwald-Hartwig, Stork-enamine, formation of azides and hydrazines, formation of amides and peptides, coupling reactions.

TEXT BOOKS

1. Modern Organic Synthesis, Dale L. Boger, The Scripps Research Institute, Rush Press, San Diego, California, 2001
2. Francis A.Carey and Richard J. Sundberg, "Advanced Organic Chemistry - Part B: Reactions and Synthesis", 5th Edition, Springer, 2008.
3. R.O.C. Norman and J.M. Coxon, "Principles of organic synthesis", CRC press, 2014

REFERENCES

1. Stuart Waren, Designing Organic Synthesis: A programmed introduction to the synthon approach, JOHN WILEY & SONS, 2nd edition, 2008
2. Name Reactions: A collection of detailed Mechanisms and synthetic applications, Jie Jack Li, Springer, fourth edition (expanded edition), 2009.
3. Michael B Smith, "March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure", 7th edition, Wiley (2015).
4. Francis A.Carey and Richard J. Sundberg, "Advanced Organic Chemistry - Part A: Structure and Mechanisms", 5th Edition, Springer, 2008

18CHY603 Solid State Chemistry and Materials Science 3 0 0 3

Unit 1 Introduction to Crystal Systems

Introduction to solids - solid state chemistry, close packing, hcp, fcc, density, coordination numbers, tetrahedral and octahedral holes, body centered and primitive structures, symmetry, proper rotation, mirror planes, inversion, improper axis symmetry elements, symmetry in crystals, Schoenflies and Hermann-Mauguin notations, unit cells, glide plane, screw axis, atom occupancy in cubic unit cells, seven crystal systems/classes, space groups, Miller indices, Bravais lattices, reciprocal lattice, inter-planar spacing in different crystal systems, fractional coordinates, ionic solids, structures of CsCl, NaCl, NiAs, zinc blende and wutzite structures, MX_2 type solids, fluorite and antfluorite structures, $CdCl_2$ and CdI_2 structures, rutile and anti-rutile, ReO_3, spinel and inverse spinel, pervoskite structures, ionic radii, crystal radii, radius ratio, Extended covalent array, diamond, graphite.

Unit 2 Bonding in Solids and Electronic properties

Bonding in crystals, metallic bonding, ionic bonding, covalent bonding, silicates, Born-Haber cycle, Hess's law, lattice energy (L) and calculation of L, free electron theory, density of states, electronic conductivity, molecular orbital theory, overlap and bonding, linear chain of H atoms, LCAO, Fermi Level, conductors, insulators and semiconductors, n- and p-type semiconductors, bands in compounds, band-gap energy, direct and indirect band gaps in semiconductors, band-gap measurements, electrical conductivity, photoconductivity.

Unit 3 Magnetic and Optical Properties of Solids

Behaviour of substances in magnetic field, magnetic moments, para magnetism, diamagnetism, ferro- and anti-ferromagnetism, ferri-magnetism, effects of temperature of magnetism, Curie & Curie-Weiss laws; mechanism of ferro- and anti-ferromagnetic ordering, super exchange. Luminescence and phosphorescence of solid materials, phosphors, lasers, non-stoichiometry and its effect in properties of solids, electronic properties of non-stoichiometric oxides. Defects in solids, Schottky defects, Frenkel defects, doping in crystals and colour features, ruby, diamond, organic conductors, preparation, mechanism of conduction in organic semiconductors, photoconductivity of polymers.

Unit 4 Materials Science-Structure and properties

Solid materials of importance. Structure and properties of SiO_2, ZrO_2, SiC, BN, ZnO, TiO_2, CdS, CdTe, GaAs, MoS_2. Band-gap properties of semiconductors like ZnO, TiO_2, CdS, CdSe, CdTe, GaAs, MoS_2 and $(CH_3NH_3)[PbX_3]$-type perovskites. Photo-catalytic properties of ZnO and TiO_2 – principle and applications. Inorganic-organic hybrid materials. High Tc superconductors (HTS) like Bi-Sr-Ca-Cu oxide based HTS (BSCCO) and Y-Ba-Cu-oxide (YBCO), their structure and properties. Metal-organic framework (MOF) materials, special features of MOF materials. Synthesis, special features and properties of MOF materials like

HKUST-1 and MOF-8. Gas storage and emission properties of MOF materials. MOFs as sensors. Zeolites, their special features and properties.

Unit 5 Materials Science-Synthesis, processing and characterization

Sol and gel, their properties, xerogels. Sol-gel synthesis - synthesis of SiO_2 and TiO_2 through sol-gel process. Calcination and sintering. Characterization of processed materials, PXRD, IR, Raman, Uv-visible and solid state NMR spectral techniques. Understanding morphological features through, SEM, EDAX and TEM methods. Chemical vapour deposition (CVD) method. Solid state synthesis, synthesis of High Tc superconducting materials like YBCO and BSCCO. Synthesis of inorganic-organic hybrid materials. Solvo-thermal and high pressure synthesis.

TEXTBOOKS:

1. *L V Azroff , 'Introduction to Solids' , Tata McGraw-Hill publishing company*
2. L. E. Smart and E. A. Moore, Solid State Chemistry – An Introduction, 4th Edition, CRC Press, 2016.
3. A. R. West, Solid State Chemistry and its Applications, Wiley, 2014
4. C N R Rao, K Biswas, Essentials of Inorganic Materials Synthesis, John Wiley, 2014
5. C N R Rao Chemical Approaches to Synthesis of Materials, Wiley, 1994

REFERENCES

1. D. Jiles, "Magnetism and Magnetic Materials", Chapman and Hall, London, 1991.
2. R. E. Hummel, "Electronic Properties of Materials", 3rd ed., Springer-Verlag, New York, 2001.
3. Schubert, U. and Hüsing, N, Synthesis of Inorganic Materials, 3rd edn, VCH-Wiley Verlag GmbH, Weinheim, 2012
4. W.D. Kingery, H.K. Dowen and R.D. Uhlman, Introduction to Ceramics, John Wiley.
5. F.H. Norton, Elements of Ceramics,.
6. M.W. Barsoum, Fundamentals of Ceramics, McGraw Hill.
7. Material Science and Engineering, S.K. Hajra Choudhury, Indian Book Dist.
8. B D Fahlman, Materials Chemistry, 2nd Edition, Springer, 2011
9. Stefan Kaskel, The Chemistry of Metal–Organic Frameworks: Synthesis, Characterization, and Applications, Wiley-VCH Verlag GmbH, 2016

18CHY604 Bio-inorganic Chemistry 3 0 0 3

Unit 1: Basics in bio-inorganic chemistry

Essential elements in biological systems, transport of ions across biological membranes, active and passive transport, metal transport and metallochaperons, Na^+/K^+ pump and active transport. Metal complexation with biological molecules. Electron transport in biology, electron transport chain (ETC), role of ETC in biological systems. Amino acids, peptides and proteins, primary and secondary structure of proteins, α-helix and β-sheets forms of proteins and their special features; tertiary and quaternary structures of proteins the type of molecular interactions involved in them . Reactive oxygen species (ROS), generation and function of organic free radicals, action of ROS in biological systems, oxidative stress, antioxidants. Photosynthesis, PS-I and PS–II.

Unit 2: Oxygen take-up, transport and storage proteins

Porphine, corrin, corrole, chlorin and bacteriochlorin. Myoglobin (Mb) and hemoglobin (Hb), their prosthetic groups and functions, mechanism for reversible binding of O_2 in Mb and Hb. Cooperative effect in Hb and its consequence. Behaviour of bound O_2 to Fe(II). Difference between O_2 and CO binding to Hb and Mb, CN^- poisoning. Structure and functions of haemerythrin (Hr) and haemocyanin (Hc), O_2 binding nature in Hr and Hc, electron transfer processes in them. Cytochromes and their role in biology, cytochrome P-450, cyto-

chrome C-oxidase and oxygen transfer from O_2 to non-activated substrates, monooxygenases, methane monooxygenase (MMO). Fe-S and other non-heme iron proteins, ferredoxins-their structure and special properties, transferrin, ferritin, siderophores, enterobactin, uptake, transport and storage of iron. Sickle-cell anemia

Unit 3: Metallo-enzymes

Catalases – structure and properties reaction mechanism. Peroxidases- glutathione peroxidase, HRP, structure and properties and enzyme reaction mechanism. Cytochrome c peroxidase and lignin peroxidase. Copper enzymes-structure and function, azurin, plastocyanin. Type I, II and III copper proteins. Superoxide dismutase (SOD) - structure and enzymatic reaction mechanisms. Tyrosinase, reaction mechanism. Zn-containing enzymes, carbonic anhydrase and carboxy-peptidases-structure and enzymatic reactions. N_2 fixation, nitrogenase enzyme, Fe-S clusters, Fe-protein structure, Mo-Fe protein structure, P-cluster and M-centre, their model compounds.

Unit 4: Other functional roles of metal ions

Zn in biological systems, Zn-finger proteins – structural features and properties, classifications and their roles in biological systems. Ca^{2+} binding proteins, calmodulins. Metal ion based (Pt, V, Au) drugs, anticancer agents. Cis-platin and its properties. Chelation therapy, macrocyclic antibiotics. Role of Mn, Ni, Mo and Cr in biological systems, metal toxicity and homeostasis, therapeutic complexes. Diseases caused by both excess and deficiency of metal ions, thalassaemia, Wilson disease. DNA intercalators, diagnostic agents, MRI imaging and contrast agents, the role of Gd^{3+} and other metal ions as contrast agents.

Unit 5: Biomimetic compounds, metals in medicine

Porphyrins (H_2P) and metalloporphyrins (MP), spectral, fluorescence and redox properties of H_2P and MP. Biomimetic compounds. Fe(II), Co(II) and Cu(II) based model compounds model compounds of Mb and Hc –. 'picket-fence' porphyrin and its special features. Photodynamic therapy (PDT), principles and applications. Natural and synthetic ionophores, crown ethers, interaction and uptake of alkali metal and alkaline earth metal ions with crown ethers, cryptands and cryptates, calixarenes and their special properties, cyclo-dextrins and their special properties.

TEXTBOOKS:

1. J.E. Huheey, R.A. Keiter, R.L. Keiter, Inorganic Chemistry-Principles of Structure and Reactivity, 4th Edn., Prentice Hall, 1997.
2. F.A. Cotton, G. Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th Edn., Wiley-Interscience, 1999.
3. P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong, Shriver and Atkins Inorganic Chemistry, 4th Edn., Oxford University Press, 2006.

REFERENCES

1. S. J. Lippard, J. M. Berg, Principles of Bioinorganic Chemistry, University Science Books, 1994.
2. J. D. Atwood, Inorganic and Organometallic Reaction Mechanism, 2nd Edn., Wiley-VCH, 1997.
3. B.E. Douglas, D.H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007.
4. W. Kaim, B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, John Wiley & Sons, 1994.
5. M. N. Hughes, The Inorganic Chemistry in Biological Processes, Wiley (1981)

18CHY631 Applied Electrochemistry 3 0 0 3

Unit 1 – Electrodics: Electron transfer under an interfacial electric field, A two way traffic across the interference: equilibrium and exchange current density. Dependence of the electrochemical reaction rate on over potential-Quantitative version of the Butler Volmer equation. Electrode kinetics involving the semiconductor/solution interface. Techniques of electrode kinetics-preparation of electrode surface. Microelectrodes-applications

Unit 2: Industrial Cathodic process - Electrodeposition of copper, nickel and chromium over mild steel – zinc plating on MS – decorative plating of silver and cold – nano plating and microstructure of deposits - Tests for adhesion, hardness, thickness, uniformity and corrosion resistance of the electro deposits-post plating passivation processes-barrel plating of small components - Electroless deposition of nickel, copper, gold on metal components – making of waveguides and plated through hole boards -

Unit 3: Industrial Anodic Processes: Anodising of aluminium and its alloys – baths used, operating conditions and sequence determination of thickness – industrial applications- nano anodizing of titaniuim, and tantalum – application to sensor field

Electropolishing of ferrous and non-ferrous metals and alloys - mechanism of electropolishing –Electrochemical etching of ferrous and non-ferrous metals –

Special processes: Electrolysis of water – electrowinning of aluminium and sodium – electrolysis of brine-photoelectrochemistry

Unit4 - Electrochemical energy systems: Primary batteries: Zinc-carbon (Leclanche type), zinc alkaline (Duracell),; lithium primary cells - liquid cathode, solid cathode and lithium-ferrous sulphide cells Secondary batteries: Lead acid and VRLA (valve regulated (sealed) lead acid), nickel-cadmium, nickel-zinc, nickel-metal hydride batteries, lithium ion batteries, ultra thin lithium polymer cells (comparative account) Advanced Batteries for electric vehicles, requirements of the battery - sodium-beta and redox batteries. Reserve batteries thermally activated batteries - remote activation - pyrotechnic materials: Fuel Cells: Principle, proton exchange membrane (PEM), direct methanol(DMFC), molten carbonate electrolyte (MCFC) fuel cells and outline of biochemical fuel cells.

Unit5 - Electro chemical sensors: Potentiometric sensors, solid state Potentiometric chemical sensors, polymeric membrane sensors, ion selective field effect transistor, application, Hydrovolumetric technique-hydrodynamic voltammetric-application, voltammetric sensors-electrode modification application, optical sensors,-bioamperometric titration. Methods involving forced convection-hydrodynamic methods

Text books

1. *Allen J.Bard and Larry R. Faulkner, 'Text book for Electrochemical Methods',2nd edition, Wiley, 2000.*
2. *Derek Pletcher and Frank C. Walsh, 'Industrial Electrochemistry', Blackie Academic and Professional, (1993).*

References

1. *Christopher M A, Brett, 'Electrochemistry – Principles, Methods and Applications', Oxford University, (2004).*
2. *Watanabe T, 'Nano-plating: microstructure control theory of plated film and data base of plated film microstructure', Elsevier, Oxford, UK (2004).*
3. *Kanani N, 'Electroplating and electroless plating of copper and its alloy', ASM International, Metals Park, OH and Metal Finishing Publications, Stevenage, UK (2003).*
4. *Curtis, 'Electroforming', London, (2004).*
5. *Rumyantsev E and Davydov A, 'Electrochemical machining of metals', Mir, Moscow, (1989).*
6. *Peter G Sheasby 'Basics of aluminium anodising', Banbury, Oxon (2001)*
7. *Robert Brugger 'Nickel Plating' Robert Draper Ltd, Teddington, (1970)*
8. *J. K. Dennis, T. E. Such, 'Nickel and Chromium Plating, Third Edition' Woodhead Publishing Series in Metals and Surface Engineering, 3rd Edition,(1993)*

18CHY632 BIOANALYTICAL CHEMISTRY 3 0 0 3

Unit 1 Enzymes

Enzyme nomenclature, Enzyme commission numbers, Enzymes in bioanalytical chemistry, Enzyme kinetics - Enzyme activators, Enzyme inhibitors.

Unit 2 Quantification of Enzymes and their substrates
Instrumental methods, Optical detection - Absorbance, Fluorescence, Luminescence, Nephlometry Electrochemical detection -Amperometry, Potentiometry, Conductometry, Other Detection Methods - Radiochemical, Manometry, Calorimetry.

Unit 3 Immobilized enzymes
Immobilization methods - nanopolymerizing covalent immobilization, Crosslinking with bifunctional reagents. Properties of immobilized enzymes, immobilized enzyme reactions, theoretical treatment of packed bed enzyme reactors.

Unit 4 Antibodies
Structural and functional properties of antibodies, Polyclonal and monoclonal antibodies Antibody-antigen interactions, analyrtical application of secondary antibody-antigen.

Unit 5 Biosensors
Response of Enzyme-based Biosensors, Examples of Biosensor Configuration, Ferrocene-mediated Amperometric Glucose Sensor, Potentiometric Biosensor for Phenyl Acetate, Potentiometric Immunosensor for Digoxin, Optical Biosensor for Glucose Based on Fluorescence Energy Transfer, Piezoelectric Sensor for Nucleic Acid Detection, Enzyme Thermistors.

TEXTBOOKS:

1. Susan R. Mikkelsen, and Eduardo Corto´n 'Bioanalytical Chemistry', 1st edition, Wiley Interscience, 2003.
2. Andres Manz, Nicole Pamme and Dimitri Lossifidis, 'Bioanalytical Chemistry', World Scientific Publishing Company, 2004.

REFERENCE:

1. Robert W. Cattrall, 'Chemical Sensors', Oxford University Press, 1997.

18CHY633 CHEMISTRY OF BIOMOLECULES 3 0 0 3

Unit 1 Amino acids, Proteins and Peptides
Classification, Stereochemical aspects, physical properties, Ionic properties, spectral properties, essential and non essential amino acids, chemical reactions of amino acids, Industrial preparation and chemical synthesis of amino acids. Ionic properties of proteins, protein structure, protein purification, protein structure determination, proteomics and protein function, solid phase peptide synthesis, biologically important peptides.

Unit 2 Enzymes Introduction to Enzymes, Classification of enzymes, mechanism of enzyme action, immobilized enzymes and enzyme technology, enzyme analog built polymers, design of molecular clefts, enzymes in synthetic organic chemistry. Enzymes in biological systems

Unit 3 Molecular biology and bioinformatics
Structure of nucleic acids, genes and genome complexity, functions of nucleic acids, isolation and separation of nucleic acids, molecular analysis of nucleic acid sequences, nucleotide sequencing of DNA.

Unit 4 Immunochemical techniques
Production of antibpodies, purification and fragmentation of immunoglobulins, immunoprecipitatipon, labeling antibodies, immunoblotting, immunoassays, immunohisto/cytochemistry.

Unit 5 Recombinant DNA and genetic analysis

Constructing gene libraries, cloning vectors, hybridization and gene probes, application of gene cloning, expression of foreign genes, pharmacogenomics.

REFERENCES:

1. *Hermann Dugas, 'Bioorganic Chemistry - A Chemical Approach to Enzyme Action', 3rd edition, Springer.*
2. *Keith Wilson and John Walker, 'Principles and Techniques of Biochemistry and Molecular Biology', 6th edition, Cambridge University Press.*

18CHY634 INDUSTRIAL CHEMISTRY 3 0 0 3

Unit 1 Water treatment

Softening of water, Ion exchange process, Lime soda process, Modified Lime soda process, Zeolite process, Chemical and physical method of sterilization, Desalination, Boiler problems. Corrosion of boiler units, industrial water treatment, water analysis.

Unit 2 Fuels

Calorific value, determination of Calorific value, classification of fuels, Solid fuels, Properties of fuels, classification of coal, coking and non-coking coals, advantages and disadvantages of solid fuels. Liquid fuels, gaseous fuels, analysis of fuel gases, Distillation of petroleum. Processing & purification of petroleum and petroleum products, Flash point, Fire point, Knocking, antiknocking, Cetane number, octane number, natural gasoline, cracking, polymerization, alkylation, isomerisation, rocket fules, fossil fules, nuclear fuels.

Unit 3 Energy resources

Renewable and non renewable sources of energy, conventional and non conventional sources of energy, solar energy, solar technology, solar photovoltaic cell - application, PV lantern system, Radiotelephone system, Application of solar energy, Environmental implication, Nuclear energy, nuclear fuel cycle in India, Energy conservation and waste heat boilers, Fuel cells, hydrogen cells.

Unit 4 Paints and Pigments

White pigment, blue, green, yellow, black and red pigments - manufacture, physical properties, characteristics, Manufacture of paints, setting of paints, requirement for good paints, emulsion paint, latex paint, luminescent paint, fire retardant paints, heat resistant paints, varnishes, manufacture of varnishes, enamels, lacquers.

Unit 5 Explosives and Toxic Chemical Weapons

Introduction, Classification. Deflagrating or low explosives. Characteristics of explosives, nitrocellulose, PETN, DNB, TNB, TNT, Picric Acid, Nitroglkycerine, Dynamite, Cirdite, Gun powder, RDX, EDNA, HMX,Tetryl, Pentryl, Hexyl, Dinol. Toxic chemical weapons, screening smokes, Incendiaries, Pyrotechniques, Explosives in India.

TEXTBOOKS:

1. *B.K.Sharma, 'Industrial Chemistry', Goel publishing.*
2. *James A Kent, 'Riegels Hand book of Industrial chemistry', 10th edition, Kluwer Academic/Plenum publishers, 2003.*

REFERENCES

1. *Alan Heaton, 'An Introduction to Industrial chemistry', 3rd edition, Blackie Academic and professional, 1996.*

2. *Chris A Clausen and Guy Mattson, 'Principles of industrial chemistry', 2nd edition Wiley, 1978.*
3. *Jonathan Steed, 'Core Concepts on supramolecular chemistry and nanochemistry', Wiley Eastern Publishers, 2006.*

18CHY635 INDUSTRIAL STOICHIOMETRY 3 0 0 3

Unit 1 Introduction to process calculation - dimensions and systems of units - fundamental quantities of units, derived quantities, definition and units of force, volume, pressure, work, energy, power, heat-unit conversions in FPS, MKS and SI systems.
Unit 2 Mixtures and solutions - methods of expressing compositions of mixture and solutions, wet and dry basis concept. Ideal and real gas laws – Gas constant – normal molal volume, calculations of pressure, volume and temperature using ideal gas law. Gas mixtures – Use of partial pressure and pure component volume in gas calculations. Dissociating gases. Relation between mole%, volume% and pressure% of ideal gases calculation of average molecular weight, density, mole%, weight% in gas mixture in SI/MKS systems – applications of real gas relationship in gas calculation.
Unit 3 Description and simple material balance calculation of physical processes such as drying, distillation, absorption, mixing, crystallization, Evaporation.
Unit 4 Single stage material balance calculation of leaching and extraction, calculations involving recycling and by passing operation - limiting reactant, excess reactant, conversion, yield and selectivity - simple numerical for finding yield, conversion and composition.
Unit 5 Calculation of material and energy balance based on reactions involving heat capacity and specific heat - mean heat capacity of gases - heat capacity of gas mixture and liquid mixture. Calculations of heat capacity by integral equation up to three terms - sensible and latent heats of fusion, sublimation, vaporization. Calculations of standard heat of formation from heat of combustion data. Calculations for heat of reaction from heat of formation and heat of combustion data – Fuels - calorific values proximate and ultimate analysis - air requirement and composition of flue gases.

TEXTBOOKS:
1. *Bhatt,B.L. Vora,S.M., "Stoichiometry", 3rd Edition, Tata McGraw-Hill (1996).*
2. *Felder,R.M. and Rousseau,R.R. "Elementary Principles of Chemical Processes" 3rd Edn., John Wiley & Sons, New York 2000.*

REFERENCE BOOKS:
1. *Hougen O.A., Watson K.M. and Ragatz R.A., "Chemical Process Principles" Part I, CBS Publishers (1973).*
2. *Warren. K Lewis, Arthur H. Radash & H.Clay Lewis, "Industrial Stiochiometry", McGraw Hill Book C., NY 1995.*

18CHY636 MATERIAL SCIENCE AND NANOCHEMISTRY 3 0 0 3

Unit 1 Introduction to NanomaterialsIntroduction to Material Science, Interdisciplinary nature, Structure of nanomaterials, Length scales, de-Broglie wavelength & exciton Bohr radius, Foundations of Quantum Mechanics: wave function, Schrödinger equation, ucertainty principle, quantum wells, quantum wires, quantum dots, articles.
Unit 2 Nanomaterials: Synthesis, PropertiesSize effect and properties of Nanoparticles - Particle size - Particle shape - Particle density, Specific surface area and pore - Composite structure, Crystal structure - Functionality of nanostructures and their characteristic evaluation - Optical properties - Catalytic property; Synthesis - Methods and Strategies, Top-down and bottom-up approaches, Chemical vapor deposition, Laser ablation, Electric-arc, Sol-Gel Processing, Lithography - Surface modification of inorganic nanoparticles by organic functional groups.
Unit 3 Surface Science and Characterization of NanomaterialsElectron Microscopy, MFM, SNOM, SEM, TEM, EDAX, X-ray Diffraction and Electron diffraction, Atomic Force Microscopy, Scanning Tunneling Microscopy, Spec-

troscopy: UV-Visible spectroscopy, Photoluminescence spectroscopy, IR spectroscopy, FTIR and ATR, Raman spectroscopy, Self-Assembled Monolayers.

Unit 4 Nanotechnology: Applications and DevicesNanoscale materials, Nano transfer printing, Biomaterials applications, MEMS and NEMS, selforganisation, nanoscale (opto) electronics, Fullerenes, Devices - Actuators and motors for nanodisplacements, Nanosensors, development of optical memory using semiconductor nanoparticles - Nozzle-free inkjet technology - Dendrimers and their application to organic electronics devices - Nanomedicines, Bio-imaging with quantum dots.

Unit 5 Environmental Issues in NanotechnologyNanoparticles and environment - Nanoparticles in atmosphere - Ground water, exhaust gases – wastewater and Indoor environments; Safety of nanoparticles - Problems caused by nanoparticles, Safety assessment for the nanoparticles; Removal of nanoparticles.

TEXTBOOKS:

1. T.Pradeep, 'Nano - The Essentials Understanding Nanoscience and Technology', McGraw-Hill Professional Publishing, 2008.
2. Charles P. Pool and Frank J. Ovens, 'Introduction to Nanotechnology', John Wiley and sons, 2006.

REFERENCES:

1. Ozin, Geoffrey Alan, Arsenault, 'Nanochemistry: A Chemical Approach to Nanomaterials', Royal Society of Chemistry, 2008.
2. C.N.R. Rao, A.Muller, A.K.Cheetham, 'The Chemistry of Nanomaterials: Synthesis, Properties and Applications', Wiley-Vch Verlag Gmbh & Co., 2004.
3. Alexei Nabok, 'Organic and Inorganic Nanostructures', Artech House, 2005.
4. C. Richard Brundle, Charles A. Evans Jr., and Shaun Wilson, 'Encyclopedia of Materials Characterization', Butterworth-Heinemann Publishers, 1992.
5. Masuo Hosokawa, Kiyoshi Nogi, Makio Naito and Toyokazu Yokoyama, 'Nanoparticle Technology Handbook', Elsevier Publishers, 2007.

18CHY637 MEDICINAL CHEMISTRY 3 0 0 3

Unit 1 Medicinal chemistry: Introduction, drugs – classification of drugs – mechanism of drug action. Drug-receptor complex, nomenclature – agonist,

Unit 2 Physicochemical properties of drugs in relation to biological action: solubility**,** Partition coefficient, dissociation constant, hydrogen bonding, ionization, drug shape, surface activity, complexation, protein binding, molar refractivity, bioisosterism – stereo chemical aspects of drug action.

Unit 2: Enzymes, hormones and Vitamins - representative cases, nomenclature, classification and characteristics of enzymes, mechanism of enzyme action, factors affecting enzyme action, co-factors and co-enzymes, enzymes in organic synthesis, mechanism of enzyme catalysis, enzyme inhibition. Hormones and vitamins – representative cases.

Unit 3 Essentials of drug design

Molecular mimetics, drug-lead modification, drug design using QSAR and computer assisted design, assessment of drug activity, receptors and drug action, mechanism of drug action, drug metabolism pathways, Drug potentiation, drug antagonism and drug resistance

Unit 4 Medicinal agents from natural products

History of the use of natural products as therapeutic agents, medicinal plants, active principle, Isolation methods of alkaloids, terpenes, antioxidants, natural oils from plants

Unit 5 Medicinal agents

Medicinal agents belonging to alkaloids, steroids, polypeptides, modified nucleic acid bases, sulphonamide and sulpha drugs, antibacterials - sulpha drugs, substituted sulphonamides, anticonvulsants, anticoagulants, antiamoebic agents, antihelmintic agents, anti-malarial agents, diuretics and cardio vascular agents, , medici-

nal agents affecting CNS, analgesics, antipyretics, antiseptics and disinfectants, Histamine and anti-histaminic agents. Infectious and non infectious diseases (malaria, AIDS, Cancer) introduction, mechanism of action types of cure,

TEXTBOOKS:

1. *John M beak and John H Block, 'T Wilson, O. Gisvold and R. F. Deorge - Text book of Organic, Medicinal and Pharmaceutical Chemistry', 7th edition, J.B. Lippincott Williams and Wilkons Company, 1977.*
2. *A.Burger, 'Medicinal Chemistry', 3rd edition, Wiley Interscience, 1970.*
3. *V.K.Ahluwalia and Madhu Chopra, 'Medicinal Chemistry', Ane Books pvt Ltd, 2008.*

REFERENCES

1. *V.Kothekar, 'Essentials of Drug Designing', 14th edition, Dhruv publications, 2005.*
2. *V.K.Ahluwalia, Lalita S.Kumar and Sanjiv Kumar, 'Chemistry of Natural Products', Ane Books India.*
3. *L.P.Graham 'An introduction to Medicinal Chemistry', 3rd edition, Oxford University Press, 2005.*

18CHY638 SUPRAMOLECULAR CHEMISTRY 3 0 0 3

Unit 1 Introduction to Supramolecular Chemistry

From molecular to supramolecular chemistry: Factors leading to strong binding, hydrogen bonding and stacking interactions, Bottom-up approach, Top-Down Approach, Energy and Signals Semiochemistry, photo switching devices, electro switching devices, mechanical switching processes,

Unit 2 Processing of Energy and Signals by Molecular and Supramolecular system

Fundamental principles of photo induced electron and energy transfer, Molecular electronics, Molecular photonics, Molecular Chemionics, Molecular electro photonics, Molecular Photochemionics.

Unit 3 Molecular Recognition

Molecular receptors: crown ethers, siderophores, cyclophanes, cyclodextrin and their application in specific recognition processes. Metal guided self assembly reactions, molecular knot with double helical complexes, Self assembly of polynuclear metal complexes.

Unit 4 Electrochemistry of Supramolecular Systems

Electroluminescent systems as sensors and devices, Redox controlled molecular switches, Biohybrid electrochemical devices, Dendrimers as multielectron storage devices, Redox-active Metal-Polypyridinedendrimers as light harvesting antennae.

Unit 5 Molecular Scale Mechanical Devices Introduction to mechanical devices, Spontaneous mechanical like motions, Allosteric movements, Tweezers and Harpoons, A natural proton pump, Twisters, Tweezers, Threading-Dethreading movements, Ring switching processes in Rotaxanes and Catenanes, Molecular valves, Molecular Muscles.

TEXTBOOKS:

1. *VincezoBalzani, 'Supermolecular Chemistry', Kluwer Academic, 1992*
2. *Vincenzo Balzani, Alberto Credi and MargheritaVenturi, 'Molecular Devices and Machines: A Journey Into the Nanoworld', Wiley, 2006.*
3. *Paola Ceroni, Alberto Credi and MargheritaVenturi, 'Electrochemistry of Functional Supramolecular Systems', Wiley, 2010.*

REFERENCES:

1. *Jonathan W. Steed Atwood, Jerry L.Chich, 'Supramolecular Chemistry', 2nd edition, Wiley, 2009.*

2. *Fritz Vögtle and F.Alfter 'Supramolecular Chemistry: An Introduction', John Wiley & Sons, 1999.*
3. *Jean-Marie Lehn, 'Supramolecular Chemistry', RCS pubs., 2005*
4. *Jonathan Steed, David Turner and Carl Wallace, 'Core concepts in Supramolecular Chemistry and nanochemistry', John Wiley & Sons, 2007*
5. *Katsuhiko Ariga and ToyokiKunitake, 'Supramolecular chemistry – Fundamentals and applications advanced textbook', Springer-Verlag, 2000*

18CHY639 Nanomaterials for Biomedical Applications 3 0 0 3

Unit 1: Introduction to Nanomaterials: Size dependence of properties – Surface to volume ratio and Quantum confinement. Microscopic techniques to study nano structures - SEM, AFM – TEM and STM. Spectroscopic techniques to characterize nanostructures - Raman, XPS, Auger, EDAX.
Unit 2: Synthetic approaches: Colloidal, Self-Assembly (Self assembled monolayers-SAMs) and electrostatic self-assembly, electrochemical methods (cathodic and anodic processes), sol-gel, Langmuir-Blodgett (LB) technique, chemical vapour deposition, plasma arcing and ball milling, lithography.
Unit 3: Electrical, optical, mechanical, chemical and magnetic properties of nanomaterials. Surface Plasmon resonance – Fluorescence Resonance energy transfer (FRET).
Unit 4: Carbon Clusters: Synthesis, properties and biomedical applications of Fullerenes, Carbon nanotubes and Graphenes. Quantum Dots, wells and wires (metallic and semiconducting) - Preparation, properties and biomedical applications. Dendrimeric structures and their applications.
Unit 5: Biofunctionalisation of nanomaterials - Noncovalent Assembly - Covalent assembly - Biofunctional Nanomaterials - Semiconductor Nanoparticles - Magnetic Nanoparticles. Applications of Biofunctional nanomaterials – Optical and Electrochemical Sensing.

REFERENCES:

1. Alexei Nabok, "Organic and Inorganic Nanostructures", Artech House, Inc., 2005
2. Huangxian Ju, Xueji Zhang and Joseph Wang, "NanoBiosensing, Principles, Development and Application", Springer, 2011.
3. M. Reza Mozafari (Editor), "Nanomaterialsand Nanosystems for Biomedical Applications", Springer 2007.
4. Zhong Lin Wang (Editor), "Characterisation of Nanophase Materials", Wiley VCH, 2000.

18CHY640 INDUSTRIAL METAL FINISHING PROCESSES 3 0 0 3

Unit 1 Background Theory: Review of reversible and irreversible processes - electrodes, indicator and reference - Nernst and Butler-Vohmer equation - phenomenon of polarization - factors influencing - Tafel experiment and Tafel plot - Significance.
Unit 2 Electrodeposition: Industrial plating of copper-nickel (dull and bright) - chromium on mild steel – operating conditions and sequence – pre-treatment processes - plant layout – electroplating of zinc on MS and post plating chromating, yellow and blue passivation processes – decorative plating of silver and gold on non-ferrous metals – brief discussion on nano plating of metals and micro structure of the deposition.
Properties of deposits: Tests for adhesion, hardness, thickness, uniformity and corrosion resistance of the electro deposits.
Electroless deposition: Nickel, copper, gold on metal components – bath composition and operating conditions - immersion plating - plating on plastics – pre-treatment processes – long duration plating – electroforming, operating conditions and sequence.

Unit 3 Anodising: Industrial anodizing of aluminium and its alloys – baths used, operating conditions and sequence – plant layout – effect of temperature and current density on the thickness of anodic film – determination of thickness – industrial applications.
Nano anodizing of titaniuim, aluminium and tantalum – application to sensor field.
Plasma electrolytic oxidation: power supply requirements – baths used – process sequence for aluminium, magnesium and titanium – properties of the coating and industrial applications.
Unit 4 Electropolishing: Mechanism of electropolishing – electropolishing of ferrous and non-ferrous metals – industrial baths used – operating conditions and sequence - industrial applications.
Unit 5 Electrochemical etching: Etching of ferrous and non-ferrous metals – special properties of matt and satin finish – DC and AC processes – operating conditions and sequence.
Special Topics: Electrochemical and chemical metal colouring of ferrous and non-ferrous metals.
Black nickel coating – Hard chromium deposition – Hard anodizing of aluminium – Electrochemical machining of hard steels – Electro-winning process – Barrel plating – Electrodeposition of paint.

TEXTBOOK:

1. *Derek Pletcher and Frank C. Walsh, 'Industrial Electrochemistry', Blackie Academic and Professional, (1993).*

REFERENCES:

1. *Christopher M A, Brett, 'Electrochemistry – Principles, Methods and Applications', Oxford University, (2004).*
2. *Watanabe T, 'Nano-plating: microstructure control theory of plated film and data base of plated film microstructure', Elsevier, Oxford, UK (2004).*
3. *Kanani N, 'Electroplating and electroless plating of copper and its alloy', ASM International, Metals Park, OH and Metal Finishing Publications, Stevenage, UK (2003).*
4. *Curtis, 'Electroforming', London, (2004).*
5. *Rumyantsev E and Davydov A, 'Electrochemical machining of metals', Mir, Moscow, (1989).*
6. *Peter G Sheasby 'Basics of aluminium anodising', Banbury, Oxon (2001)*
7. *Robert Brugger 'Nickel Plating' Robert Draper Ltd, Teddington, (1970)*
8. *J.K.Dennis, T.E.Such, 'Nickel and Chromium Plating, Third Edition' Woodhead Publishing Series in Metals and Surface Engineering, 3rd Edition, (1993)*

18CHY641 Biosensors : Fundamentals and Applications 3 0 0 3

Unit 1: Introduction to biosensor – classification based on the signal transduction and biorecognition element. Enzymatic and non-enzymatic sensors, DNA and protein based sensors-immunosensors.

Unit 2: Biosensing using nanomaterials: Concepts of surface to volume ratio, quantum confinement, surface plasmon resonance, fluorescence, chemiluminescense and electroluminescence and FRET in biosensing. Application of metal, semiconducting quantum dots, carbon nanotubes, graphene and carbon dots in biosensing.

Unit 3: Electrochemical principle in biosensing: Principles of potentiometry, voltammetry, amperometry and impedimentary in biosensing. Principle, fabrication and working of optical, electrochemical biosensors. Construction and working of potentiometric, amperometric and impedemetric sensors. Development and applications of piezoelectric sensors.

Unit 4: Optical and electrochemical sensors for glucose, vitamins, cholesterol, dopamine, nitric oxide, nitrates, and pesticides. Biocompatibility of sensors.

Unit 5: Biochips and wearable devices: lab-on-a-chip - fabrication of microfluidics- lithography, wearable sensors, epidermal electronic system, lab-on-skin-devices.

REFERENCES

1. Xueji Zhang, Huangxian Ju, Joseph Wang, “Electrochemical Sensors, Biosensors and Their Biomedical Applications”, Elsevier, 2008

2. Joseph Wang, "Analytical Electrochemistry", Wiley, 2006

3. Huangxian Ju, Xueji Zhang, Joseph Wang, "NanoBiosensing: Principles, Development and Application", Springer, 2011.

4. Peter Grundler, “Chemical Sensors – An Introduction for Scientists and Engineers”, Springer-Verlag, Berlin Heidelberg, 2007

5. Arben Merkoci, “Biosensing using nanomaterials” Wiley, 2009.

18CHY642 COMPUTATIONAL CHEMISTRY 3 0 0 3

Unit 1 - Introduction

Introduction to computational chemistry (molecular modelling), questions commonly investigated computationally, principle and application of methods (tools) of computational chemistry - molecular mechanics, ab initio method, semiempirical methods, density functional theory and molecular dynamics, STOs, GTOs, basis sets, specification of molecular geometry using Cartesian coordinates and internal coordinates, Z-matrix, Z-matrix of simple molecules (water, ethanol), potential energy surface (PES), potential energy surface of diatomic molecules and triatomic molecules (H_2O and HOF) - hypersurface and process of “slicing”, stationary points on apotential energy surface - potential energy surface of the isomerization reaction of ozone to isoozone, stationary points (ozone, isoozone and transition state), intrinsic reaction coordinate, minimum, relative minimum, saddle-shaped surface, saddle point, higher-order saddle point and mathematical treatment of stationary points, Born-Oppenheimer approximation and its significance and frozen-nuclei energy.

Unit 2 - Molecular Mechanics

Introduction to molecular mechanics, forcefield, developing a force field - expression for potential energy of a molecule, bond stretching term, angle bending term, torsional term and nonbonded interaction term,parameterizing a forcefield -parameterizingbond stretching term, angle bending term, torsional term and nonbonded interaction term, calculation using forcefield - compare the energies of two 2, 2, 3, 3-tetramethylbutane geometries, illustration of application (use) ofmolecular mechanics - calculation of geometries and energies of small-sized and medium-sized molecules, polymers and transition states (transition state for the Diels-Alder reaction of butadiene with ethene to form cyclohexene), in organic synthesis for predicting the more suitable path for carrying out the synthesis and calculation of normal-mode vibrational frequencies for characterizing a species as a minimum or a transition state or higher-order saddle point, for obtaining zero-point energies to correct frozen-nuclei energies and for interpreting or predicting IR spectra, strength (merit) and weakness (demerit) of molecular mechanics.

Unit 3 - Semiempirical methods - Part 1

Introduction to semiempirical (SE) methods, Simple Huckel Method (SHM) - theory - expression for calculating energy of a molecular species, expression for molecular wave function based on LCAO approximation, secular equations and the single matrix equation, H, C, S and ε matrices and their interpretation, the values of

H_{ij} as zero, coulomb integral α and bond integral β and their physical significance, the H matrix in terms of α, β and zero for ethene system(ethene neutral molecule, ethene radical cation and ethene radical anion), propenyl system (propenyl cation, propenyl neutral radical and propenyl anion) and cyclobutadiene system (square cyclobutadiene dication, square cyclobutadiene neutral molecule and square cyclobutadiene dianion), the H matrix in terms of zero, α = 0 and β =− 1for ethene systems (ethene neutral molecule, ethene radical cation and ethene radical anion), propenyl system (propenyl cation, propenyl neutral radical and propenyl anion) and cyclobutadiene system (square cyclobutadiene dication, square cyclobutadiene neutral molecule and square cyclobutadiene dianion), result of diagonalization of the H matrices written for ethene system, propenyl system and cyclobutadiene system, molecular orbital energy level diagrams and expressions for energy and molecular wave functionsfor ethene system, propenyl system and cyclobutadiene system based on the result of diagonalization of the H matrices, and molecular orbital energy level diagrams for ethene system, propenyl system and cyclobutadiene system showing ground state and excited state electronic configurations.

Unit 4 - Semiempirical methods - Part 2

Application of SHM - nodal properties of molecular orbitals and Woodward-Hoffmann orbital symmetry rule, stability towards oxidation and reduction of various species in ethene system, propenyl system and cyclobutadiene system, geometry of cyclobutadiene molecule as predicted by SHM and its Jahn-Teller distortion, aromaticity and Huckel's (4n + 2) π electron rule,and calculation of resonance (stabilizing) energy, bond order and atomic charges of various species in ethene system, propenyl system and cyclobutadiene system, strength of SHM, weakness of SHM (detailed explanation) - basis set is limited to p orbitals (p_z orbitals), it treats only π electrons, and the overlap integrals, Fock matrix elements, electron spin and electron-electron repulsion are not calculated/accounted properly, Extended Huckel Method (EHM) - minimal valence basis set, calculation of Fock matrix elements, and calculation of overlap integrals by Lowdin orthogonalization, EHM procedure, EHM calculation on protonated helium molecule, application of EHM - an overall idea, strength and weakness of EHM, SCF SE methods - Pariser-Parr-Pople (PPP) method and Complete Neglect of Differential Overlap (CNDO) method - basic principle (an exhaustive treatment is **not** expected).

Unit 5 - Density Functional theory and ab initio method

(An exhaustive treatment is **not** expected)

Introduction to Density Functional theory and calculations, Kohn-Sham approach - the first and the second Hohenberg-Kohn theorems, introduction to ab initio method and calculation, basis sets for H, He and first, second and third row elements used in ab initio calculations - STO-3G, 3-21G, 3-21G$^{(*)}$ and 6-31G*, these basis sets for a few molecular species (water, methane and carbene), basic principles of ab initio method (an idea only).

Text Book

1. Computational Chemistry-Introduction to the Theory and Applications of Molecular and Quantum Mechanics - Errol Lewars

18CHY643 Sustainable Chemical Science 3 0 0 3

Unit 1 Green Chemistry and Sustainability

History of green chemistry, Chemical composition of the, environment (Air, water & soil- Role of organic and inorganic molecules in pollution), the twelve principles of green chemistry (detailed description with examples), green chemistry as an expression of environmental ethics (Thrift Chemistry),the concept of sustainability, from green to sustainable chemistry, sustainable use of chemical feedstock, water and energy,

quantifying greenness of a chemical reaction, green chemistry metrics- mass based, energy and environmental metrics, designing greener process, life cycle assessment (introduction and scope),Green toxicology- the need, principles of toxicology, Disposition of Toxicants in Organisms, Non-Organ System Toxicity, Mechanistic Toxicology, Quantitative Structure–Activity Relationships, (Environmental Toxicology-Persistence and bio-accumulation), Non-Cancer risk assessment, Cancer risk assessment, stakeholders in sustainable policy implementation.

Unit 2Chemistry in water

Definition and attributes of a green solvent, the principle and reasons for use of water in green chemistry- hydrophobicity- cyclodextrin chemistry, Lewis acids in aqueous media, Michael addition in water using triflates, green processes with base in water, green oxidations and reduction in water, on water conditions, use of water in microwave and ultrasonic technology.

Unit 3 Green solvents

Ionic liquids as green solvents- definitionand notation- properties, synthesis and use in organic reactions, oxidation, oxidative carbonylation of aniline,Friedel–crafts reaction, Michael addition, Fischer Indole synthesis, Benzoin condensation, dimethyl carbonates synthesis in ionic liquids.

Super critical fluids- super critical water and carbondioxide- properties and organic transformations.(Diels Alder, Clasen rearrangement, Fisher Indole, Friedel–crafts reaction, oxidation and hydrogenation.

Properties and application in organic transformation of green solvents like polyethylene glycol, glycerol, cyclopentyl methyl ether, 2-methyltetrahydro furan, Perfluorinated (Fluorous) Solvents- FluorousBiphase Concept and dimethyl carbonate.

Unit 4 Green Chemistry and Catalysis

Importance of catalysis, turn over number and frequency, the basis of catalysis-kinetic phenomenon, basics of homogeneous, heterogeneous and biocatalysis, sabatier's principle, catalyst -deactivation, sintering, thermal degradation, inhibition and poisoning, catalyst promoters, modifiers, supported catalysts and reagents for green chemistry- heterogenized reactions for green chemistry, preparation of solid catalyst-slurry and co-precipitation, impregnation, hydrothermal synthesis- drying, calcination, activation and forming, selecting the right support, catalyst characterization- surface characterization methods, temperature programmed techniques, spectroscopy and microscopy.Common mechanism in enzyme catalysis immobilized enzymes, developing biocatalyst- rational design and directed evolution, non-enzymatic biocatalysts.

Unit 5 Green Chemistry Technologies and Alternate Energy Sources

Design for Energy Efficiency, Photochemical Reactions Advantages of and Challenges Faced by Photochemical Processes (Examples)

Microwaves as energy source in chemistry- properties of microwaves, microwave heating (Effects), Approaches to Microwave-assisted Organic Chemistry- solvent free methods, MORE chemistry, continuous microwave reactor (CMR)-microwave batch reactor (MBR), examples of organic transformations.

Sonochemistry and Green Chemistry-Theoretical Basis- Cavitation Inception, Nucleation-Bubble Dynamics- examples of organic transformations, Sono-chemical synthesis of nano-structured materials,

Electrochemical Synthesis- materials manufactured using the process, organic electrosynthesis- 3-bromothiophen from thiophene

Renewable Sources of Energy, Solar Energy, Wind Power, Geothermal Solution, Hydropower (Sources, Merits and Difficulties in widespread applications), Indian Energy scenario- Energy Conservation act (2001)- features.

Reference

1. Green chemistry and engineering A Pathway to Sustainability, Anne E. Marteel-Parrish, Martin A. Abraham, American Institute of Chemical Engineers, Inc, John Wiley & Sons, Inc 2014.
2. Synthetic organic Sonochemistry, Jean-Louis luche, Springer Science+Business Media New York, 1998
3. New Methodologies and Techniques for a Sustainable Organic Chemistry, Alessandro Mordini and FerencFaigl, Springer, 2008.
4. Green chemistry, Fundamentals and Applications, Suresh C. Ameta and RakshitAmeta, CRC press, Taylor & Francis Group, 2013
5. Handbook of Green Chemistry, Vol5 Green Solvents- Reactions in Water, PualT Anastas, Chao Jun Li
6. Sonochemistry: theory, reactions, syntheses, and applications, Filip M. Nowak, Nova Science Publishers, Inc, 2010.
7. Green Chemistry Metrics, A Guide to Determining and Evaluating Process Greenness, Dicks, Andrew, Hent, Andrei, SpringerBriefs in Green Chemistry for Sustainability, 2015
8. Catalysis: concepts and applications, Gadi Rothenberg,Wiley-VCH Verlag& Co. KGaA, Weinheim, Germany, 2008

18CHY681 ORGANIC QUALITATIVE ANALYSIS LAB. 0 0 6 2

1. Separation of binary mixtures

Includes separation, preliminary investigations, determinations of saturation/unsaturation, detection of elements by Lassaigne's test, functional group identification, derivative preparation, determination of melting points of the derivatives and calculation of Rf values from TLC

The following mixtures can be given:

(a) Acid and hydrocarbon
(b) Phenol and aldehyde
(c) Phenol and acid
(d) Phenol and amine
(e) Acid and ester
(f) Halo compound and aldehyde
(g) Acid and aldehyde
(h) Amine and aldehyde
(i) Amine and ketone
(j) Alcohol and hydrocarbon

2. Thin layer chromatography to determine Rf values of compounds

(a) 2-nitroaniline
(b) 4-nitroaniline
(c) Cinnamic acid and 2-nitroaniline
(d) Acetophenone
(e) Ethyl benzoate

3. Simple column chromatography to separate the components of binary mixtures

(a) Hydrocarbon and ester

(b) Aldehyde and amine

REFERENCES:

1. P.W.G. Smith, A.J.Hannaford, B.S.Furnis and A.R. Tatchell, "Vogel's Textbook of Practical Organic Chemistry", ELBS/Longman, 1989.

2. Ralph L.Shriner, Christine K.F.Hermann, Terence C.Morrill, David Y.Curtin, Reynold C.Fuson, 'Systematic Identification of Organic Compounds', John Wiley & Sons, 2003.

3. Mann and Saunders, 'Practical Organic Chemistry', Pearson edition, 2009

18CHY682 INSTRUMENTAL METHODS OF ANALYSIS LAB. 0 0 5 2

1. Determination of strengths of halides in a mixture potentiometrically**.**
2. To find the redox potential of the given sample using cyclic voltametry.
3. Determination of half wave potential of Cd & Zn by polarography.
4. Determination of pKa of an indicator in aqueous and micellar medium using UV-Vis spectroscopy.
5. Determination of stoichiometry and stability constant of inorganic (ferric-salicylic acid) and organic (amineiodine) complexes using UV–Vis spectroscopy.
6. Determination of copper and cadmium in a mixture by electrogravimetry.
7. Determination of rate constant for enzyme kinetics-inversion of sucrose.
8. Determination of molecular weight of a polymer by Viscometry.
9. Determination of a molecular weight of a solute using Beckmann thermometer.
10. Refractrometric determination of composition of solutions.

TEXTBOOKS:

1. Alexander Findly, 'Practical physical chemistry', 9th edition, Wiley, 1972.

2. R.C. Das and B.Behera, 'Experimental Physical Chemistry', Tata McGraw-Hill, 1983.

REFERENCE BOOKS:

1. J.B.Yadav, 'Advanced Practical Physical Chemisty', Krishna Prakashan Media, 29th edition, 2010.

2. Francis William Gray, 'A Manual of Practical Physical Chemistry' Macmillan and Co., Limited, 1914.