UNIVERSITY DEPARTMENTS

ANNA UNIVERSITY CHENNAI :: CHENNAI 600 025

REGULATIONS - 2009

CURRICULUM I TO IV SEMESTERS (FULL TIME)

M.Sc. APPLIED CHEMISTRY

SEMESTER I

COURSE	COURSE TITLE	L	Т	Р	С
THEORY					
AC 9111	Inorganic Chemistry	3	0	0	3
AC 9112	Organic Chemistry - I	3	0	0	3
AC 9113	Physical Chemistry - I	3	0	0	3
AC 9114	Analytical Chemistry	3	0	0	3
PRACTICAL					
AC 9115	Organic Chemistry Practicals	0	0	12	6
E1	Elective I	3	0	0	3
	Total	15	0	12	21

SEMESTER II

Course Code	Course Title		L	Т	Р	С	
THEORY							
AC 9121	Co-ordination Chemistry		3	0	0	3	
AC 9122	Organic Chemistry II		3	0	0	3	
AC 9123	Physical Chemistry II		3	0	0	3	
AC 9124	Introductory Principles of Chemical		3	0	0	3	
	Engineering						
PRACTICAL							
AC 9125	Inorganic Chemistry Practicals		0	0	12	6	
AC 9126	Seminar		0	0	2	1	
E2	Elective II		3	0	0	3	
		Total	13	0	18	22	

SEMESTER III

COURSE CODE	COURSE TITLE	L	Т	Р	С	
THEORY						
AC 9131	Advanced Inorganic Chemistry	3	0	0	3	
AC 9132	Organic Chemistry III	3	0	0	3	
AC 9133	Physical Chemistry III	3	0	0	3	
AC 9134	Molecular Spectroscopy	3	0	0	3	
PRACTICAL						
AC 9135	Physical Chemistry Practicals	0	0	12	6	

E3	Elective III		3	0	0	3
	Tot	al	15	0	12	21

SEMESTER IV

COURSE CODE	COURSE TITLE	L	Т	Р	С
THEORY					
E4	Elective IV	3	0	0	3
E5	Elective V	3	0	0	3
AC 9141	Project work	0	0	20	10
	Total	6	0	20	16

TOTAL CREDITS: 80

ELECTIVES

COURSE	COURSE TITLE	L	Т	Р	С		
THEORY							
AC 9151	Organic Chemical Technology	3	0	0	3		
AC 9152	Inorganic Chemical Technology	3	0	0	3		
AC 9153	Polymer Chemistry	3	0	0	3		
AC 9154	Polymer Technology	3	0	0	3		
AC 9155	Textile Chemistry	3	0	0	3		
AC 9156	Textile Processing	3	0	0	3		
AC 9157	Environmental Chemistry	3	0	0	3		
AC 9158	Water and Wastewater Treatment	3	0	0	3		
AC 9159	Solid Waste Management and Air Pollution	3	0	0	3		
AC 9160	Industrial Electrochemistry	3	0	0	3		
AC 9161	Corrosion and Corrosion Control	3	0	0	3		
AC 9162	Chemical Process Equipments and	3	0	0	3		
	<u>Instrumentation</u>						
AC 9163	Bio-organic Chemistry	3	0	0	3		
AC 9164	Bio-Process Technology	3	0	0	3		
AC 9165	Pharmaceutical Chemistry	3	0	0	3		
AC 9166	Industrial Catalysis	3	0	0	3		
AC 9167	Computational methods in Chemistry	3	0	0	3		
AC 9168	Chemistry of Nanomaterials	3	0	0	3		

INORGANIC CHEMISTRY

LTP C 3 0 0 3

UNIT I ATOMIC STRUCTURE

9

Wave equation – hydrogen atom and polyelectron atoms; electronic configuration and term symbols, periodic properties of elements – atomic size, ionisation energy, electron affinity, electronegativity, covalent and ionic radii, magnetic properties.

UNIT II NON-VALENCE FORCES

9

Van der Waals'forces, hydrogen bond –clathrates, metallic bond – free electron theory of metals, ionic solids – lattice energy – Born-Haber cycle.

UNIT III CRYSTAL STRUCTURE

9

Radius ratio, structures of AX, AX₂, A₂X₃, ABX₃ and A₂BX₄ type solids – layer structure – cadmium iodide; covalent solids – diamond, graphite.

UNIT IV COVALENT BOND

9

Valence bond theory – hybridization and resonance – diatomic and polyatomic systems; VSEPR theory; molecular orbital theory – LCAO approximation for diatomic and polyatomic systems.

UNIT V AQUEOUS AND NON-AQUEOUS CHEMISTRY

9

Acid-base concepts, HSAB theory, non-aqueous solvents – reactions in liquid ammonia, sulphuric acid, aprotic solvents; molten salts; electrode potentials and applications in inorganic systems.

TOTAL PERIODS 45

- 1. F.A. Cotton, G.Wilkinson and P.L.Gaus, "Basic Inorganic Chemistry", 6rd Edn. John Wiley and Sons (2004)
- 2. D.F. Shriver and P.W.Atkins, "Inorganic Chemistry", 3rd Edn. Oxford University Press (2004).
- 3. J.E. Huheey, E.A. Keiter and R.L. Keiter, "Inorganic Chemistry", 5th Edn. Pearson Education (2005).
- 4. James E. Huheey, "Inorganic chemistry-Principle, structure and reactions', 1st edition, Dorley Kindesely Pvt. Ltd. (2006)
- 5. A.G. Sharpe, "Inorganic Chemistry", 3nd Édn. Pearson Education (2004).
- 6. W.L.Jolly, "Modern Inorganic Chemistry", 2nd Edn. Tata McGraw –Hill Pub.Co. (2007)
- 7. J.D.Lee, Concise Inorganic Chemistry, 5th Edn. Blackwell Science (2006).

UNIT I STEREOCHEMISTRY

10

Optical activity and chirality - classification of chiral molecules as asymmetric and dissymmetric - Newman, Sawhorse Wedge and Fischer projection formulae and interconversion - R,S-nomenclature - diastereoisomerism in acylic and cyclic systems - enantiotopic, homotopic and diastereotopic hydrogens and prochiral carbons - optical activity of biphenyls, allenes and spirans - stereospecific and stereoselective syntheses- asymmetric synthesis - Cram's rule - Prelog's rule - conformational analysis of cyclic and acyclic compounds - conformation and reactivity - conformation and stereochemistry of cis and trans decalin and 9-methyl decalin - E,Z-nomenclature - E,Z-isomerism of olefins containing one double bond and more than one double bond - determination of configuration of geometrical isomers using physical and chemical methods.

UNIT II ADDITION REACTIONS

8

Reactive intermediates - formation and stability of carbonium ions, carbanions, carbenes and carbenoids, nitrenes, radicals and arynes - addition to carbon-carbon and carbon-hetero multiple bonds - electrophilic, nucleophilic and free radical additions - stereochemistry of addition to carbon-carbon multiple bonds - orientation and reactivity - addition to conjugated systems and orientation -addition to α,β -unsaturated carbonyl compounds.

UNIT III SUBSTITUTION REACTIONS

10

Aliphatic nucleophilic substitutions - S_N1 , S_N2 and S_Ni mechanisms - effects of substrate, attacking nucleophile, leaving group and solvent - stereochemistry of nucleophilic substitution reactions - mechanism of ester hydrolysis (B_{AC}^2 , A_{AC}^2 and A_{AL}^1) - alkylation of active methylene compounds - substitutions at carbonyl, bridgehead, vinylic and allylic carbons - neighbouring group participation - labelling and kinetic isotope effects - norbornyl cation and other non-classical carbocations, ambident nucleophiles - O versus C alkylation - aromatic nucleophilic substitution - mechanisms - effects of substrate, structure, leaving group and attacking nucleophile - various methods of benzyne generation and reactions of benzyne, reactions of aryl diazonium salts - vicarious nucleophilic substitution (VNS) - aromatic electrophilic substitution reactions and mechanisms.

UNIT IV ELIMINATION REACTIONS

7

E1, E2 and ElcB mechanisms - stereochemistry of E2 elimination - Hofmann and Saytzeff rule - competition between elimination and substitution reactions - orientation effects in elimination reactions - effects of substrate structures, attacking base, leaving group and medium on E1 and E2 reactions - pyrolytic eliminations - Bredt's rule.

UNIT V REACTIONS 10

Birch, Clemmensen, Wolff-Kishner and Meerwein-Ponndorf-Verley reductions - Oppenauer oxidation - Claisen, Dieckmann, Benzoin, Darzens and Stobbe condensations - Chugaev and Cope eliminations - Michael addition - Mannich reaction - Wittig reaction - Chichibabin reaction - Hunsdiecker reaction - Robinson annulation - Hell-Volhard-Zelinsky reaction - Japp-Klingemann reaction - Stork enamine alkylation - Ziegler alkylation - Vilsmeier-Haack reaction - Heck reaction - Shapiro reaction - Polonovski reaction - Sharpless asymmetric epoxidation - Hofmann-Loffler-Freytag reaction - Reformatsky reaction - Simmons-Smith reaction - Gattermann-Koch reaction - Schiemann reaction - Ene reaction - von Braun reaction - Ullmann reaction - Thorpe reaction.

TOTAL PERIODS 45

- 1. J. March, Advanced Organic Chemistry, 4th edition, Wiley Intersciences, New York (2003).
- 2. F.A. Carey and R.J. Sundberg, Advanced Organic Chemistry, Part A and Part B, 5th edition, Plenum Press, New York (2006).
- 3. T.W. Graham Solomons, Organic Chemistry, 5th edition, John Wiley & Sons, New York (2002).
- 4. R.T. Morrison and R.N. Boyd, Organic Chemistry, 6th edition, Prentice-Hall of India Private Ltd., New Delhi (2006).
- 5. P.Y. Bruice, Organic Chemistry, Prentice Hall, New Delhi (1998).
- 6. S. Pine, Organic Chemistry, 5th edition, McGraw-Hill Book Company (1987).
- 7. E.L. Eliel, S.H. Wilen and L.N. Mander, Stereochemistry of Carbon Compounds, John Wiley and Sons, New York (2005).
- 8. D. Nasipuri, Stereochemistry of Organic Compounds, 2nd edition, Wiley Eastern Limited (1991).
- 9. P.S. Kalsi, Stereochemistry of Organic Compounds, Wiley Eastern Ltd., New Delhi (1992).
- 10. R. Bruckner, Advanced Organic Chemistry Reaction Mechanism, Elsevier, New Delhi (2002).

PHYSICAL CHEMISTRY I

LTPC 3 0 0 3

UNIT I CHEMICAL THERMODYNAMICS

9

First law of thermodynamics – Joule Thomson effect – second law of thermodynamics - free energy and work function - Maxwell relations – third law of thermodynamics - entropies of chemical reactions – partial molar properties – chemical potential - Vant Hoff's equation - Gibbs – Duhem equation.

UNIT II PHASE EQUILIBRIA

9

Gibb's Phase rule-two component systems – classification – liquid-liquid and liquid vapour equilibria (fractional distillation) solid – gas (dehydration and rehydration of $CuSO_4$. $5H_2O$), solid-liquid systems(Bi-Cd, Al-Mg and – benzene – picric acid systems),– three component systems involving liquid–liquid equilibria.

UNIT III MOLECULAR SYMMETRY AND GROUP THEORY

9

Symmetry elements and symmetry operations – group postulates – types of groups – point groups – representation of molecular point groups – great orthogonality theorem – character tables – reduction of reducible representations –construction of character tables - applications of group theory.

UNIT IV ELECTROCHEMISTRY

9

Ion-solvent and ion-ion interaction, ion transport in solutions-electrochemical cells electrical double layer – various models – electrocapillary phenomena –electrokinetic phenomena–electro-osmosis -streaming potential and electrophoresis –kinetics of electrode processes – Butler–Volmer equation – Tafel equation

UNIT V APPLIED ELECTROCHEMISTRY

9

Electrochemical energy conversion – Ag – Zn cells- dry cells – Batteries- lead acid, Ni-Cd and lithium ion-fuel cells (Hydrogen – Oxygen) galvanic corrosion – methods of –corrosion control – electroplating – electroforming and electrochemical machining – electrorefining – electrolytic oxidation and reduction

TOTAL PERIODS 45

- 1. P. W. Atkins, and J.D. Paula, Physical Chemistry, 7th Edn. Oxford University Press, London (2002).
- 2. P.A. Alberty and R.U. Silbey, Physical Chemistry 1st Edn. John Wiley and Sons Inc. (1995).
- 3. G.W.Castellan, Physical Chemistry 3rd Edn. Narosa Publishing House (2004).
- 4. Philip H.Reiger, Electrochemistry, Prentice Hall Inc., New Delhi (1987).
- 5. J.C. Kuriacose and J.Rajaram, Thermodynamics for students of Chemistry, 4rd Edn. S.Chand & Co., New Delhi (2002).
- 6. D.R. Crow, Principles and application of electrochemistry, Chapman and Hall (1988).
- 7. Cotton F.A. Chemical Application of group theory, 3rd Edn. Wiley, New York (2003).

ANALYTICAL CHEMISTRY

LTPC 3 0 0 3

UNIT I WET CHEMICAL METHODS OF ANALYSIS

9

Volumetric analysis –neutralization, precipitation, complexometric and redox titrations- theoretical titrations curves - theory of indicators; Gravimetric analysis-volatilization and precipitation methods- homogeneous precipitation; Colorimetric analysis - principles and applications- estimation of iron and nickel.

UNIT II SPECTRAL METHODS

9

Molecular and atomic spectroscopy - interaction of electromagnetic radiation with matter - Beer-Lambert law - UV / Visible absorption spectroscopy- photometric titrations, IR absorption spectroscopy; Fluorescence, phosphorescence and chemiluminescence methods; Atomic spectroscopy - atomic absorption spectrometry; Emission spectroscopy - flame photometry and ICP-AES; atomic fluorescence spectroscopy; Principles, instrumentation and analytical applications of spectral methods.

UNIT III ELECTROANALYTICAL TECHNIQUES

a

Conductometry, and high frequency titrations; Potentiometry, pH-metry, Ion selective electrodes; Electrogravimetry and coulometry; Voltammetry –polarography, amperometric titrations and anodic stripping voltammetry; principles, practice and applications.

UNIT IV SEPARATION TECHNIQUES

9

Solvent extraction and lon exchange techniques – principles and applications; Chromatographic techniques – adsorption chromatography, thin layer chromatography, gas chromatography, high performance chromatography, size exclusion chromatography; Supercritical fluid chromatography.

UNIT V THERMAL METHODS OF ANALYSIS, SAMPLING AND EVALUATION OF ANALYTICAL DATA

Thermal analytical techniques – TGA, DTA, DSC – principles, instrumentation and applications; Sampling methods - Types of errors-evaluation of analytical data-statistical methods.

TOTAL PERIODS 45

- 1. D.A.Skoog, D.M.West, F.J. Holler and S.R.Crouch, "Fundamentals of Analytical Chemistry". 8th Edn.. Thomson Brooks/Cole Pub. (2005).
- 2. J.Mendham, R.C.Denney, J.D. Barnes and M.J.K.Thomas, "Vogel's Text book of quantitative chemical analysis", 6th Edn., Pearson Education (2008).
- 3. F.W. Fifield and D.Kealey, "Principles and Practice of Analytical Chemistry, 1st Indian Reprint, Blackwell Pub. (2004).
- 4. H.H Willard, L.L Merritt, J.A Dean, and F.A Settle, "Instrumental Methods of Analysis", 7th Edn., -CBS Pub (2004).
- 5. G. D.Christian, "Analytical Chemistry", 6th Edn., John Wiley Press (2006).
- 6. K.A. Rubison and J.F. Rubison, "Contemporary Instrumental Analysis, Printice Hall, Inc. (2000).

ORGANIC CHEMISTRY PRATICALS

L T P C 0 0 12 6

UNIT I QUALITATIVE ANALYSIS OF TWO-COMPONENT MIXTURES

30

Separation of two component mixture, analysis for hetero atoms, functional group analysis, derivative preparation and confirmatory tests

UNIT II QUANTITATIVE ORGANIC ANALYSIS

30

Percentage purity of aniline, phenol, acetone, glucose and glycerol. Determination of acid value, saponification value and iodine value of oils. Determination of fatty acid content, total alkali content and moisture content of soap

UNIT III PURIFICATION OF SOLVENTS AND REAGENTS

45

Purification of liquids by distillation Purification of solids by recrystallisation Determination of melting point Determination of boiling point by capillary method Analysis with thin layer and column chromatographic techniques

UNIT IV ORGANIC PREPARATIONS

45

Preparation of dimethylamino propiophenone hydrochloride by Monnicer reaction. Two-stage preparation of a few organic compounds. Phase transfer catalysis. Synthesis of azo dyes

UNIT V IDENTIFICATION OF ORGANIC COMPOUNDS BY INSTRUMENTAL METHODS 30

UV, IR, NMR, Mass spectroscopy and TGA

TOTAL PERIODS 180

- 1. Daniel R.Palleros, "Experimental Organic Chemistry" John Wiley & Sons, Inc., New York (2001).
- 2. Furniss B.S, Hannaford A.J, Smith P.W.G and .Tatchel A.R., Vogel's Textbook of Practical Organic Chemistry, LBS, Singapore (1994).
- 3. William Horwit, "Official methods of Analysis of the Association of official Analytical Chemists", 13th edition, Washington, D.C. (2004).

COORDINATION CHEMISTRY

LTPC 3 0 0 3

UNIT I COORDINATION COMPOUNDS

9

Nomenclature; coordination geometry and isomerism – structural and stereoisomerisms; absolute configuration – ORD and CD spectra; stability of complexes – successive and overall formation constants - experimental methods – polarography and potentiometry- thermodynamic aspects,

UNIT II THEORIES OF METAL LIGAND BOND

9

Valence bond theory – hybridization; crystal field theory – crystal field splitting, crystal field stabilization energy – thermodynamic, structural, spectral and magnetic characteristics, Jahn-Teller effect, ligand field theory; molecular orbital theory – pi bonding

UNIT III SPECTRA OF COORDINATION COMPOUNDS

9

Spectral characteristics - Free ion terms, transformations in crystal field, energy diagrams in weak and strong field cases – Tanabe-Sugano diagrams, selection rules; magnetic properties – Van Vleck equation, magnetic susceptibility –Guoy and Faraday methods; ESR spectra of transition metal ions.

UNIT IV REACTIONS OF COORDINATION COMPOUNDS

9

Inert and labile complexes; substitution reactions in square-planar and octahedral complexes – factors affecting reactivities; electron transfer reactions- outer sphere and inner sphere mechanisms; photochemical reactions of coordination compounds – substitution, red-ox and rearrangement reactions

UNIT V COMPARATIVE CHEMISTRY OF OXIDATION STATES OF D AND F BLOCK METALS 9

Lanthanides – occurrence, isolation, lanthanide contraction, oxidation states, spectral and magnetic properties, coordination complexes; actinides- configuration, properties; nuclear reactions of uranium, thorium and plutonium- power generation by nuclear reactors, breeder reactor, fusion reaction, radioisotopes and their applications.

TOTAL PERIODS 45

- 1. D.F.Shriver and P.W. Atkins, "Inorganic Chemistry 3rd Edn., Oxford University Press (2004).
- 2. W.L.Jolly, "Modern Inorganic Chemistry", 2nd Edn., Tata McGraw-Hill Pub.Co., (2007).
- 3. J.E. Huheey, E.A. Keiter and R.L. Keiter, "Inorganic Chemistry, 5th Edn., Peasron Education (2005).
- 4. F.A. Cotton, G.Wikinson and P.Gaus, "Basic Inorganic Chemistry", 3rd Edn., John Wiley and Sons (2003).
- 5. F.A.Cotton, G.Wikinson, C.A.Murillo, M.Bochmann, "Advanced Inorganic Chemistry", 6th Edn., John Wiley and Sons (2003).
- 6. G.L.Miessler and D.A.Tarr, "Inorganic Chemistry", 3rd Edn., Pearson Education, (2004).

ORGANIC CHEMISTRY-II

LTPC 3 0 0 3

UNIT I REARRANGEMENTS

10

General mechanistic considerations - nature of migration - migratory aptitude - nucleophilic, electrophilic and free radical rearrangements - Wagner-Meerwein, McLafferty, Demyanov, Benzil-benzilic acid, Favorskii, Fritsch-Buttenberg-Wiechell, Neber, Hofmann, Curtius, Beckmann, Schmidt, Lossen, Wolff, Baeyer-Villiger, Dienone-phenol, Pinacol, Stevens, Wittig, Chapman, Wallach, Orton, Bamberger, Pummerer and von Richter rearrangements.

UNIT II REAGENTS IN ORGANIC SYNTHESIS

11

Diborane - lithium aluminium hydride - sodium borohydride - selenium-di-oxide - osmium tetroxide - phenyl isothiocyanate - N-bromo succinamide (NBS) - lead tetraacetate - dicyclohexylcarbodiimide (DCC) - pyridinium cholorochromate (PCC) - Swern oxidation - p-toluenesulphonyl chloride - trifluoroacetic acid - lithium diisopropylamide (LDA) - 1,3-dithiane (reactive umpolung) - crown ethers - trimethyl silyl iodide - Gilman reagent - dichlorodicyanobenzoquinone (DDQ) - lithium dimethylcuprate - tri-n-butyltin hydride - di-tert-butoxy dicarbonate - dihydropyran - phase transfer catalysts - Wilkinson's catalysts - Peterson synthesis - and diethylaluminium cyanide- IBX and Swern oxidations

UNIT III MULTISTEP SYNTHESIS

7

Concepts in multistep synthesis - strategies for retrosynthetic analysis, synthon and planning - functional group introduction - removal and interconversion - protective groups - hydroxyl, amino, carbonyl and carboxylic acid groups - retrosynthetic analysis - disconnections - synthons - synthetic equivalents - a,d synthons - C-C, C=C bond forming reactions - control of stereochemistry.

UNIT IV HETEROCYCLICS AND ALKALOIDS

9

Synthesis and reactivity of furan, thiophene, pyrrole, thiazole, pyridine, indole and their derivatives, quinoline, isoquinoline, pyrimidine, purine and flavone - Skraup synthesis - Fischer indole synthesis and Pachmann coumarin synthesis - alkaloids - sources and classification - structural elucidation by chemical degradation - total synthesis of quinine, morphine, reserpine, papaverine and nicotine.

UNIT V PROTEINS AND NUCLEIC ACIDS

8

Classification - structure and synthesis of amino acids - peptides - Merrifield solid phase peptide synthesis - structure determination - peptide sequence and synthesis of - primary, secondary, tertiary and quaternary structures- Merrifield solid phase peptide synthesis - nucleic acids - structure and synthesis of DNA - structure and synthesis of RNA-WC Model

TOTAL PERIODS 45

- J. March, Advanced Organic Chemistry, 5th edition, Wiley-Intersciences, New York (2003).
- 2. F.A.Carey and R.J. Sundberg, Advanced Organic Chemistry, Part A and Part B, 5th edition, Plenum Press, New York (2005).
- 3. T.H. Lowry and K.S. Richardson, Mechanism and Theory in Organic Chemistry, 2nd edition, Harper and Row Publishers (1981).
- 4. R.K. Mackie and D.M. Smith, Guide book to Organic Synthesis, 2nd edition, ELBS Publications, London (1998).
- 5. R.K. Mackie and D.M. Smith, Guide book to Organic Synthesis, 2nd edition, ELBS Publications, London (1998).
- 6. R.K. Mackie and D.M. Smith, Guide book to Organic Synthesis, 2nd edition, ELBS Publications, London (1998).
- 7. R.M. Achesen, Chemistry of Heterocyclic Compounds, Wiley Eastern (1973).
- 8. W. Carruthers, Some Modern Methods of Organic Synthesis, 3rd edition, Cambridge University Press (1993).
- 9. B.I. Smith, Organic Synthesis, Chapman and Hall, New York (1980).

PHYSICAL CHEMISTRY II

LTPC 3 0 0 3

UNIT I FOUNDATION TO QUANTUM CHEMISTRY

8

Inadequacy of classical mechanics- black body radiation, photo electric effect, heat capacity of solids- Planck's quantum theory - quantum mechanical operators- Hamiltonian operators, momentum operators, permutation operators — matrix representations —eigen value — eigen function equations.

UNIT II QUANTUM CHEMISTRY OF ATOMS AND MOLECULES

10

Schrodinger wave equation and its solution to a particle in a box, rigid rotor, harmonic oscillators – H-atom solutions – variation method – perturbation method – He atom - SCF & Hartree-Fock method. Born Oppenheimer approximation of H_2^+ and H_2 , Huckel theory of conjugated molecules

UNIT III CATALYSIS 9

Acid – base catalysis – general scheme – Arrhenius complex – Vant Hoff's complex – specific and general catalysis – catalytic constants – Bronsted relationship – Hammett acidity functions – mechanism of acid-base catalysed reaction - catalysis by transition metal ions and their complexes, supported transition metal complexes as catalysts – enzyme catalysis – theory and applications

UNIT IV SURFACE PHENOMENA AND HETEROGENEOUS CATALYSIS 9

Diffusion, adsorption – unimolecular and bimolecular surface reactions- types of - various adsorption isotherms – determination of surface area - pore volume and pore size – thermodynamics of interfaces - solid catalysts – metal - metal oxides, zeolites – geometric factor – electronic factor.

UNIT V SOLID STATE 9

Cyrstallography-optical crystallography, laws of crystal structures, crystal systems, crystal structure, X-Ray crystallography - X-Ray, neutron and electron diffraction, structure and types of crystalline solids, chemical bonding in solids- cohesive energies of solids-

TOTAL PERIODS 45

- 1. P.W.Atkins, and J.D.Paula, Physical Chemistry, 7th edition, Oxford University Press. London (2002).
- 2. G.W. Castellan, Physical Chemistry 3rd Edn. Narosa Publishing House (2004)
- 3. D.A.McQuarrie, Quantum Chemistry, 1st Edn. University Science Books, Mill Valley, California (2003)
- 4. M.W. Hanna, Quantum Mechanics in Chemistry, 3rd edition, Addition Wesley, London (1981).
- 5. J.Rajaram and J.C. Kuriacose, Kinetics and mechanism of chemical transformation, McMillan India Ltd., New Delhi (1993).
- 6. I.N.Levine, Physical Chemistry, Tata McGraw-Hill (2007).
- 7. I.N. Levine, Quantum Chemistry, 5th Edn. Pearson Education (2000).
- 8. A.R.West, Solid State Chemistry and its applications" John Wiley (1984).
- 9. Lesley Smart and Elaine Moore, "Solid State Chemistry an introduction" Chapman and Hall (1992).

AC 9124 INTRODUCTORY PRINCIPLES OF CHEMICAL ENGINEERING

LTPC 3 0 0 3

UNIT I CHEMICAL ENGINEERING CONCEPTS

9

Stoichiometric principles – material and energy balances. Fluid flow – Bernoullis equation and its applications – pipes and fittings – Industrial pumps – flow through equipments.

UNIT II HEAT AND MASS TRANSFER

9

Fouriers law – simple numerical problems on conduction – natural and forced convection – heat transfer equipment –Drying - Different types of dryers-Distillation – vapour liquid equilibria –distillation methods – continuous rectification of binary systems – design method for theoretical plates – HETP concepts.

UNIT III MASS TRANSFER OPERATIONS

9

Adsorption and adsorption principles—equilibrium relationships—methods of calculation — various types of equipments. Extraction—liquid extraction—ternary diagram—selection of solvent and equipment—method of calculation for co-current and counter-current extraction operations Crystallization — types of crystallization equipment — material and energy balances.

UNIT IV MECHANICAL OPERATIONS

9

Laws of crushing – closed and open circuit grinding – various types of crushers and grinders – settling, floatation and filtration concepts.

UNIT V UNIT PROCESSES

9

Nitration, sulphonation, halogenation, esterification, amination, saponification and hydrogenation, role of the above unit processes in such industries as petroleum, drugs, pharmaceuticals and organic synthesis

TOTAL PERIODS 45

- 1. W.I.Badger and I.T.Banchero Introduction to Chemical Engineering, McGraw Hill Book co., Inc., Kogakusha, 1988.
- 2. W.L.McCabe, J.C.Smith and P. Harriot, Unit Operations of Chemical Engineering, 6th Edition, McGraw Hill Book Co.2001.
- 3. P.H.Groggins, Unit Processes in Organic Synthesis, McGraw Hill Book Co., Kogakusha. 1984.
- 4. J.H.Perry, Handbook of Chemical Engineers, McGraw Hill Book Co.2002.

INORGANIC CHEMISTRY PRATICALS AC 9125 LTP C 0 0 12 6 UNIT I QUANTITATIVE INORGANIC ANALYSIS 36 (i) Ores: oxides and carbonate ores (ii) Alloys: ferrous and nonferrous alloys-brass and solder (iii) Spectrophotometry- estimation of copper, nickel, iron and manganese **UNIT II ESTIMATION OF INDUSTRIAL PRODUCTS** 36 (i) Active CaO in lime (ii) Chlorine in bleaching powder (iii) Analysis of cement -silica, mixed oxide - Fe₂O₃, Al₂O₃ & CaO/MgO (iv) Lead content in red lead (v) BaSO₄ in lithophone. **UNIT III WATER ANALYSIS** 36 (i) total dissolved solids (ii) carbonate and non-carbonate hardness by EDTA (iii) Dissolved oxygen, BOD, COD (iv) Alkalinity (v) F, Cl, SO₄²⁻, Fe³⁺ (vi) Turbidity UNIT IV PREPARATION OF TYPICAL INORGANIC COMPLEXES 36 UNIT V QUALITATIVE INORGANIC SEMI-MICRO ANALYSIS 36 Detection of atleast four cations (2 common and 2 uncommon) in a mixture of salts.

TOTAL PERIODS 180

- 1. G.H.Jeffery, J.Bassett, J.Mendham and R.C.Denney Vogel's ext book of quantitatives chemical analysis, ELBS 5th Edn. Longman, Singapoor Publishers, Singapore, 1996.
- R. Mukhopodhyay, P.Chatterjee, "Advanced practical Chemistry"
 Dinesh Sharma, "A hand book of Analytical Inorganic chemistry", First Published (2004).
- 4. I.M.Kolthoff, E.B.Sandell et.al. Quantitative chemical analysis, Macmillan, Madras 1980

ADVANCED INORGANIC CHEMISTRY

LTPC 3 0 0 3

UNIT I ORGANOMETALLIC COMPOUNDS

9

18 electron rule: metal carbonyls, metal nitrosyls, metal alkyl and aryl and aryl complexes; preparation, structure, bonding, stereochemical non-rigidity; Metal – alkene, alkyne and allyl complexes, cyclopentadiene and benzene complexes – preparation, structure and bonding; catalysis by organometallic compounds-hydrogenation, hydroformylation, stereoregular polymerization, Wacker process.

UNIT II BIO-INORGANIC CHEMISTRY

9

Metals and non-metals in biological systems; metal ion transport; oxygen carriers-haemoglobin, myoglobin; metallo-enzymes – carboxypeptidase A, carbonic anhydrase, vitamins B_{12} , nitrogenase; eletron transfer and redox systems; photosynthesis.

UNIT III BONDING AND MOLECULAR POLYHEDRA IN INORGANIC SOLIDS 9

Boranes, borazines, silicates, phosphorous-nitrogen, sulphur-nitrogen compounds, metal atom clusters; inert gas compounds.

UNIT IV INORGANIC SOLID STATE

9

Preparation of non-molecular solids; band theory of solids; defects and non-stoichiometry, electrical and magnetic properties, superconductivity, amorphous solids, nanosolids.

UNIT V PHOTOCHEMISTRY

9

Photophysical processes, spontaneous and stimulated emission of radiation, chemical actinometry, solar energy conversion and applications.

TOTAL PERIODS 45

- 1. F.A.Cotton, G.Wilkinson and P.Gaus Basic Inorganic Chemistry, 3rd Edn. John Wiley and Sons (2003)
- 2. D.F.Shriver and P.W.Atkins Inorganic chemistry 3rd Edn. Oxford University Press (2004)
- 3. J.E. Huheey, E.A. Keiter and R.L. Keiter, Inorganic Chemistry, 5th Edn. Pearson Education (2005)
- 4. W.L.Jolly, Modern Inorganic Chemistry, 2nd Edn., Tata McGraw-Hill Pub.Co. (2007).

ORGANIC CHEMISTRY III

LTPC 3 0 0 3

UNIT I PHOTOCHEMISTRY AND AROMATICITY

9

Photochemistry –Jablonski diagram – photochemistry of olefins and carbonyl compounds - photo oxidation and reduction, cis – trans isomerism, Paterno – Buchi , Barton, Norrish type I and II reactions, di-pi- methane rearrangement. Aromaticity-concept – Huckel and Craig rules – NMR and X – ray diffraction as a tool – diatropy and paratropy. Aromatic and anti aromatic compounds. Benzenoid, non-benzenoid and homo aromatic compounds. Alternant and nonalternant hydrocarbons. Annulenes (discussion of spectral data) - Aromaticity in ferrocenes, fullerenes, heterocyclic rings and charged ring systems.

UNIT II PERICYCLIC REACTIONS

12

Definition-electrocyclic, cycloaddition, sigmatropic and ene reactions. Woodward – Hoffmann rules – Frontier orbital, Mobius- Huckel and orbital symmetry correlation approaches. Stereospecificity and regiospecificity of pericyclic reactions - pericyclic reactions in organic synthesis. Diels –Alder reaction, 1,3 dipolar cycloaddition, Claisen, Cope, chelotropic reactions. Fluxional molecules.

UNIT III TERPENOIDS

7

Classification – isolation of terpenes – isoprene rule, methods of structural elucidation. Synthesis and structure of α -Terpeniol, Camphor, car – 3 – ene, , zingiberene, santonin, abietic acid and β - caryophyllene.

UNIT IV STEROIDS

8

Structural elucidation and stereochemistry of cholesterol, ergosterol, estrone, testosterone, progesterone, and cortisone, bile acids and prostaglandins.

UNIT V VITAMINS

9

Structure and synthesis of vitamins A, B₁, B₂, B₆, C, D, E and K

TOTAL PERIODS 45

- 1. Jerry March, Advanced Organic Chemistry, -Reactions, Mechanisms and Structure 5th edition, Wiley Inter Science, New York, 2003.
- 2. Francis A. Carey and Richard J. Sundberg, Advanced Organic Chemistry, Part A & B, 6rd Edition, Plenum Press, New York, 2007.
- 3. I.Fleming, Frontier Orbitals and Organic Chemical Reactions, Wiley, 1976.
- 4. T.H. Lowry and K.S.Richardson, Mechanism and Theory in Organic Chemistry, 2nd edition, Harper and Row, 1981.
- 5. S.Sankararaman, Pericyclic Reactions A Textbook: Reactions, Applications and Theory, 1st Edition, Wiley-VCH, Weinheim, 2005.
- 6. I.L. Finar, Organic Chemistry, Vol. II, 6th Edition, 9th Indian reprint, ELBS Longman Group Ltd., London, 2004

PHYSICAL CHEMISTRY III

LTP C 3 0 0 3

UNIT I KINETICS 9

Methods of determining rate laws – reversible, consecutive and competing reactions – theory of absolute reaction rates – transmission coefficient – quantum mechanical tunneling – thermodynamic formulation of reaction rates – kinetics – classical treatment – stochastic methods, principle of microscopic reversibility.

UNIT II MECHANISM OF GAS PHASE REACTIONS

12

Lindeman's theory - Hinshelwood, Kassel and Slater treatments - abnormal frequencies - ortho-para conversions - explosion limits - reaction rates in solution - effect of dielectric constant and ionic strength - kinetic isotope effect - linear free energy relationships - Hammett equation - Taft equation - fast reactions - study of kinetics by stopped flow techniques - flash photolysis - shock tubes.

UNIT III STATISTICAL THERMODYNAMICS

8

Objectives of statistical thermodynamics – probability – microstates and macrostates for distinguishable and indistinguishable particles – permutation and combinations – Maxwell – Boltzmann statistics - use of partition function for obtaining thermodynamic functions, entropy and third law.

UNIT IV QUANTUM STATISTICS

7

Molar partition functions – evaluation of translational, rotational, vibrational and electronic partition functions – rotational heat capacity for the hydrogen molecule. Quantum statistics – Fermi - Dirac and Bose – Einstein statistics

UNIT V NON-EQUILIBRIUM THERMODYNAMICS

9

Steady state – conservation of energy and mass-entropy production and entropy flow in open system – fluxes and forces – transformation of properties of rates and affinity – microscopic reversibility and Onsager reciprocal relation, thermokinetic effect.

TOTAL PERIODS 45

- 1. K.J.Laidler, Chemical Kinetics, Pearson, 3rd edition, New Delhi 2004.
- 2. J. Rajaram and J.C. Kuriacose, Kinetics and Mechanism of Chemical Transformation, Macmillan India Ltd., 1993
- 3. J.C. Kuriacose and J.Rajaram, Thermodynamics for students of Chemistry 3rd Edn. Shoban Lal Nagin Chand and Co. 1999.
- 4. L.K. Nash and Addison, Elements of Statistical Thermodynamics, Wiley Pub Co. 1971
- 5. M.C. Gupta, Statistical Thermodynamics, Wiley Eastern, New Delhi 1990
- 6. F.W. Sears and G.L. Salinger, Thermodynamics, Kinetic theory and Statistical Thermodynamics 3rd Edn. Narosa Publishing House, New Delhi 1998

MOLECULAR SPECTROSCOPY

LTPC 3 0 0 3

UNIT I ELECTROMAGNETIC RADIATION AND ROTATIONAL SPECTROSCOPY

9

Characterization of electromagnetic radiation – regions of the spectrum-basic elements of practical spectroscopy—enhancement of spectra – Microwave spectroscopy – rotational spectra of molecules – applications.

UNIT II ABSORPTION SPECTROSCOPY

12

Applications of group theory, Infra-red spectroscopy - harmonic and anharmonic vibrations -dissociation energy of diatoms- vibrating rotator - PQR branches in IR spectra - Fermi resonance - Raman spectroscopy - mutual exclusion principle - UV-vis spectroscopy - electronic transitions - solvent effects - Woodward's rule.

UNIT III SPIN RESONANCE SPECTROSCOPY

12

Proton magnetic resonance spectroscopy – relaxation processes – chemical shift – coupling – simplification of complex NMR spectra – 13 C NMR spectra - Electron spin resonance spectroscopy – hyperfine interactions.

UNIT IV MASS SPECTROMETRY

7

Reactions of ions in gas phase – effect of isotopes – nitrogen rule - determination of molecular formula - fragmentations and rearrangements - metastable ions – fragmentation of organic compounds.

UNIT V MOSSBAUER SPECTROSCOPY

5

Mossbauer nuclei – Doppler effect – isomer shift – quadrupole splitting – magnetic hyperfine interactions.

TOTAL PERIODS 45

- 1. C.N.Banwell and E.M.McCash, Fundamentals of molecular spectroscopy, 5th Edn., Tata McGraw Hill, New Delhi,2002.
- 2. D.L.Pavia, G.M.Lampman and G.S.Kriz, Introduction to spectroscopy, 3rd Edn. Cole Pub, Singapore, 2001.
- 3. W.Kemp, Organic Spectroscopy, 3rd Edn, ELBS, McMillan, London, 2004.
- 4. R.Drago, Physical methods for chemists, Saunders, Philadelphia, 1992.
- 5. D.H.Williams and I.Fleming, Spectroscopic methods in organic chemistry, 4th Edn, McGraw Hill, New York, 1989.
- 6. D.Pasto, C.Johnson and M.Miller, Experiments and techniques in organic chemistry Prentice- Hall Inc., New Jersey, 1992.
- 7. G.Aruldhas, "Molecular structure and spectroscopy", 2nd Edn.,Printice –hall of India (2007)

PHYSICAL CHEMISTRY PRACTICALS

LTPC 00126

UNIT I CONDUCTOMETRY

20

Equivalent conductance of strong electrolytes and verification of Debye-Huckel-Onsager equation. Degree of hydrolysis of aniline hydrochloride. Basicity of an acid. Verification of Ostwald dilution law using weak acid and determination of its dissociation constant. Conductometric titrations — acid- base, mixed acid-base, precipitation titrations.

UNIT II POTENTIOMETRY AND PH-METRY

20

Emf measurement - Potentiometric titrations - red-ox and precipitation titrations; pH measurement, pH-metric titrations - acid-base reactions

UNIT III KINETICS 20

Determination of order - acetone-iodine reaction; Determination of rate constantsaponification of ethyl acetate; Study of primary salt effect on the kinetics of ionic reaction

UNIT IV HETEROGENEOUS EQUILIBRIA

20

Determination of CST in phenol-water system; Phase diagram of a ternary systemnitrobenzene-acetic acid-water or water- acetic acid-chloroform. Two component solid solutions – eutectic formation

UNIT V THERMODYNAMICS

20

Temperature dependence of solubility of benzoic acid in water and DMSO – water and calculation of partial molar heat of solution. Activity coefficients of weak or strong electrolyte by solubility method. Determination of activity coefficients of an electrolyte at different molalities.

UNIT VI SPECTROPHOTOMETRIC AND FLAME PHOTOMETRIC METHODS 20

Determination of molar absorptivity – verification of Beer-Lambert equation – Simultaneous estimation of Mn and Cr in solutions containing KMnO₄ and K₂Cr₂O₇. Photometric titration of Fe(III) by EDTA; Estimation of Na/K by flame photometer.

UNIT VII POLAROGRAPHY

20

Determination of half-wave potential – quantitative estimation of Cd/Zn Determination of Pb²⁺ and SO₄²⁻ by amperometric titration

UNIT VIII OPTICAL METHODS

20

Polarimetry - Determination of sucrose content in cane sugar / cane juice Kinetics of hydrolysis of sucrose - effect of acid strength. Abbe's refractometer- Percentage composition of binary mixtures

Verification of Freundich isotherm – adsorption of acetic acid, oxalic acid on carbon–, Relative and absolute viscosities - Molecular weight of a polymer by viscometry Demonstration experiments-TGA and DTA, Atomic absorption spectrometry, G.C, HPLC, TOC analyser, FT-IR spectrophotometer, X-Ray Diffraction and GPC

TOTAL PERIODS 180

- 1. Khosla, A.Gulnti and V.C. Garg, Senior Practical Physical Chemistry, 7th Edn. S.Chand & Co., New Delhi 1994.
- 2. D.R.Satiya, Practical Chemistry, 2nd Edn. Allied Publishers, Madras 1991
- 3. V.D. Athawale and P. Mathur, Experimental Physical Chemistry, New Age International Publishers 2001
- 4. B. Viswanathan and P.S. Ragavan, Practical Physical Chemistry, 1st Edn. Viva Books (P) Ltd., Chennai 2005

ORGANIC CHEMICAL TECHNOLOGY

LTPC 3003

UNIT I BASIC PRINCIPLES OF CHEMICAL TECHNOLOGY

9

Classification of chemical technological processes – chemical equilibrium in technological processes - rates of technological processes – designing and modeling chemical technological processes and reactors .

UNIT II INDUSTRIAL ORGANIC SYNTHESIS

9

Raw materials - manufacture of methyl alcohol, ethyl alcohol, ethylene, 1,3-butadiene, acetylene - ethyl benzene, cumene, linear alkyl benzenes alkyl phenols.

UNIT III SYNTHETIC ORGANIC CHEMICALS

9

Chemicals derived from ethylene – polyethylene, ethylene oxide, ethylene dichloride chlorinated hydrocarbons – chemicals derived from propylene – isopropyl alcohol, polypropylene, acrylonitrile, propylene oxide – oxidation of butane – esters – maleic anhydride - acetone- ethyl methyl ketone - bisphenol - DDT - aniline.

UNIT IV PHARMACEUTICALS AND PESTICIDES

9

Introduction – manufacture - aspirin, phenobarbital, penicillin – malathion, parathion, naled.

UNIT V DYES 9

Classification - raw materials - intermediates - manufacture - azodyes - triphenylmethane dyes - xanthene dyes. Indigoid and thioindigoid dyes, sulphur dyes, phthalocyanines - optical brighteners.

TOTAL PERIODS 45

- 1. P.H. Groggins, Unit Processes in Organic Synthesis, McGraw Hill Book Co., Kogakusha (1984).
- 2. Peter Wiseman, An Introduction to Industrial Organic Chemistry, 2nd Edition, Applied science publishers Ltd., London (1979).
- 3. J.A. Kent, Riegel's Hand book of Industrial Chemistry, 7th Edn, Van Nostrand Reinhold Co., New York (1974).

INORGANIC CHEMICAL TECHNOLOGY

LTPC 3 003

UNIT I FUEL AND INDUSTRIAL GASSES

q

Fuel and industrial gases – production and uses of producer gas, water gas, coke oven gas, acetylene, natural gas, LPG: Liquefaction of gases– noble gases, carbon dioxide, hydrogen, oxygen, nitrogen.

UNIT II HEAVY CHEMICALS

9

Chloralkali industry – soda ash, caustic soda, chlorine: Chemicals from sea- sodium chloride, magnesium chloride, bromine

UNIT III ACIDS AND FERTILIZERS

9

Sulphur and sulphuric acid – nitric acid – ammonia –nitrogenous fertilizers – phosphorus – phosphoric acid – phosphatic fertilizers – potassic fertilizers

UNIT IV SILICATE INDUSTRIES

9

Silicate industries - refractories - abrasives - ceramics - glass - cement, lime, gypsum

UNIT V PRINCIPLES OF METALLURGICAL PROCESSES

9

Principles of metallurgical processes – ore beneficiation pyrometallurgy, hydrometallurgy powder metallurgy, electrometallurgy: Explosives and propellants: Nuclear materials.

TOTAL PERIODS 45

- 1. B. Norris Shreve and Joseph A.Brink, Chemical Process Industries,. McGraw Hill, Kogakusha Ltd. (1991).
- 2. Dryden's outlines of Chemical Technology, (Ed) M.Gopala Rao and Marshall Sitty Affliated East West Press Pvt. Ltd. (1992).
- 3. B.K. Sharma Industrial Chemistry, GOEL Publishing House (1991)
- 4. Riegel's Industrial Chemistry, edited by James A. Kent, Asia Publishing House (1989).

POLYMER CHEMISTRY

LTPC 3 003

UNIT I BASIC CONCEPTS OF POLYMERS

11

Basic concepts of polymers – classification of polymers – oranic and inorganic polymers.- classification based on occurrence, end use, thermal properties and structure. Tacticity and its determination using ¹H NMR. Crystalline and amorphous polymers – Factors affecting crystallinity and crystallisability. Effect of crystallinity on properties- Glass transition temperature and its determination.- thermal transitions-dialatometer-variation of specific volume of polymers with temperature- Factors affecting glass transition temperature.

UNIT II CHAIN POLYMERISATION

9

Kinetics and mechanism of free radical, cationic and anionic polymerization Trommsdorff's effect – chain transfer reactions and constants – living polymers – alfin catalysts — coordination polymerisation -Ziegler-Natta catalysts-iniferters -Atom transfer radical polymerization.

UNIT III STEP GROWTH POLYMERSIATION

9

Kinetics of polycondensation reactions – copolymerization – co-polymer equation – copolymer compositions from ¹H-NMR, FT-IR, UV spectra and chemical methods – Monomer reactivity ratios- Mayo-Lewis and Fineman-Ross methods- significance of reactivity ratios-Sequence length–Metathetical, Group transfer, Electrochemical and Ring-opening polymerisation

UNIT IV POLYMERISATION TECHNIQUES

6

Polymerisation techniques— homogeneous and heterogeneous polymerisation — bulk (liquid, gas and solid monomers), solution, suspension and emulsion polymerisation—merits and demerits—interfacial, and melt polycondensation.

UNIT V MOLECULAR WEIGHT AND ITS DISTRIBUTION

10

Number, weight and viscosity average molecular weights of polymers— determination of constants in Mark Houwink's equation. Poly dispersity index and molecular weight distribution — Molecular weight determination by GPC and viscometry; Polymer dissolution, thermodynamics of polymer dissolution —solubility parameter — Fractionation of polymers-fractional precipitation and fractional dissolution methods.

TOTAL PERIODS 45

- 1. V.R.Gowarikar, N.V.Viswanathan and Jayadev Sreedhar, Polymer Science, Wiley Eastern Limited, Madras (2006).
- 2. F.N. Billmayer, Text Book of polymer Science, 3rd Edn. John Wiley & Sons, New York (2002).
- 3. George Odian, Principles of Polymerisation, 3rd Edn, McGraw Hill Book Company, New York (2003).
- 4. M.S.Bhatnagar, "A Text Book of Polymers (chemistry and Technology of
- 5. polymers), Vol I, II & III, 1st Edn., S.Chand and Company, New Delhi (2007). R.S. Young, Introduction to Polymers, Chapman and Hall Ltd., London (1999).

POLYMER TECHNOLOGY

LTP C 3 0 0 3

UNIT I POLYMERIC MATERIALS

9

Introduction – classification – thermoplastics - cellulose derivatives - LDPE, HDPE, PVC, PMMA, PTFE, PET, Nylons – thermosetting resins – phenolic resins, epoxy resins, silicones, polyurethanes – polymer blends and alloys reinforced plastics

UNIT II ELASTOMERS

9

Natural rubber – processing – vulcanization – synthetic rubber – SBR, neoprene, butyl, thiocol rubber – thermoplastic elastomers – high performance polymers – polyethers – PEEK, polysulphones, polyimides.

UNIT III MOULDING TECHNIQUES

9

Moulding constituents – functions –moulding techniques – compression – injection - extrusion – blow moulding – thermoforming – vacuum forming – pultrusion – casting – calendering – RIM – lamination

UNIT IV CHARACTERISATION AND TESTING

9

Characterisation of polymers by IR and NMR – Thermal properties by TGA and DSC, Testing tensile strength, Izod impact, Compressive strength, Rockwell hardness, Vicot softening point. Test for electrical resistance, dielectric constant, dissipation factor, arc resistance and dielectric strength – water absorption.

UNIT V POLYMER PROPERTIES

9

Effect of structure on mechanical, chemical, thermal, electrical and optical properties.

TOTAL PERIODS 45

- 1. Michael L. Berins, Plastics Engineering hand book, 5th Edn. Chapman & Hall, New York (1991).
- 2. Jacqueline.I. Kroschwitz, Concise Encyclopedia of Polymer Science and Engineering, John Wiley & sons, New York (1998).
- 3. R.W.Iyson, Specialty Polymers, Blackie Academic & Professional, London (1992).
- 4. Mourice Morton, Rubber Technology, Van Nostrand, Reinhold, New York (1987).

TEXTILE CHEMISTRY

LTPC 3 0 0 3

UNIT I PROPERTIES OF TEXTILE MATERIALS

10

Classification of textile fibres – chemical structure, physical and chemical properties of textile fibers – cotton, wool, silk, viscose, rayon, synthetic fibres.

UNIT II PREPARATORY PROCESSES

10

Brief outline on desizing, singeing and mercerisation, scouring – bleaching with hypochlorites and peroxides.

UNIT III DYEING 15

Theory of colours – dye chemistry - preparation of simple dyes and intermediates. Introduction to theory of dyeing. Application of direct, vat , azoic, reactive, sulphur, disperse and acid dyes and mineral colours.

UNIT IV PRINTING 5

Stages involved in printing –printing paste ingredients, styles and methods of printing. Outline on printing of cotton fabrics with reactive dyes, polyester fabrics with disperse dyes.

UNIT V FINISHING 5

Classification – calendering, crease proofing and shrink proofing.

TOTAL PERIODS 45

- 1. R.Trotman, Dyeing and Chemical Technology of Textile Fibres, Charles Griffin and Co., Ltd., London (1985).
- 2. V.A. Shenai, Technology of Textile Processing, Vol II, IV and V, Sevak Publications, Bombay (1976).
- 3. F. Sadov, M.Korchagin and A.Matetsky, Chemical Technology of Fibrous Materials, Mir Publishers, Moscow (1978).
- 4. J.T. Marsh, Textile Science An Introductory Manual, B.I. Publications (1979).
- 5. J.T. Marsh, An Introduction to Textile Finishing, B.I. Publications, New Delhi (1979).

TEXTILE PROCESSING

LTPC 3 0 0 3

UNIT I PREPARATORY PROCESSES

7

Preparation to colouration and finishing of natural, manmade fibres and their blends – desizing, singeing, scouring, mercerizing and bleaching.

UNIT II DYEING 11

Theory of dyeing fundamentals involved in the theory of dyeing. Dyeing of various textile fibres and their blends – dyeing of coton, wool, silk and man made fibres with direct, acid, basic, reactive, sulphur, vat, aryo, disperse dyes and other speical dyes

UNIT III MACHINERY FOR PREPARATION AND DYEING

10

Machines used for preparation and dyeing processes- singeing, mercerizing, scouring machines - bleaching ranges dyeing machines - jigger, winch padding ranges, HTHP machines, jet dyeing machines and overflow dyeing machines

UNIT IV PRINTING & MACHINERIES

10

Printing – methods and styles – direct, discharge and resist styles, block, roller and screen printing –transfer printing. Printing of various classes of dyes and pigments – printing of natural and synthetic materials with direct, reactive, disperse and other dyes – pigment printing. Printing machinery and post printing operations – roller printing machinery, hand, flat and rotatory screen printing machines – transfer printing machine – dryers, steamers, curing chambers and washing ranges.

UNIT V FINISHING 7

Finishing of textile materials – scutching, calendering, starching, creeping, antishrinking, crease-proofing, wool-finishing and other finishes.

TOTAL PERIODS 45

- 1. R.H. Peters, "Textile Chemistry, Vol II. Impurities in Fibers and Purification of Fibers", Elsevier Pub. (1975).
- 2. E.R. Trotman, "Textile Scouring and Bleaching", Griffins Pub. (1968).
- 3. R.R. Chakravarthy and S.S.Trivedi, "Technology of Bleaching and Dyeing of Textile Fibres", Vol.I mahajan Bros. (1979).
- 4. J.T. Marsh, "Textile Finishing", B.I. Publications (1979).
- 5. V.A. Sheni, "Technology of Textile Processing", Vol.II, 'Textile Printing', Sevak Pub. (1976).

ENVIRONMENTAL CHEMISTRY

LTPC 3 0 0 3

UNIT I CHEMISTRY AND THE ENVIRONMENT

7

Chemistry and the environment - environmental pollution - causes - pollutants - air pollution - effects of air pollution: Environmental fate of pollutants - transformation process - bio concentration - fate of air, water and soil pollutants

UNIT II BIOLOGICAL ACTIVITY

11

Biological activity - biodegradation of carbohydrates, proteins, fats and oil, detergents, pesticides; Metabolic fate of pollutants - adsorption - distribution - metabolism - excretion.

UNIT III TOXIC EFFECTS OF POLLUTANTS

9

Toxic effects of pollutants - toxicity - carcinogenicity - mutagenecity- teratogenicity - biochemical effects of arsenic, cadmium, lead, mercury, carbon monoxide, nitrogen oxides, sulphur dioxide, ozone and pan, cyanide, pesticides, asbestos

UNIT IV WATER POLLUTION

10

Water pollution - water quality parameters - turbidity, colour, pH, acidity, alkalinity, solids, hardness, chlorides, residual chlorine, sulphates, fluorides, phosphates, iron and manganese, DO, BOD, COD, nitrogen, grease, volatile acids, gas analysis.

UNIT V POLLUTION AND WASTEWATER TREATMENT

10

Soil pollution - noise pollution - thermal pollution; Wastewater treatment - volume reduction - strength reduction - neutralisation - equalisation - proportioning - primary and secondary treatment - solid waste disposal.

TOTAL PERIODS 45

- 1. AK De Environmental chemistry, Wiley Eastern Ltd., Madras (1994).
- 2. M. S. Sethi Environmental chemistry, Shri Sai Printographers, New Delhi (1994).
- 3. Clair N. Sawyer, Perry L. Mc Carty and G. F. Parkin Chemistry for Environmental Engineering, McGraw Hill Inc. New York (1994).
- 4. Standard methods for the examination of water and wastewater, American Public Health Association, Washington DC (1998).
- 5. Metcalf & Eddy Wastewater engineering: Treatment, Disposal and Reuse, McGraw Hill Inc. New York (1991).

WATER AND WASTEWATER TREATMENT

LTPC 3003

9

UNIT I REQUIREMENTS OF WATER AND PRELIMINARY TREATMENT

Requirements of water – quality standards for drinking water – object of water treatment – conventional treatment – turbidity removal – cause of turbidity – coagulation – common coagulants – theory of coagulation – mixing basins – flocculation – principle and design of flocculators – sedimentation – settling tanks – settling velocity – surface loading rate – efficiency of settling tanks – sludge removal mechanism.

UNIT II INDUSTRIAL WATER TREATMENT

9

Filteration – size and shape characteristics of filtering media – sand filters hydraulics of filteration – design considerations – radial, upflow, highrateand multimedia filters, pressure filter. Water softening – lime soda, zeolite and demi mineralisation processes – industrial water treatment for boilers.

UNIT III TREATMENT METHODS

9

Taste and odour control – adsorption – activated carbon treatment – removal of colour – iron and manganese removal – aeration, oxidation, ion exchange and other methods – effects of fluorides – fluoridation and defluoridation –desalination – corrosion prevention and control – factors influencing corrosion – Langelier index – corrosion control measures.

UNIT IV WASTEWATER TREATMENT

9

Wastewater treatment – pre and primary treatment – equalization neutralisation – screening and grid removal – sedimentation – oil separation gas stripping of volatile organics – biological oxidation – lagoons and stabilisation basins – aerated lagoons – activated sludge process – trickling filtration – anaerobic decomposition.

UNIT V ADSORPTION AND OXIDATION PROCESSES

9

chemical process – adsorption – theory of adsorption – ion exchange process – chemical oxidation – advanced oxidation process – sludge handling and disposal – miscellaneous treatment processes.

TOTAL PERIODS 45

- W. Wesley Eckenfelder, Jr. Industrial water pollution control, 2nd Edn., McGraw Hill Inc. (1989).
- 2. Metcalf & Eddy Wastewater engineering, 3rd ed., McGraw Hill Inc. (1991).
- 3. C.S. Rao Environmental pollution control engineering, Wiley Eastern Ltd. (1994).
- 4. S.P. Mahajan Pollution control in process industries, Tata McGraw Hill Publishing Company Ltd. (1994).
- 5. Howard S. Peavy, Donald R. Rowe and George Tchobanoglous Environmental Engineering, McGraw-Hill Inc. (1985).

AC 9159 SOLID WASTE MANAGEMENT AND AIR POLLUTION

LTPC 3 0 0 3

9

UNIT I SOLID WASTE

Solid waste - definition - characteristics - perspectives - types of solid waste - sources - properties of solid waste - physical and chemical composition - changes in composition - solid waste management-materials flow - reduction in raw materials usages and solid waste quantities - reuse of solid waste materials

UNIT II SOLID WASTE COLLECTION AND DISPOSAL

9

Solid waste generation - on-site handling, storage and processing-collection of solid waste-transfer and transport-processing techniques - ultimate disposal

UNIT III ENERGY RECOVERY

9

Energy recovery - processing techniques-materials recovery systems - recovery of biological conversion products and thermal conversion products - materials and energy recovery system

UNIT IV AIR POLLUTION

9

Air pollution - global implication of air pollution-units of measurement - sources of pollutants - classification of pollutants - meteorology and natural purification processes - influence of meteorological phenomena on air quality-effects on man and vegetation. Effects of pollutants on human beings, animals, vegetation, buildings and materials

UNIT V ANALYSIS AND CONTROL DEVICES

9

Sampling and analysis - particulates and gaseous pollutants - methods for monitoring air pollutants - air quality control devices for particulate and gaseous contaminants-major polluting industries - measures to check industrial pollution.

TOTAL PERIODS 45

- 1. Howard S. Reavy, Donald R. Rowe & George Technobanoglous-Environmental Engineering, McGraw-Hill Inc.(1985).
- 2. Gilbut M.Masters Introduction to environmental engineering and science, Prentice-Hall of India Pvt. Ltd. (1991)
- 3. S.K. Garg Sewage disposal and air pollution engineering, Khanna publishers, (1990).
- 4. V.P.Kudesia Air pollution, Pragati Prakashan publishers, (1992).
- 5. M.N. Rao and H.V.N Rao Air pollution, Tata McGraw Hill publishing company Ltd., (1994).

INDUSTRIAL ELECTROCHEMISTRY

LTPC 3 0 0 3

UNIT I CHLORALKALI INDUSTRY

8

General concepts of brine electrolysis – modern technological developments – chlorine cell technologies – mercury and diaphragm cell – membrane cell

UNIT II ELECTROMETALLURGY

8

Metal extraction and refining – electrowinning – aluminum extraction – manufacture of sodium, lithium and magnesium – hydrometallurgical processes – electrorefining – aqueous and molten salt electro refining

UNIT III METAL FINISHING

12

Pretreatment – conversion coatings – phosphating – types –methods – properties and influencing factors – evaluation and testing – applications – anodizing – principle – applications. Electroplating – objectives – theory – method – electroplating of nickel (only) – electroless plating – galvanizing – tinning

UNIT IV ELECTROSYNTHESIS

9

Electrolytic preparation of inorganic compounds – fluorine – peracids and their salts – $KMnO_4$ -- $K_2Cr_2O_7$. organic electrosynthesis – hydromerisation of acrylonitrile – Monsanto process – Manufacture of ethylene glycol – electrolysis of organic compounds with the use of ion – exchange membranes.

UNIT V INDUSTRIAL ELECTROCHEMICAL PROCESSES

8

Water treatment and environmental protection – metal ion removal and metal recovery – electro-filtration of particulates from gases – electrodialysis – desalination – electroflotation

TOTAL PERIODS 45

- 1. P.H. Rieger, Electrochemistry, Prentice Hall, Inc, New York (1987).
- 2. D Fletcher, Industrial electrochemistry, Chapman and Hall, London (1982).
- 3. J.Bockris and A.K.M.Reddy, "Modern electrochemistry, Vol.II, Mac Donold, London (1970).
- 4. C.Rajagopal and K. Vasu, Conversion Coatings, 1st Edn. Tata McGraw Hill, New Delhi (2000).

CORROSION AND CORROSION CONTROL

L TPC 3 0 0 3

UNIT I CORROSION

Ç

Causes and effects of corrosion – theories of corrosion - oxidation - direct atmospheric effect – electrochemical corrosion – hydrogen evolution- presence and absence of oxygen – corrosion by gaseous reduction.

UNIT II FORMS OF CORROSION

9

Galvanic bimetal corrosion – differential aeration corrosion – concentration cell corrosion – erosion corrosion – pitting corrosion – underground soil corrosion – intergranular corrosion - stress corrosion - seasonal cracking of alloys – caustic embrittlement – corrosion fatigue

UNIT III CORROSION TESTING

8

Rate of corrosion – calculation of ΔG and other related thermodynamic parameters – potential measurement - electrochemical series – redox reactions – emf measurement and corrosion current - anodic and cathodic behaviour of metals – passivity – testing of virgin metals – alloy – Pourbaix and Evans diagrams.

UNIT IV FACTORS INFLUENCING CORROSION

9

Nature of metal – overvoltage – areas of anodic / cathodic – purity of metal - physical state of metals – passive nature of metal – solubility – volatility of corrosion products – corroding environment – influence of pH – ions – formations of cells – polarization of electrodes.

UNIT V CORROSION CONTROL

10

Design – selection of materials – pure metals and alloys – annealing – elimination of galvanic action – cathodic protection – sacrificial anodic protection – impressed current cathodic protection – modification of environment – deaeration – dehumidification – inhibitors - protective coatings - preparation of materials for coating – metallic and non metallic – organic coatings – special paints – varnish, enamel and lacquers.

TOTAL PERIODS 45

- 1. M.G. Fontana and N.G.Green, Corrosion Engineering, McGraw Hill Book Company, New York (1984).
- 2. J.H.Brophy, R.M. Rose and J.Walf, The structure and properties of materials Wiley Inter Science Inc., New York (1984).
- 3. B.T. Kelly, Irradiation diamagneto solids, Pergamon Press, New York (1992).
- 4. D.R.Cross, Principles and application of electrochemistry, Chapman and Hall, U.K, (1988).

AC 9162 CHEMICAL PROCESS EQUIPMENT AND INSTRUMENTATION

LTPC 3 0 0 3

UNIT I CHEMICAL REACTOR

9

Chemical reactors – Batch reactor – Flow reactor – Fixed bed, Fluidised bed and slurry reactor – fluid moving machinery – pumps – blowers – compressors.

UNIT II PROCESS EQUIPMENT

9

Storage vessels – humidification –cooling towers. Agitation – Mixing – Industrial driers, crystallisers, absorbers. Extractors – Absorbers –Distillation – Extractive distillation, H.T.equipment, furnaces, heaters

UNIT III MEASURING DEVICES

9

Industrial measurement of temperature –pressure – level – flow – humidity –density – pH – characteristics of measuring devices – concepts of automatic control recorders.

UNIT IV PHYSICAL PROPERTIES

9

Measurement of physical parameters like surface tension –viscosity – melting point – Boiling point – optical rotation – Refractive Index – Thermal properties – molecular wt determination.

UNIT V COMPUTER INSTRUMENTATION

9

Elements of analogue and digital computers – computer instrumentation interfacing – microprocessor – controlled instruments – outlines of on-line and automatic analysers.

TOTAL PERIODS 45

- 1. Feeder and R.W.Roussean, "Elementary Principles of Chemical Processes", 2nd Edn. John Wiley andSons (1986).
- 2. G.J. Shugar, etal., "Chemical Technicians" Ready Reference Hand book, 3rd Edn. McGraw-Hill (1991).
- 3. K.Weissermel, and Arpe, "Industrial Organic Chemistry", Verlag Chemie, Weinheim, NewYork (1993).

BIO-ORGANIC CHEMISTRY

LTPC 3003

UNIT I CELL STRUCTURE AND FUNCTION

9

Cell structure and function: Molecular logic of living matter, Origin of biomolecules, cell structure – structure of prokaryotic and eukaryotic cells, intracellular organelles and their functions, comparison of plant and animal cells.

UNIT II INTRODUCTION TO BIOMOLECULES

9

Introduction to biomolecules: Examples of biomolecules, Building blocks of biomacromolecules, Nature of biomoleculear interactions. Types of reactions occurring in cells.

UNIT III PROTEINS, NUCLEOSIDES AND NUCLEIC ACIDS

9

Proteins, Nucleosides and nucleic acids: Primary structure of proteins, End group determination, Secondary structure of proteins tertiary structure, oligomeric proteins, ribonuleotides and deoxyribonucleotides, RNA and DNA, Base pairing, double helical structure of DNA and genetic code, transcription, Ribosomes.

UNIT IV ENZYMES LIPIDS AND MEMBRANES

9

Enzymes Lipids and membranes: Enzymes categorization catalysis, kinetics –single substrate enzyme catalysed reactions, Inhibition, common class of lipids, self association of lipids, Formation of micelles, membranes, bilayer and hexagonal phases. Membrane bound proteins structure, properties and transport phenomena.

UNIT V BIOENERGETICS

9

Bioenergetics: Basic principles, glycolytic pathways, kreb's cycle, oxidative phosphoylation, hydrolysis of esters and amids, c-c and c=c bond formation, oxidation, reduction, Decarboxylation, Biomimetic reactions, Drug design.

TOTAL PERIODS 45

- R.J. Simond, Chemistry of Biomolecules, Royal Society of Chemistry, U.K. London (1992).
- 2. A.L. Lehninger, Biochemistry: The molecular Basis of cell structure and function, Worth Publishers (1982).
- 3. D.E. Metzier, Biochemistry The chemical reactions of a living cell, Academic Press (1977).
- 4. H. Dugas, Bio organic Chemistry, A.Chemical approach to enzyme action, 2nd Edn. Springer Verlay (1989).
- 5. Lehninger, Nelson, and Cox, Principles of Bio chemistry, 2nd Edn. CBS Publishers, (1993).

BIO-PROCESS TECHNOLOGY

LTPC 3003

UNIT I BIOPROCESS PRINCIPLES

10

Bioprocess principles – components and objectives; microorganisms – bacteria, yeasts and molds, animal and plant cells – cell structure, biomolecules, cellular organisation, metabolic processes, stochiometry and energetics elementary aspects of molecular genetics.]

UNIT II ENZYME TECHNOLOGY

8

Enzyme technology – classification of enzymes, enzyme activity; kinetics of enzyme catalysis; modulation and regulation; immobilization of enzymes; applied enzyme catalysis.

UNIT III MICROBIAL PROCESSES

8

Microbial processes – bacterial and yeast strains for industrial processes; fermentation – aerobic and anaerobic fermentation; fundamentals of bioreactors—types – batch, fed-batch and CSTR; substrate utilization, product formation and biomass production.

UNIT IV PRODUCT RECOVERY AND PURIFICATION OPERATIONS

9

Product recovery and purification operations—principles of filtration, centrifugation, cell disruption, extraction, adsorption, precipitation, membrane separation, chromatographic and affinity technique.

UNIT V BIOPROCESSES AND ENZYME TECHNOLOGY IN INDUSTRIES 10

Bioprocesses and enzyme technology in industries – fuel generation ethanol and methane production; industrial enzymes; food production and processing – SCP, fermented foods, beverages, dairy products, vegetable and fruit products - pharmaceuticals – antibiotics and monoclonal antibodies.

TOTAL PERIODS 45

- 1. J.E.Bailey and D.F.Ollis Biochemical Engineering Fundamentals, McGraw Hill Book Co. (1986).
- 2. BIOTOL (Biotechnology by Open Learning) A series of books (Butter worths J.E.Smith, Biotechnology Principles, Van Nostrand (1985).

PHARMACEUTICAL CHEMISTRY

L T P C 3 0 0 3

UNIT I INTRODUCTION TO DRUG DESIGN

g

Factors governing drug design – Advantages - types of drug-lit survey for prep of drugs - characterisation /structural elucidation of drugs using diff. Spectral methods. Analgesics – Narcotic analgesics – morphine analogues – synthesis of codeine – Synthetic narcotic analgesics – synthesis and use of pethidines, methodones, dexdtropropoxyfene- narcotic antagonists – nalorphine – naloxone – Antipyretic analgeics – salicylic acid analogues – methyl salicylate, phenyl salicylate – paraamino phenol derivatives – structure synthesis and use of paracetamol, phenacetin, aspirin and salol

UNIT II ANTIHISTAMINES AND ANTIMALARIALS

9

Antihistamines – classification H1 & H2 receptor antagonists – structure, synthesis and their action & use of Diphenhydramine, cyclizinc, chlorpheneraminemaleate, Promethazine, Antimalerials classification – Quinine-4-aminoand 8-amino quinolines – chloroquine phosphate-Pyrimidines –Acidines; Sedatives – Barbiturates – structure, synthesis, action & use of Phenobarbitol-Benzodiazepines – mode of action structure and synthesios of Diazepam, Nitrazepam

UNIT III ANTIBIOTICS AND ANTIBACTERIALS

9

Antibiotics - penicillin, D-pencillamine, Phenoxy methyl pencillin -chloramphenicol-Antibacterials - norfloxacin, ciprofloxacin, Trimethoprim sulphadrugs - mode of action - preparation of sulphanilamide, sulphadiazine, sulphathiazole, sulphapyridine, sulphadimidine, sulphagauidine, sulphamethoxazole Antifungals - action, use and synthesis of clotrimazole, micronazole, Isoconazole.

UNIT IV ANTIHYPERTENSIVE AND ANTITUBERCULAR DRUGS

9

Anthihypertensive drugs— synthesis and mode of action of methyldopa, pargyline, bertyline, hydralazine, propranolol- Antitubercular drugs — synthesis of PAS, ethambutol — pyrazinamide, isoniazid-

UNIT V ANTIDIARRHEAL AGENTS

9

Antitussives and antineoplastic drugs, antidiarrheal agents – cimetidine, domperidone, loperamide; Expectorants – antitussives – guaiphenesin, ambroxal, bromohexine, dextromethorphan, Antineoplastic drugs - alkylating agents –nitrogen mustards – sulphonic acid esters -

TOTAL PERIODS 45

- 1. Berger, A.Medicinal chemistry, Vol 1&2, Wiley Interscience, New York (1990)
- 2. Asutoshkar Medicinal Chemistry, Wiley Eastern Ltd., Chennai (1992).
- 3. Bentely and Driver's Textbook of Pharmaceutical Chemistry, Oxford Univ. Press. (1985).
- 4. H.J Roth, A. Kleemann, Pharmaceutical chemistry vol.1 Drug synthesis (2001).

INDUSTRIAL CATALYSIS

LTPC 3 0 0 3

UNIT I CATALYSTS PREPARATION AND STRUCTURAL ASPECTS

9

Catalysts Preparation: Zeolite Y, Beta, ZSM-5, AIPO-5, 11, MCM- 4I, MesoporousAIPO's, Super acids, Supported catalysts, perovskites and spinels.

UNIT II CATALYSTS CHARACTERIZATION TECHNIQUES

12

Physical characterization – shapes; XRD, FTIR, SEM, TEM, AES, ESCA, BET, Si-Al-MAS NMR, DTA, TPD, TPR, ESR, DRSUV

UNIT III HOMOGENEOUS AND HETEROGENEOUS CATALYSIS

9

Conversion, selectivity, contact time, time on stream, Kinetics of heterogeneous catalysis, adsoprtion, phase transfer catalysis, super acid catalysis, intramolecular catalysis, enzyme catalysis, semi-conductor catalysis and photocatalysis. Promoters, stabilizers, catalyst deactivation by poisoning, fouling and sintering,

UNIT IV OPERATING CATALYTIC PROCESS

6

Mechanism of performing mass and heat balance, reactors – batch reactor, flow reactor and fluidised bed reactor - plug-flow and back - mixed reactors, isothermal and adiabatic reactors

UNIT V INDUSTRIAL CATALYTIC PROCESSES

9

Cracking, reforming, alkylation, isomerization, hydrogenation / dehydrogenation, dehydrocyclisation, dehydrosulphurization, hydrocracking, oxidation, metathesis, carbonylation, polymerization, synthetic fuels, hydrogen generation.

TOTAL PERIODS 45

- 1. Jens Hagen,Industrial catalysis, 2nd Edition, Wiley-VCH Verlay Gambh & Co, . (2006).
- 2. Herman Pines, The chemistry of catalytic hydrocarbon conversions, Academic Press, New York (1981).
- 3. R. Pearce and W.R.Patterson, Catalysis and chemical processes, Leonard Hill, London (1981).
- 4. Charles, N. Satterfield, Heterogeneous catalysis in industrial practice, 2nd Edn. Mc.Graw Hill, International Edition, Singapore (1993).

COMPUTATIONAL METHODS IN CHEMISTRY

LTPC 3003

UNIT I INTRODUCTION TO COMPUTERS

7

Binary System - Processor - Storage devices - I/O devices - Introduction to operation systems - DOS, WINDOWS and Unix - Algorithms - Flow charts - Introduction to e mail and internet - world wide web.

UNIT II NUMERICAL METHODS

7

Roots of equations – Bisection method – Newton-Raphson method- Curve fitting – Principle of Least squares – Correlation and Regression Analysis – Sample distributions, Students' t distribution.

UNIT III BASIC PROGRAMMING

11

Introduction – I/P & Read statements, Library functions, Statements – if-then, if-thenelse, go-to, for-to-next, for-to-next-step, for-to-next-loops, One dimensional and two dimensional arrays – writing simple programs for applications in chemistry.

UNIT IV C PROGRAMMING

11

Fundamentals and input/output statements: Constants – Variables- Data types-Operators – standard input output functions. Control structures: The decision control structure-The loop control structure- The case control structure. Functions: assessing a function - multidimensional arrays – pointer declarations – passing pointers to a fuction – operations on pointers.

UNIT V APPLICATIONS of C PROGRAMMING

9

Applications of C Programming to Simple Chemistry problems. Determination of rate constants of Ist, 2nd and 3rd order reactions- consecutive, parallel and equilibrium reactions - enzyme catalysed reactions- Reactivity ratios in copolymerization- determination of spectroscopic data and error analysis - simple quantum chemical calculation for simple molecules.

TOTAL PERIODS 45

- 1. K.V.Raman, Computers in Chemistry, Tata McGraw-Hill Publishing Co. Ltd., New Delhi(2003).
- 2. K.Arora Computer applications in chemistry, Anmol Pub. New Delhi (2004).
- 3. E. Balagurusamy, E. "Programming in ANSI C", 3rd Edn., Mc-Graw Hill Pub. Co., New Delhi, (2004).

CHEMISTRY OF NANOMATERIALS

LTPC 3 0 0 3

UNIT I 9

Nanotechnology – scope and emerging trends - bottom-up and top-down approaches; chemistry of solid surfaces – surface energy – chemical potential of curved surfaces; stabilization of colloidal dispersions by electrostatic and steric interactions; different types of nano materials.

UNIT II 9

General methods of synthesis of zero-dimensional nano particles – homogeneous nucleation and heterogeneous nucleation, growth of nuclei and factors of importance; synthesis of metallic, semiconductor and metal oxide nano particles;

UNIT III 9

Nanotubes - carbon nanotubes - synthetic methods for single walled and multi walled nanotubes; physical properties- optical, mechanical, magnetic and electrical properties, quantum size effects, structural characterization by scanning electron microscopy, x-ray diffraction and Raman spectroscopy. Inorganic nanotubes - synthesis and properties.

UNIT IV 9

One-dimensional Nanowires and nanorods, two-dimensional thin films, nano composites and nano-structured polymers, nano catalysts, nano clusters – preparation and properties

UNIT V 9

Physical techniques for fabrication of nanostructures – photolithography, electron beam lithography and related techniques– nanolithography by scanning tunneling microscopy and atomic force microscopy; assembly of nano particles and nanowires. Applications of nano materials in electronic and optoelectronic devices

TOTAL PERIODS 45

- 1. G. Cao Nanostructures and nanomaterials- Synthesis, properties and applications Imperial College Press (2004).
- 2. P. Yang (ed.)The chemistry of nanostructured materials- World Scientific (2005).