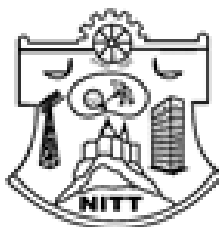
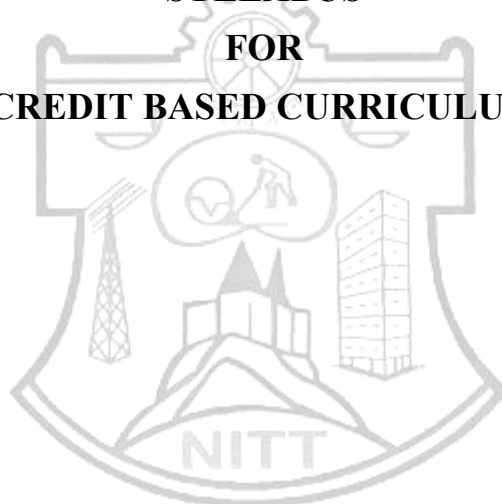


**M. Sc. DEGREE
CHEMISTRY**

**SYLLABUS
FOR
CREDIT BASED CURRICULUM**



**DEPARTMENT OF CHEMISTRY
NATIONAL INSTITUTE OF TECHNOLOGY
TIRUCHIRAPPALLI – 620 015, INDIA.**

M. Sc. Chemistry

Total minimum credits required for completing the M. Sc program in Chemistry is 68

SEMESTER I

Code	Course of Study	L	T	P	C
CH 601	Stereochemistry and Reaction Mechanisms	4	0	0	4
CH 603	Coordination and Transition Metal Chemistry	4	0	0	4
CH 605	Quantum Chemistry and Group Theory	3	0	0	3
CH 607	Fundamentals of Analytical Chemistry	3	0	0	3
CH 609	Organic Chemistry Practicals (Quantitative Analysis)	0	0	6	2
CH 611	Inorganic Chemistry Practicals (Qualitative Analysis)	0	0	6	2
					18

SEMESTER II

Code	Course of Study	L	T	P	C
CH 602	Photochemistry, Reactions and Reagents in Organic Synthesis	3	0	0	3
CH 604	Organometallic and Bioinorganic Chemistry	4	0	0	4
CH 606	Thermodynamics, Electrochemistry and Kinetics	4	0	0	4
CH 608	Instrumental Methods of Chemical Analysis	3	0	0	3
CH 610	Physical Chemistry Practicals	0	0	6	2
CH 612	Analytical Chemistry Practicals	0	0	6	2
					18

SEMESTER III

Code	Course of Study	L	T	P	C
CH 613	Bioorganic Chemistry	3	0	0	3
CH 615	Solid State, Nuclear and Main Group Chemistry	3	0	0	3
CH 617	Statistical Thermodynamics and Surface Chemistry	4	0	0	4
CH 619	Applications of Spectroscopy	0	0	0	2
CH 621	Comprehensive Viva voce	0	0	6	2
CH 623	Physical Chemistry and Organic Chemistry Practicals	0	0	6	2
CH 625	Analytical Chemistry and Inorganic Chemistry Practicals	0	0	6	2
					20

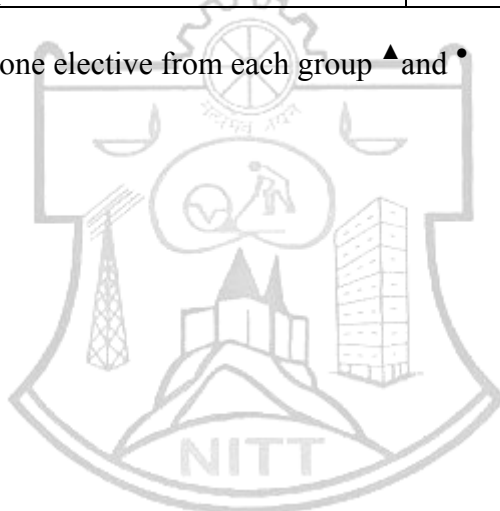
SEMESTER IV

Code	Course of Study	L	T	P	C
	▲ELECTIVE I	3	0	0	3
	●ELECTIVE II	3	0	0	3
CHE 630	M. Sc. Project and Viva voce	0	0	0	6

LIST OF ELECTIVES

Code	Course of Study	L	T	P	C
CHE 614	▲Nuclear Chemistry	3	0	0	3
CHE 616	▲Medicinal Chemistry	3	0	0	3
CHE 618	▲Polymer Chemistry	3	0	0	3
CHE 620	▲Biochemistry	3	0	0	3
CHE 622	●Catalysis	3	0	0	3
CHE 624	●Nano Science and Technology	3	0	0	3
CHE 626	●Computational Methods in Chemistry	3	0	0	3
CHE 628	●Unit Operations and Processes	3	0	0	3

The student has to choose one elective from each group ▲ and ●



CH 601- Stereochemistry and Reaction Mechanisms

Theories of Aromaticity and Antiaromaticity, Huckel's rule, annulenes and heteroannulenes, fullerenes (C₆₀). Other conjugated systems, Ylides, Aromatic Nucleophilic substitution of activated halides, Chichibabin reaction.

Optical activity and chirality, absolute and relative configuration, Classification of chiral molecules as asymmetric and dissymmetric, R-S Notation system, Fischer projection, Interconversion of Sawhorse, Newman and Fischer projections. Molecules with more than one asymmetric center. Enantiotopic and diastereotopic atoms, groups and faces. Stereo specific and stereo selective synthesis Optical isomerism of biphenyls, allenes and spiranes. Compounds containing chiral nitrogen and sulfur. Geometrical isomerism, E, Z-nomenclature of olefins, Geometrical isomerism of cyclic compounds (disubstituted cyclopropane, cyclobutane and cyclopentanes), cumulenes and oximes.

Conformational analysis of ethane and disubstituted ethane derivatives, cycloalkanes and substituted cyclohexane. Effects of conformation on reactivity in acyclic compounds and cyclohexanes (oxidation and acylation of cyclohexanol, reduction of cyclohexanone, esterification and hydrolysis of cyclohexane carboxylic acid). Conformation and stereochemistry of cis and trans decalin and 9-methyldecalin.

Reaction mechanism: Definition of reaction mechanism, transition state theory, kinetics, qualitative picture. Substituent effects, linear free energy relationships, Hammett equation and related modifications. Basic mechanistic concepts like kinetic vs thermodynamic control, Hammond postulate, Curtin-Hammett principle, isotope effects, general and specific acid-base catalysis, and nucleophilic catalysis.

Aliphatic Nucleophilic Substitution— reactivity, structural and solvent effects, substitution in norbornyl and bridgehead systems, substitution at allylic and vinylic carbons, substitution by ambident nucleophiles, substitution at Carbon doubly bonded to oxygen and nitrogen – alkylation and acylation of amines, halogen exchange, Von-Braun reaction, alkylation and acylation of active methylene carbon compounds, hydrolysis of esters, Claisen and Dieckmann condensation.

Text Books

1. M. B. Smith, J. March, March's Advanced Organic Chemistry, John Wiley & Sons, 6th Edn, 2007
1. R. R. Carey and R. J. Sundburg, Advanced Organic Chemistry, Part A and Part B, Springer, 5th Edn, 2007

References

1. Peter Sykes, A guide book to mechanism in Organic chemistry, Orient-Longmans, 6th Edn, 1996.
2. E. J. Eliel, Stereochemistry of Carbon Compounds, John Wiley, 1997
3. P. Y. Bruice, Organic Chemistry. Pearson Education, 3rd edition, 2006

CH 603 – Coordination and Transition Metal Chemistry

EAN rule - Theories of coordination compounds - VB theory - CFT - splitting of d orbitals in

ligand fields and different symmetries - CFSE - factors affecting the magnitude of $10 Dq$ - evidence for crystal field stabilization - spectrochemical series - site selection in spinels - tetragonal distortion from octahedral symmetry - Jahn-Teller distortion - Nephelauxetic effect - MO Theory - octahedral - tetrahedral and square planar complexes - π -Bonding and molecular orbital theory - experimental evidence for π -bonding.

Term states of dn ions – Origin of Electronic spectra of coordination compounds - selection rules - band intensities and band widths - energy level diagrams of Orgel and Tanabe – Sugano diagrams and spectra of dn systems. Calculation of Δ . Calculation of Racah parameters. Magnetic properties of coordination compounds - change in magnetic properties of complexes in terms of spin orbit coupling - temperature independent paramagnetism - spin cross over phenomena.

Substitution reactions in square planar complexes - the rate law for nucleophilic substitution in a square planar complex - the trans effect - theories of trans effect - mechanism of nucleophilic substitution in square planar complexes - kinetics of octahedral substitution - ligand fields effects and reaction rates - mechanism of substitution in octahedral complexes - reaction rates influenced by acid and bases - racemisation and isomerisation - mechanisms of redox reactions - outer sphere mechanisms - excited state outer sphere electron transfer reactions - inner sphere mechanisms - mixed valent complexes.

Structure of coordination compounds with reference to the existence of various coordination numbers - complexes with coordination number two - complexes with coordination number three - complexes with coordination number four - tetrahedral and square planar complexes - complexes with coordination number five - regular trigonal bipyramidal and square pyramidal - site preference in trigonal bipyramidal complexes - site preference in square planar complexes - isomerism in five coordinate complexes - coordination number six - distortion from perfect octahedral symmetry - trigonal prism - geometrical isomerism in octahedral complexes – optical isomerism in octahedral complexes - absolute configuration of complexes - stereo selectivity and conformation of chelate rings - coordination number seven and eight.

Periodicity, General properties of lanthanides and actinides: Electronic configuration, oxidation state, oxidation potential, atomic and ionic radii- Cause and consequences of lanthanide and actinide contractions- Comparison of spectral and magnetic properties of lanthanide and actinide complexes- separation of lanthanides – use of lanthanide compounds as shifting agents- The transactinide elements- Extraction details of cerium, thorium and uranium – Chemistry of their important compounds: Oxides, nitrates and sulfates.

Text Books

1. J. E. Huheey, E. A. Keiter and R. L. Keiter “ Inorganic Chemistry, Principles of Structure and Reactivity”, 4th Edition, Harper Collin College Publishers, 1993
1. F.A. Cotton and G.Wilkinson “ Advanced Inorganic Chemistry” 4th & 5th Editions, Wiley Interscience, New York, 1998

References

1. B. E. Douglas, H. Darl , McDaniel and J. J. Alexander, ‘Concepts and Models of Inorganic Chemistry’, John Wiley & Sons, Inc. 3rd Edn, New York, 1994.
2. D. F. Shriver, P. W. Atkins and C. H. Langford, ‘Inorganic Chemistry’, Oxford University Press, Oxford, 1994.
3. F. Basolo and R. G. Pearson, Mechanism of Inorganic reactions.

CH 605-Quantum Chemistry and Group Theory

Quantum Chemistry-I: The Failures of Classical Physics – Block Body Radiation-photoelectric effect-Bhor's Quantum theory, Wave Particle Duality-Uncertainty Principle. Operator Algebra, Linear and Hermitian operators, Quantum mechanical postulates, Schrodinger equation and its solution to the problem of a particle in one and three dimensional boxes.

Quantum Chemistry-II: Schrodinger equation for hydrogen atom and its solution, the origin of electronic quantum numbers and physical significance - radial probability density-significance of magnetic quantum number with respect to angular momentum. Hydrogen molecule ion and hydrogen molecule-Pauli's exclusion principle. Term symbols for electronic state in atoms –LS and JJ coupling. Born Oppenheimer approximation, Mulliken designation of molecular orbitals.

Quantum Chemistry-III: Quantum mechanical results for a simple harmonic oscillator and rigid rotator, Solution of Schrodinger equation for harmonic oscillator, rigid rotor, derivation of Eigen function and Eigen value for hydrogen atom - MO theory of bonding, and MO treatment of Hbonded systems, ethylene, butadiene and benzene. Approximation methods; Perturbation and variation method, wave functions for many electron atoms –Hartree – Fock SCF method, Slater Orbitals.

Group Theory-I: Symmetry Elements and Symmetry Operations, Point Groups, Representation of Groups, Reducible and Irreducible Representation; Character Tables, Orthogonality Theorem– Its Consequences.

Group Theory-II: Application of group theory to atomic orbitals in ligand fields, molecular orbitals, hybridization, classification of normal vibrational modes, selection rules in vibrational and electronic spectroscopy, systematic procedure for determining Symmetries of Normal Modes of Vibrations, Chemical applications of group theory – AB₂ and AB₃.

Text Books

1. I. N. Levine, 'Quantum Chemistry', 4th Edn., Prentice Hall India, 1994.
2. A. K. Chandra, Introductory Quantum Chemistry, Tata McGraw Hill 1994.
3. M. S. Gopinathan and V. Ramakrishnan, Group Theory in Chemistry, Vishal Publishers, 1988.

References

1. D. A. McQuarrie, 'Quantum Chemistry', University Science Books, 1983.
2. F.A.Cotton, 'Chemical Applications of Group Theory', 2nd Edn., Wiley Eastern Ltd., 1990.
3. R.K.Prasad, Quantum Chemistry, TMH, 1995
4. P.W. Atkins, 'Physical Chemistry', 6th Edn., Oxford University Press, 1998.

CH 607- Fundamentals of Analytical Chemistry

Tools of Analytical Chemistry – Factors affecting the choice of Analytical methods. Data acquisition and treatment, Common apparatus and Basic Techniques, Errors in chemical analysis, Statistical data treatment and Evaluation, Accuracy and Precision, , Students T-test, Ftest & Q-test, Sampling

Classical methods of Analysis: Theoretical concepts of Titrimetric Analysis-Theory of indicators, titrations, Applications of Complexometric titrations- Metal ion indicators Determination of cations and Analysis of mixture of cations. Gravimetric determination- Principles and examples. Applications of Coordination chemistry in analytical methods

Separation Techniques: Solvent and synergistic extraction. Countercurrent extraction, super critical fluids, Electrophoresis- theory and applications. Chromatography-classification-columnpaper and thin layer chromatography. HPLC-instrumentation, Ion – exchange chromatography- Theory. Gel Permeation Chromatography. Gas chromatography – basic instrumental set upcarriers, columns, different detectors and comparative study. Qualitative and quantitative studies using GC, CHN analysis by GC.

Thermal methods of Analysis: TG, DTA and DSC - Instrumentation and Theory. TG of copper sulfate pentahydrate and calcium oxalate monohydrate. Calculations of thermodynamic parameters.

Atomic Emission Spectroscopy: DCP and ICP, Flame Emission and Atomic Absorption Spectrometer. Instrumentation of AAS, the flame spectra, flame characteristics. Atomizers used in spectroscopy, Hollow cathode lamp interference in AAS-applications. Atomic emission spectroscopy-flame photometry-simultaneous multi element analysis.

Text Books

1. G. H. Geffery et al., Vogel's Text Book of Quantitative Chemical Analysis, ELBS Edn, 1989
2. D.A. Skoog, D.M. West, F.J Holler, S.R Crouch , Fundamentals of Analytical Chemistry, 8th edition, Thomson Brooks Cole , 2004

References

1. H.H. Willard, L.L. Merrit, J.A. Dean and F.A. Settle, Instrumental Methods of Analysis, D, CBS Publishers, New Delhi, 1986.
2. D.A. Skoog, E. J. Holler, S. R. Crouch , Principles of Instrumental Analysis, 6th edition, Thomson Brooks Cole , 2007
3. F.W. Fifield and D. Kealey, Principles and Practice of Analytical Chemistry, 2nd Edition, International Book Company, London, 1983

CH 609 - Organic Chemistry Practicals

- a. Estimations
Estimation of Phenol, Aniline, Ascorbic Acid.
Estimation of ketone by volumetric method & gravimetric method.
Estimation of Lactose in milk.
Estimation of glucose by Fehlings method.
Estimation of glucose by Bertrand's method.
- b. (b) Analysis of Oils
Determination of Saponification value of an oil., Determination of Acetyl value of an oil.
Determination of Iodine value of an oil., Determination of Acid value of an oil.
- c. (c) Drug Analysis
Estimation of Isoniazid by KMnO₄ method and bromine method.

Estimation of Ascorbic acid in a given tablet., Estimation of pot. phenoxy methyl penicillin in a given tablet.

d. Preparations - Double Stage

Preparation of m-nitrobenzoic acid from methyl benzoate. , Preparation of Acetyl Salicylic acid from methyl salicylate., Preparation of Triacetoxy benzene from Hydro Quinone. , Preparation of m-nitroniline from nitro benzene., Preparation of Tribromo benzene from Aniline. , Preparation of p-nitroaniline from Acetanilide.

e. Extraction

Extraction of caffeine from tea leaves.

f. Chromatography

Paper chromatography.

i. Separation of Anthocyanidine from Hibiscus Rosasinens., ii. Separation of sugars.

iii. Separation of Amino Acids.

Text Books

1. I. A. I. Vogel, 'Text book of Practical Organic Chemistry', 5th Edn. ELBS, London, 1989.
2. B. B. Dey and M. V. Sitharaman, 'Laboratory Manual of Organic Chemistry' Revised by
3. T.R. Govindachari, Allied Publishers Ltd., New Delhi. 4th Revised Edn., 1992.

CH 611- Inorganic Chemistry Practicals

I. Semi-micro analysis: Analysis of mixture containing two common cations and any two of the following less familiar cations. Tl, W, Se, Te, Mo, Ce, Th, Ti, Zr, V, Be, U and Li.

II. Preparation of the following:

1. Chrome alum 2. Copper (I) chloride 3. Tris(thiourea) copper (I) complex 4. Potassium tris (oxalato) aluminate (III) 5. Hexaamminecobalt (III) chloride 6. Tetraamminecopper (II) sulphate.

Text Books

1. I. G., Svehla , 'Vogel's Qualitative Inorganic Analysis', 6th Edn., Orient Longman New Delhi, 1987.
2. V.V., Ramanujam , 'Inorganic Semi-micro Qualitative Analysis', 3rd Edn., National Publishing Company, Madras, 1990.

SEMESTER 2

CH 602-Photochemistry, Reactions and Reagents in Organic Synthesis

Fundamentals of Photochemistry, Qualitative introduction about different transitions, Cis-Trans isomerization, Paterno-Buchi reaction, Norrish type I and II reactions, photo reduction of ketones, di-pi-methane rearrangements, photochemistry of arenes. Barton reaction, Photosynthesis, Photochemistry of vision, Pericyclic reactions: Classification, electrocyclic, sigmatropic, cycloaddition and ene reactions, Woodward-Hoffmann rules, and FMO theory, Claisen, Cope, Sommelet, Hauser, and Diels-Alder reactions in synthesis, stereochemical aspects.

Carbonyl compounds: Modern methods of synthesis from alcohols, Swern and Dess-Martin oxidations. Reactions of carbonyl compounds, addition of N, O, and S nucleophiles. Reduction

using hydride reagents, chemo - and stereoselectivity, formation of enols and enamines, kinetic and thermodynamic enolates, lithium and boron enolates in aldol and Michael reactions, stereoselective aldol condensations, alkylation and acylation of enolates, condensation reactions, Claisen, Dieckman, Knoevenagel, Stobbe and Darzen glycidic ester, acyloin,

Rearrangement reactions involving electron deficient carbon, nitrogen, oxygen centers, emphasis on synthetic utility of these rearrangements. Baker–Venkataraman, Benzilic acid, [1,2]- Meisenheimer, [2,3]-Meisenheimer, Wagner-Meerwein, Pinacol, Demjanov, Dienone-Phenol, Favorskii, Wolff, Hofmann, Curtius, Lossen, Schmidt, Beckmann, Benzidine, Hofmann-Löffler rearrangements

Synthesis of alkenes, Wittig and related reactions, modern methods of synthesis, Peterson, McMurry, Shapiro reaction, , synthesis from 1,2-diols, pyrolytic elimination of sulfoxides and selenoxides, synthesis of alkynes, allenes and cumulenes, Pd catalysed coupling reactions, Heck, Suzuki, Glazer-Ellington coupling. Reactions of alkenes and alkynes, stereo – and enantioselective hydroboration, hydrogenation, hydroxylation, epoxidation (Sharpless, Jacobson methods), oxymercuration, halolactonisation. Preparation and synthetic uses of lithium and copper acetylides.

Use of the following reagents in organic synthesis and functional group transformation, Complex metal hydrides, Gilman's reagent, lithium dimethyl cuprate, lithium diisopropylamide (LDA), dicyclohexylcarbodiimide, trimethylsilyl iodide, tri-n-butyl hydride, , Woodward and Prevost hydroxylation, osmium tetroxide, DDQ, SeO₂, lead tetraacetate, H₂O₂, phase transfer catalyst, crown ethers and Merrified resin, , Wilkinson's catalyst, Baker yeast.

Text Books

1. S. Warren, Organic Synthesis The Disconnection approach, Wiley and sons, 2002.
2. House, Modern Synthetic Reactions, 1973.

References

1. R.O.C. Norman and J. M. Coxon, Principles of organic synthesis, ELBS, 1994.
2. J. J. Li, Name Reactions, Springer, 3rd Edn, 2006.
3. B. P. Mundy, M. G. Eller, F. G., Jr. Favalaro Name Reactions and Reagents in Organic Synthesis, Wiley-Interscience, 2005.

CH 604 - Organometallic and Bio Inorganic Chemistry

Bonding in Organometallics, 18-electron rule, Metal Carbonyls, Nitrosyls, dinitrogen complexes. Fluxional Molecules, Metal Alkyls, Aryls, Hydrides and related σ -bonded ligands, Carbenes, Complexes of π -Bound Ligands, Metal-Metal Bonding, Isolobal Analogy.

Reactions of Organometallics: Ligand substitution, Oxidative Addition and Reductive Elimination, Insertion reactions, Elimination Reactions, Alkene isomerization, Hydroboration, Hydrogenation of olefins: Wilkinson's catalyst, Hydroformylation of olefins, Wacker-smidt Synthesis, Monsanto Acetic Acid process, Polymerization of olefins, Cyclo-oligomerization of acetylenes, Alkene Metathesis, C-H bond Activation, Carbon-Carbon bond formation.

Metalloenes, Electronic Structure and Bonding in Ferrocene, Synthesis and Physical and Spectroscopic properties of metalloenes, Reactions and Applications of Metalloenes. Multi decker sandwich complexes. Applications of Metalloenes in polymers, non linear optics, medicines, molecular recognition, Catalysis.

Occurrence and availability of inorganic elements in organisms, Uptake, transport and storage of metal ions by organisms, Structure and functions of biological membranes, The generation of concentration gradients (the Na⁺-K⁺ pump), Mechanisms of ion-transport across cell membranes, Bleomycin, Siderophores (e.g. enterobactin and desferrioxamine). Transport of iron by transferrin, Storage of iron by ferritin, bio chemistry of calcium as hormonal messenger.

Metal ions and electron transfer in biological systems, Background, Types of electron transfer, Universal electron carriers, Cytochromes, structure. Structure of Hemoglobin and Myoglobin, Dioxygen transport and storage by hemoglobin and Myoglobin respectively. Oxidation and spin states of iron in deoxyHb and oxyHb. Blue copper proteins (Cu), Iron-sulfur proteins (Fe), Carbon monoxide poisoning. Oxygen atom insertion reactions: monooxygenases (e.g. Cytochrome P-450), Protective metalloenzymes I. (The Cu, Zn superoxide dismutase), Vitamin B12 (Co), Cisplatin (Pt),

Text Books

1. J. E. Huheey, E. A. Keiter and R. L. Keiter “ Inorganic Chemistry, Principles of Structure and Reactivity”, 4th Edition, Harper Collin College Publishers, 1993
1. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, University Science Books, Mill Valley CA 1994.

References

1. R.H. Crabtree, The Organometallic Chemistry of Transition Metals, 4th Edn, Wiley, 2005
2. G.O. Spessard and G. L. Miessler, Organometallic Chemistry, Prentice Hall 1996.
3. F.A. Cotton and G.Wilkinson “ Advanced Inorganic Chemistry” 4th & 5th Editions, Wiley Interscience, New York.

CH 606-Thermodynamics, Electrochemistry and Kinetics

Thermodynamics I: the second law of thermodynamics, Maxwell’s relations and Thermodynamic Equations of state, (Cp-Cv) in terms of Coefficient of Expansion and Coefficient of Compressibility. Closed and Open Systems, Partial Molal Quantities, Chemical Potential, Gibbs-Duhem Equation, Variation of Chemical Potential with Temperature and Pressure. Real Systems, Fugacity and Activity, Activity Coefficients and their Determination:

Thermodynamics II: Standard States for Gases, Liquids and Solids and its Applications. Thermodynamics of Ions in Solution, Free Energies, Enthalpies and Entropies of Ions in Solutions. Activity and Mean Activity Coefficients of Electrolytes and their Determinations, Debye-Huckel Limiting Law. Thermodynamics of Mixing–Mixtures of Volatile Liquids–Real Solutions and Activities-Excess Functions. Thermodynamic Derivations of Phase Rule, Applications to Three Component Systems Involving Solids and Liquids –Acetic Acid–Chloroform-Water, NaCl-Na2SO4-H2O, NH4NO3-(NH4)2SO4-H2O.

Electrochemistry-I: Ion transport in solution –migration, convection and diffusion –Fick’s laws of diffusion conduction –influence of ionic atmosphere on the conductivity of electrolytes-The Debye Huckel-Onsager equation for the equivalent conductivity of electrolytes –experimental verification of the equation –conductivity at high field and at high frequency –conductivity of non aqueous solutions-effect of ion association on conductivity. The electrode-electrolyte interface-electrical double layer-electro capillary phenomena-Lippmann equation –the Helmholtz –Perrin –Guoy-Chapmann and Stern models, Electrokinetic phenomena Tiseiius method of separation of protons of proteins - membrane potential.

Electrochemistry-II: Electrode reactions - Mechanism of electrode reactions-polarization and overpotential –The Butler volmer equation for one step and multistep electron transfer reaction– significance of equilibrium exchange current density and symmetry factor-significance of transfer coefficient-mechanism of the hydrogen evolution reaction and oxygen evolution reactions. Some electrochemical reactions of technological interest- corrosion and passivity of metals-construction and use of Pourbaix and Evans diagrams- methods of protection of metals from corrosion, Fuel cells - electro deposition.

Chemical Kinetics: Simultaneous reactions –opposing , parallel and consecutive reactions , the steady state approximation –Theories of reaction rates-transition state theory and collision theory a comparison – enthalpy , entropy and free energy of activation , potential energy surfaces, reaction coordinates, kinetic isotope effects, factors determining reaction rates in solution solvent dielectric constant and ionic strength. Chain reactions –linear reactions, branching chains– explosion limits; Rice–Herzfeld scheme; kinetics of free radical polymerization reactions. Enzyme catalysis–rates of enzyme catalysed reactions–effect of substrate concentration, pH and temperature –determination of Michael is parameters.

Text Books

1. S. Glasstone, Thermodynamics for chemists, Affiliated East West Press, 1965.
2. Atkins, P.W. ‘Physical Chemistry’, 6th Edn., Oxford University Press, 1998.

References

1. K, J. Laidler, ‘Chemical Kinetics’, 3rd Edn., Harper and Row Publishers, 1987.
2. J. O. M. Bockris and A. K. N. Reddy, Modern Electrochemistry, Plenum Press, 1970.
3. J. Rajaram and J. C. Kuriacose, Thermodynamics for Students of Chemistry, Shobanlal Nagin Chand Co, 1986.

CH 608- Instrumental Methods of Chemical Analysis

Electrogravimetry- Coulometry- Current-Voltage relationship during electrolysis, constant current and constant potential coulometry-applications- primary and secondary coulometry, Potentiometry, Ion-Selective electrodes- Construction, membrane indicator electrodes, ionselective FET, immobilized enzyme electrodes and molecular selective electrodes.

Polarography – current – voltage curve. Stripping voltammetry, DME- Construction, supporting electrolyte – polarographic maxima. Half-wave potential- Instrumentation- Applications of Polarography. Pulse and differential pulse polarography- Voltammetry, Excitation signals in voltammetry, Amperometric titrations – Applications. Cyclic voltammetry-Theory and applications.

Vibrational and Electronic Spectroscopy- Theory, rotational, vibrational and electronic energy levels, rigid rotator and harmonic oscillator, vibrational transitions, selection rules. Raman Spectroscopy, Laser Raman rotational & vibrational Raman spectra. Definition of normal modes and normal coordinates vibrational coupling; overtones, sum and difference combinations, Fermi resonance. Electronic Transitions, selection rules, Theory of Electronic spectroscopy of Atoms and Molecules, potential energy curves, Frank Condon principle.

UV- Vis and IR Spectroscopy- Beer-Lambert Law, Basic Instrumentation, Sources, Sampling and Detectors, single beam and double beam instruments, Photometric Titrations, Spectrophotometric Kinetic methods, Nephelometry and Turbidimetry. Fluorescence and Phosphorescence, IR spectrophotometry- Instrumentation, IR sources and Transducers.

X- Ray Diffraction: Theory, The growth and form of crystals - the crystal systems and Bravais lattices - Miller indices and labelling of planes - symmetry properties - crystallographic point groups and space groups - fundamentals of X-ray diffraction - powder and rotating crystal methods - systematic absences and determination of lattice types - analysis of X-ray data for cubic system - structure factor and Fourier synthesis - Fundamentals of Electron and Neutron diffraction and structure determination.

Text Books

1. G. H. Geffery et al., Vogel's Text Book of Quantitative Chemical Analysis, ELBS Edn
2. D.A. Skoog, E. J. Holler, S. R. Crouch , Principles of Instrumental Analysis, 6th edition, Thomson Brooks Cole , 2007

References

1. H.H. Willard, L.L. Merrit, J.A. Dean and F.A. Settle, Instrumental Methods of Analysis, D, CBS Publishers, New Delhi, 1986
2. D.A. Skoog, D.M West, F.J Holler, S.R Crouch , Fundamentals of Analytical Chemistry, 8th Edition, Thomson Brooks Cole , 2004
3. F.W. Fifield and D. Kealey, Principles and Practice of Analytical Chemistry, 2nd Edition, International Book Company, London, 1983

CH 610 – Physical Chemistry Practicals

1. Kinetic study of hydrolysis of ester. Determination of order, I- and $S_2O_8^{2-}$.
2. Determination of partition co-efficient and equilibrium constant. $KI + I_2 \rightleftharpoons KI_3$.
3. Kinetics of iodination of acetone by spectrophotometer.
4. Adsorption of oxalic acid on activated charcoal.
5. Determination of heat of solution and heat of fusion.
6. Study of three component system.
7. Partition coefficient of NH_3 between water and chloroform.
8. Determination of solubility product.
9. Partial molar volume of NaCl.

Text Books

1. Shoemaker, D.P., Garland, C.W.& Nibber, J.W., 'Experiments in Physical Chemistry', McGraw Hill 5th Edn., 1989.

CH 612 – Analytical Chemistry Practicals

1. Water Analysis - Alkalinity, Carbonate and Non-carbonate hardness, Chloride, Sulphate, Ca and Mg, Microbial Quality.
2. Analysis of Cement. Determination of percentage purity of caustic soda and washing soda.
3. Determination of flash and fire point of a lubricating oil
4. Determination of calorific value of solid fuel using Bomb Calorimeter.
5. Analysis of a mixture by Gas Chromatography.
6. Analysis of an alloy by Polarography.
7. Determination of Lead and Sulphate by Amperometry
8. Estimation of Phosphate by Nephelometry.
9. Estimation of Na, K and Ca in a mixture using Flame photometer.

Text Books

1. Manual Provided by the Department
2. A. I. Vogel, Text Book of Quantitative Inorganic Analysis, 5th Edn, Longman, 1989

SEMESTER 3

CH 613- Bio Organic Chemistry

Introduction to retrosynthesis, synthon, synthetic equivalent, target molecule, functional group interconversion, disconnection approach, one group disconnection (disconnection of alcohols, olefins, ketones), Chemoselectivity, importance of the order of events in organic synthesis. Two group disconnections C-C & C-X.

C-C bond formation via free radicals and carbenes, methods of generation of free radicals and carbenes, reactions of free radicals, coupling, addition, substitution, fragmentation and rearrangements. Umpolung reagents, definition of umpolung, acyl anion equivalent, equivalents of ketene, $\text{RCOCH}_2 + \text{RCOCH}_2\text{CH}_2\text{CH}_2 + \text{RCOCH}_2\text{CH}_2\text{CH}_2 -$ etc. Protecting groups, protection of hydroxyl, carboxyl, carbonyl, amino groups. Protection of carbon-carbon multiple bonds. Illustration of protection and deprotection in synthesis.

Classification of natural products, classification based on chemical structure, physiological activity, taxonomy and biogenesis Alkaloids – classification, structure elucidation based on degradative reactions (morphine, quinine and atropine). Terpenoids classification, structure elucidation and synthesis of abietic acid.

Carbohydrates: Structure of ribose, glucose, fructose, maltose, sucrose, lactose, starch cellulose and cyclodextrins. Preparation of alditols, glycosides, deoxysugars. Synthesis of vitamin C from glucose. Synthesis of amino acids – strecker and azalactone synthesis, enantioselective synthesis of amino acids, reactions of amino acids. Structure of proteins.

Steroids– classification, structure elucidation of cholesterol, conversion of cholesterol to progesterone, androsterone and testosterone. Bio polymer, -nucleosides and nucleotides-RNA and DNA, Watsons and Creig model. Lipids-Prostaglandin-E and Pheromones.

Text Books

1. I. L. Finar, Organic Chemistry Vol. I & Vol. II- Pearson Education, 6th edn
2. House, Modern Synthetic Reaction, 1973

References

1. S. Warren, Organic Synthesis The Disconnection approach, Wiley and sons, 2002
2. S. Warren, Organic Synthesis The Synthons approach, 2nd Edn, Wiley and sons, 1991

CH 615 – Solid State, Nuclear and Main Group Chemistry

Types of solids - close packing of atoms and ions - bcc , fcc and hcp voids - Goldschmidt radius ratio - derivation - its influence on structures - structures of rock salt - cesium chloride – wurtzite - zinc blende - rutile - fluoroite - antiferite - diamond and graphite - spinel - normal and inverse spinels and perovskite - lattice energy of ionic crystals - Madelung constant - Born-Haber cycle and its applications.

Band Theory of solids. Free electron Theory, Zone Theory, M.O. Theory of solids- Dislocation in solids: Schottky and Frenkel defects. Line defects and plane defects- non-stoichiometric compounds Electrical properties: Energy bands, insulators, semiconductors and conductors.- super conductors-dielectric properties, piezo-electricity, Ferro electricity - Conductivity in pure metals; superconductivity: Occurrence, BCS Theory, High temperature super conductors.

Nuclear structure: mass and charge, nuclear moments, binding energy, mass defect, packing fraction, stability, magic numbers. Modes of radioactive decay and rate of radioactive decay- Half-life, average life, radioactive equilibrium: Transient and secular-Nuclear reactions: Energetics and Types-Nuclear Fission- Liquid drop model- Nuclear Fusion- Essential Features of nuclear reactors- Tracer techniques, Neutron Activation Analysis- Carbon and Rock dating – Application of tracers in chemical analysis, reaction mechanisms, medicine and industry.

Inorganic chains - rings - cages and clusters, catenation, heterocatenation, intercalation chemistry, one dimensional conductor, Polymeric sulfur nitride – Preparation, properties, structure and uses of inorganic polymers of boron, silicon, germanium and tin. Isopoly anions - Heteropoly anions - borazines - phosphazenes - phosphazene polymers - ring compounds of sulphur and nitrogen.

Inorganic Cages - structure and bonding of boron hydrides, carboranes and heteroboranes - metal clusters - dinuclear clusters - trinuclear clusters - tetranuclear clusters – hexanuclear clusters - structural prediction of organometallic clusters. Interhalogen compounds - Oxoacids of selenium and tellurium. Noble Gas Chemistry and their halides and pseudohalides.

Text Books

1. L.V. Azaroff “ Introduction to solids” Mc.Graw hill, New York.
2. H. J. Arnikar, ‘Essentials of Nuclear Chemistry’, 4th Edn., New Age International Publishers Ltd., New Delhi, 1995.

References

1. F. A. Cotton, Wilkinson, G. and Paul, L. Gaus, ‘Basic Inorganic Chemistry’, 3rdEdn., John Wiley & Sons, New York, 1995.
2. J. D. Lee, ‘Concise Inorganic Chemistry’, 5th Edn., ELBS. with Chapman and Hall, London, 1996.
3. J. E. Huheey, Ellen, A. Keiter and Richard, L. Keiter , ‘Inorganic Chemistry - Principles of Structure and Reactivity’, 4th Edn., Harper Collins, New York, 1993.

CH 617- Statistical Thermodynamics and Surface Chemistry

Statistical Thermodynamics I: Maxwell's Law of distribution of molecular speeds, graphical representation, experimental verification –derivation of expressions for average, most probable and root mean square velocity. Concept of velocity space and phase space-perturbation and combination-laws of probability-microstates for distinguishable and indistinguishable particles. Derivation of Maxwell Boltzmann distribution law – partition functions and their calculation. Expressions for thermodynamic quantities, in terms of partition functions-translational, rotational, vibrational, and electronic contributions to the thermodynamic properties of perfect gases-Intermolecular forces in imperfect gases.

Statistical Thermodynamics-II: Statistical interpretation of laws of thermodynamics, Third law of thermodynamics and apparent expression to it. Quantum statistics: Limitation of classical statistics –quantum statistics and classical statistics, comparison-heat capacities of gases in general and hydrogen in particular-heat capacities of solids. Einstein and Debye models –Bose Einstein statistics and Fermi Dirac statistics and corresponding distribution functions- Applications of quantum statistics to liquid helium, electrons in metal and Planck's radiation Law.

Photochemistry: Absorption and emission of radiation, Franck Condon principle decay of electronically excited states, radiative and non radiative processes, fluorescence and Phosphorescence, spin –forbidden radiative transitions, inter conversion and Intersystem crossing. Theory of energy transfer –resonance and exchange mechanism, triplet –triplet annihilation, photosensitization and quenching. Spontaneous and induced emission. Einstein transition probability- inversion of population –laser and masers. Flash photolysis: Chemi and thermoluminescence.

Colloids: Colloidal and amphoteric electrolytes. Wetting and Degeneracy. Surface Chemistry and Catalysis: Adsorption Isotherms–Freundlich, Langmuir and BET, Surface Films, Surface Area and Mechanism of Heterogeneous Catalysis, Phase Transfer Catalysis. Chemical Analysis of surfaces: Surface preparations-Spectroscopic Surface methods, electron spectroscopy, ion scattering spectrometry secondary ion scattering microscopy (SIMS)-Auger electron spectroscopy- instrumentation and application. Electron stimulated micro analysis. Scanning probe microscopes.

Text Books

1. P. W. Atkins, 'Physical Chemistry', 6th Edn., Oxford University Press, 1998.
2. D. McQuarrie, and J. D. Simmen, 'Physical Chemistry', 1st Edn., University Science Books, 1998.
3. S. Glasstone, Thermodynamics for chemists, Affiliated East West Press, 1965.

References

1. B. C. McClelland, Statistical Thermodynamics, Chapman and Hall, 1973.
2. L. K. Nash, Elements of classical and statistical thermodynamics, Addison-Wesley, 1970.
3. K. K. Rohatgi - Mukkerjee, "Fundamentals of Photochemistry", Wiley Eastern Ltd., (1992).
4. P. K. Ghosh, 'Introduction to Photoelectron Spectroscopy', Wiley Interscience, 1983.

CH 619 Applications of Spectroscopy

Nuclear Magnetic Resonance- Concept of nuclear and electronic theory of magnetic resonance, nuclear magnetic resonance, chemical shift and spin coupling. Different Experimental schemes and their working, Polarization Transfer schemes, INEPT/DEPT, NOE.

Nuclear Magnetic Resonance: Analysis and applications of ^1H , ^{13}C , ^{19}F , ^{31}P , spectra in different organic and inorganic compounds. Working of 2-D methods COSY, TOCSY, NOESY, and INADEQUATE and their applications in organic Chemistry

Electron Paramagnetic Resonance: principles, selection rules for transitions, hyperfine interaction and zero-field energy levels, Applications of multifrequency CW-EPR in radicals and complexes. Pulse EPR basics, Model system for pulse EPR and ENDOR experiments, Pulse Schemes and Applications, nuclear modulation experiments, 2- pulse and 3- pulse ESEEM, HYSCORE, Davies and Mims ENDOR, Spin labeling in EPR, Interpretation of EPR parameters, Distance measurements using ELDOR.

Mass spectroscopy: Methods of desorption and ionization (EI, CI, LD, MALDI, PD, FAB, SIMS), Instrumentation, determination of molecular formula, meta stable ions and their significance, study of fragmentation pattern. Applications in Organic Chemistry.

Principles and applications Mossbauer and Photo-Electron spectroscopy. Applications of EPR & NMR in identifying fluxional molecules in Organometallics. Woodward-Fieser rules for prediction of λ_{max} for dienes, trienes, α - β unsaturated carbonyl compounds, aromatic and hetero cyclic systems. Applications of IR spectroscopy to organic compounds. Case studies and structural identification of organic compounds using Uv-Vis, IR, NMR and Mass spectral data.

Text Books

1. R. M. Silverstein and F. X. Webster: Spectrometric Identification of Organic Compounds, 7th Edn, 2007
2. L. D. Field, S. Sternhell, J. R. Kalman, Organic Structures from Spectra, 4th Edn, John Wiley & Sons, Ltd, 2007

References

1. J. A. Weil, J. R. Bolton, Electron Paramagnetic Resonance, Elementary Theory and Practical Applications, 2nd Edn, Wiley-Interscience, 2007,
2. A. Schweigher, G. Jeschke, Principles of Pulse Electron Paramagnetic Resonance, Oxford University press, 1999
3. W. Kemp, Organic Spectroscopy, 3rd Edn, Palgrave, 1998
4. E. Breitmaier, Structure Elucidation by NMR in organic chemistry, A Practical Guide, 3rd Edn, John Wiley & Sons, ltd, 2002

CH 623 – Physical and Organic Chemistry Practicals

1. Estimation of an acid using pH-metry.
2. Conductometric titration of mixture of acids.
3. Precipitation titration (KCl Vs AgNO_3) using conductivity bridge.
4. Potentiometric titration: Precipitation titration Cl^- and I^- Vs AgNO_3 , Redox titration of Fe^{2+} .

5. Estimation of iron by spectrophotometry.
6. Separation and characterisation of two component and three component mixtures.
7. Chromatographic separation of amino acids, carbohydrates and natural pigments.
8. Single stage preparations involving acetylation, alkylation, condensation, hydrolysis, esterification etc.,
9. Electro organic synthesis of simple polymeric substances.

Text Books

1. D. P. Shoemaker, C. W. Garland & J. W. Nibber,, 'Experiments in Physical Chemistry', McGraw Hill 5th Edn., 1989.
2. A. I. Vogel, 'Text book of Practical Organic Chemistry', 5th Edn. ELBS, London , 1989.

References

1. B. B. Dey, and M. V. Sitharaman, 'Laboratory Manual of Organic Chemistry' Revised by T.R. Govindachari, Allied Publishers Ltd., New Delhi. 4th Revised Edn. 1992.

CH 625 – Analytical and Inorganic Chemistry Practicals

1. Quantitative analysis: analysis involving volumetric and gravimetric estimations of atleast
2. four mixtures of cations Cu & Ni; Cu & Zn; Zn & Cu; Fe & Ni; Fe(II) & Fe(III)
3. Titrimetry: Complexometric titrations involving estimations of calcium, magnesium, nickel, zinc and hardness of water.
4. Colorimetry: Colorimetric estimations of copper, nickel, iron and chromium using
5. photoelectric colorimeter.
2. Determination of N,P and K in a fertilizer sample
3. Determination of salt concentration of solution of unknown concentration using ion-
6. Exchanger.
7. Evaluation of thermal stability of primary standards by TGA and DTA.
8. Analysis of coal.

Text Books

1. Vogel, A.I., 'Text book of Quantitative Inorganic Analysis' 5th Edn. ELBS, with Longman, London, 1989.

SEMESTER 4

CHE 614 - Nuclear Chemistry

Discovery- Types of decay-Decay kinetics: Decay constant, half-life period, mean life Parentdaughter decay-growth relationships-Secular and transient equilibrium-Units of radioactivity- Alpha, beta and gamma decay: Theory of decay, energies and properties-Artificial radioactivity- Detectors: Ionization chamber, electron pulse counters, scintillation detectors, semiconductor, detectors, thermo luminescence detectors and neutron detectors.

Bethe notation-Types of nuclear reactions: The compound nucleus theory-Reaction crosssection- Transmutation reactions, elastic and inelastic scattering, spallation, fragmentation, stripping and pick-up, fission, fusion, photonuclear reactions, Thermonuclear reactions.

The fission energy – Reproduction factor - Classification of reactors- Based on Moderators, Coolant, Phase of Fuel and Generation -Principle of Thermal nuclear Reactors: The four factor formula - Reactor power – Critical size of a thermal reactor – Excess reactivity and control - Breeder reactor - Reprocessing of spent fuels - Nuclear waste management – Safety culture – Active and passive safety, containment building, nuclear criticality safety, ionizing radiation protection – enforcement agencies.

Radiation chemistry – Passage of radiation through matter – Units for measuring radiation absorption – Radiation dosimetry – Radiolysis of water – Free radicals in Water Radiolysis – Chemical dosimetry: Radiolysis of Fricke Dosimeter Solution – Radiation-induced colour centres in crystals – Effects of radiation with matter: Radiolysis of inorganic gases, organic gases, organic compounds, solids, and polymers- Annealing of radiation damage.

Application of radioisotopes: probing by isotopes, reactions involved in the preparation of radioisotopes, The Szilard-Chalmer's Reaction – Radiochemical principles in the use of Tracers – Applications of radioisotopes as tracers- Chemical investigations, analytical applications, agricultural and industrial applications -Neutron Activation Analysis – Carbon and Rock Dating – Use of nuclear reactions- Radioisotopes as source of electricity – Nuclear medicines.

Text Books

1. Walter Loveland, David Morrissey, Glenn Seaborg. Modern Nuclear Chemistry, Wiley-Interscience, Hoboken, NJ, 2006
2. Arnikar, H. J., 'Essentials of Nuclear Chemistry', 4th Edn., New Age International Publishers Ltd., New Delhi, 1995.

References

1. K. H. Lieser, Nuclear and Radiochemistry, 2nd revised ed., Wiley-VCH, Berlin, 2001.
2. G. Choppin, J. O Liljenzin and J. Rydberg. Radiochemistry and Nuclear Chemistry. 3rd ed. Butterworth-Heinemann, Oxford, 2002.
3. G Friedlander, GW Kennedy, ES Macias and JM Miller. Nuclear and Radiochemistry. 3rd ed., John Wiley & Sons, New York, 1981.

CHE 616 - Medicinal Chemistry

Introduction to the History of Medicinal Chemistry, General Mechanism of Drug action on lipids, carbohydrates, proteins and nucleic acids, drug metabolism and inactivation, receptor structure and sites, drug discovery development, design and delivery systems, gene therapy and drug resistance.

Classification of drugs based on structure or pharmacological basis with examples Synthesis of important drugs. Such as α - methyl dopa, Chloramphenicol griseofulvin, cephalosporins and nystatin Molecular modeling, conformational analysis, qualitative and quantitative structure activity relationships.

General introduction to antibiotics, mechanism of action of lactam antibiotics and non lactam anti biotics, antiviral agents, Chemistry, stereochemistry, biosynthesis and degradation of penicillins - An account of semisynthetic penicillins - acid resistant, penicillinase resistant and broad spectrum semisynthetic penicillins.

Elucidation of enzyme structure and mechanism, kinetic, spectroscopic, isotopic and stereochemical studies. Chemical models and mimics for enzymes, Design, synthesis and evaluation of enzyme inhibitors

DNA-protein interaction and DNA-drug interaction Introduction to rational approach to drug design, physical and chemical factors associated with biological activities, mechanism of drug action

Text Books

1. I. Wilson, Giswald and F. Doerge, 'Text Book of Organic Medicinal and Pharmaceutical Chemistry', J.B. Lippincott Company, Philadelphia., 1971.
2. A. Burger. Medicinal Chemistry, Wiley Interscience, New York, Vol.I and II., 1970.

References

1. Bentley and Driver's Text Book of Pharmaceutical Chemistry revised by L.M. Artherden, Oxford University Press, London, 1977.
2. A. Gringauz, Introduction to Medicinal Chemistry, How drugs act and why, John Wiley and sons, 1997
3. G. L. Patrick, Introduction to Medicinal Chemistry, Oxford Univeristy Press, 2001

CHE 618 - Polymer Chemistry

Fundamental concepts - functionality - principle of polymerisation - addition, condensation polymerisation - ring opening polymerisation - classification - production from coal tar and petrochemicals - Techniques of polymerisation - gas polymerisation, - bulk, solution, suspension and emulsion - melt condensation.

Mechanism of polymerisation and general characteristics - free radical - cationic, anionic and coordination polymerisation (Ziegler-Natta catalyst) autoacceleration - Kinetic chain length - degree of polymerisation kinetics of polymerisation (Detailed study) - copolymerisation.

Polymer characterisation - molecular weight, MWD - M_n , M_w , M_v and M_z - end group analysis - viscometry - osmometry - Light scattering - spectral analysis-Thermal properties – Electrical properties, Mechanical and dynamic properties - polymer degradation. Phase transitions of polymers, crystallization and glass transition, mechanism of glass transition , methods of determining T_g .

Studies of individual polymers - plastics - polyolefins, polystyrenes, acrylics, polyesters, polyamides, cellulose, polyurethanes, Inorganic polymers, FIR plastics - GRplastics. alkyd resins, epoxy resins - phenolics - Melamine resins - compounding of plastics - rubber - elastomer - vulcanisation, compression mouldings - injection mouldings - lamination .

Biopolymers - Biomaterials - medicinal applications of polymers - High temperature and fire resistant polymers. Polymer concrete - polymer impregnated concrete - conducting polymers - polymeric reagents.

Text books

1. P.J. Flory, 'Principles of Polymer Chemistry', Cornell Press,(Recent Edition).
2. Jr. Billmeyer, 'Test Book of Polymer Science', Fred, W. John Wiley & Sons, New York, 1984.

References

1. F. Rodrigues, 'Principles of Polymer Systems', M. Elpaw Hill Book Company, 2nd Edn., 1982.
2. K.J.Saunders, , 'Organic Polymer Chemistry', Chapman & Hall, London, 1973.
3. N. Mathur and Williams, 'Polymers as Aids in Organic Chemistry', Academic Press, 1980.

CHE 620-Biochemistry

Foundations of Biochemistry: Cellular foundations, Chemical, Physical, Genetic and Evolutionary foundations, Amino Acid structure, Essential Amino Acids, amino acid metabolism, proteins, primary structure, Hydrophobic Interaction , van der Waals Interactions and London Dispersion Forces, Secondary Structure, Protein Stability, Temperature-Sensitive Mutations, Ligand-Binding Specificity, Membranes and Membrane Proteins, General Structure, Function, the composition and transport across membranes, membrane dynamics, Movement of Ions and Molecules Across Membranes, Transport Across Membranes, The Nernst Equation

Enzyme mechanism, Active Site, Transition State, Catalysis, Lock and Key mechanism, Enzyme kinetics, Michaelis-Menten Equation, Inhibition, Allosterism and Cooperativity, The Monod- Wyman-Changeaux Model, Signal Transduction Pathways, Organization, Signals, Receptors, soluble Receptors, Transmembrane Receptors, Enzyme Coupled Receptors, G-Protein Coupled Receptors, Ion-Channel Coupled Receptors, Second Messengers

Nucleotides and nucleic acids, Expression of Genetic Information, DNA & RNA, Structure and stability. Information Metabolism, DNA Replication , Types of DNA Polymerase, Regulation of Information Metabolism , Transcription, Regulation of Transcription, High-Energy Phosphate Bonds and Translation , Recombinant DNA methodology, Restriction Analysis, Gels and Electrophoresis, Expression of genetic information, Cloning, Sequencing , Mutagenesis

Bioenergetics and metabolism, Glycolysis and gluconeogenesis and pentosephosphate pathway, Glycolysis Function, Gluconeogenesis Function, Glycogen synthesis and degradation, the citric acid cycle, Fatty acid catabolism, fatty acid synthesis and degradation, triglycerids and phospholipids synthesis, electron transport and oxidative phosphorylation, photophosphorylation, and ATP synthesis, Lipids, storage metabolism, amino acid oxidation and production of urea, carbohydrate biosynthesis in plants and bacteria

Information and Integrating Metabolic Pathways, Genes and Chromosomes, ATP, Glucose, Storage Molecules, Metabolic States and Signals, Insulin, Glucagon, Epinephrine, Fat, Metabolic Movements of Fat, Tissue Cooperation, Liver, Muscle, Adipose, Brain, Connection of Storage Pools, Feeding, Fasting, Starvation, Interorgan Cycles, Cori Cycle, Alanine Cycle, Ketone Bodies, Urea Cycle, Purine metabolism, Pyrimidine metabolism, one carbon metabolism, oxidation states of carbon, glucose to pyruvate, TCA cycle.

Text Books

1. H. F. Gilbert, Basic Concepts of Biochemistry, A Students Survival Guide, 2nd Edn, McGraw Hill, 1992.
2. L. Lehninger, Biochemistry, 4th Edn, 2000.

CHE 622-Catalysis

The Phenomenon Catalysis - Mode of Action of Catalysts - Classification of Catalysts - Comparison of Homogeneous and Heterogeneous Catalysis. Individual Steps in Heterogeneous Catalysis - Kinetics and Mechanisms of Heterogeneously Catalyzed Reactions (Langmuir– Hinshelwood, Eley–Rideal)- - Catalyst Concepts in Heterogeneous Catalysis- Catalyst Performance - Catalyst Deactivation and Regeneration - Characterization of Heterogeneous Catalysts.

Preparation and characterization methods: Catalyst preparation. Structured catalysts and zeolite. Synthesis of zeolites, - Isomorphic Substitution of Zeolites -Metal-Doped Zeolites – Applications of Zeolites and Mesoporous solids. Catalyst characterization by SEM, EDAX, XRD, XPS, Electron microscopy, Gas adsorption and other techniques.

Mechanisms of selected reactions - Acid catalysis and zeolites. Processing of petroleum and hydrocarbons. Catalytic oxidation. Synthesis gas and associated processes. Steam reforming. The water gas shift reaction. Methanation. Ammonia production. Nitric acid. Methanol and formaldehyde. Fischer-Tropsch. Catalysis for environmental protection and energy production. Three way catalysts for automobiles. hydrogenation and dehydrogenation reactions – dehydration of alcohols - olefin hydrogenation - decomposition of nitrous oxide - oxidation of COketonization of carboxylic acids, cracking of hydrocarbons.

Green Chemistry and Catalysis- Catalysts for PTC - Mechanism and Benefits of PTC –PTC Reactions - Selected Industrial Processes with PTC. Automotive Exhaust Catalysis - NOx and SOx Removal Systems -. Examples of catalytical process, Photocatalysis Basic Principles - Photoreduction and Oxidation of Water - Photocleavage of Water. Introduction to Biocatalysis - Kinetics of Enzyme-catalyzed Reactions -Industrial Processes with Biocatalysts. Introduction to Electrocatalysis and fuel cells.

Industrial application of catalysis- Petroleum Refining – Distillation, Cracking, Reforming, Hydrotreating, Alkylation and Isomerization, Steam Cracking. Ethylene-Based Processes - Ethylene Oxide and Ethylene Glycol, Polyethylene, Vinyl Chloride and PVC. Propylene-Based Processes - Acrylic Acid and Acrylonitrile, PP and Ziegler-Natta Chemistry. C4-Based Processes – Butadiene, Isobutylene, BTX Processes - Styrene and Polystyrene, Polyethylene Terephthalate (PET), Phenol, Adipic Acid and Nylon, Phthalic Anhydride

Text Books:

1. Emmett, P.H. - " Catalysis Vol.I and II, Reinhold Corp. ", New York, 1954.
2. Smith, J.M. - " Chemical Engineering Kinetics ", McGraw Hill, 1971.

References

1. Thomas and Thomas " Introduction to Hetrogeneous Catalysts ", Academic Press, London 1967.
1. Jens Hagen – “Industrial Catalysis: A Practical Approach”, 2nd Edition, WILEY-VCH, March 2006.
2. H. Bartholomew, Robert J. Farrauto, “Fundamentals of Industrial Catalytic Processes”, 2nd Edn; Wiley. 2006

CHE 624- Nano Science and Technology

Introduction to Nanoscience: Introduction - definition of nanoscience, nanochemistry - classification of the nanomaterials – zero dimensional nano structures - one dimensional nanostructures – nanowires and nanorods – two dimensional nanostructures – films, nanotubes and biopolymers – three dimensional nanostructures – fullerenes and dendrimers – quantum dots and their properties. Basic instrumentation and imaging techniques.

Synthesis of Nanomaterials: Introduction - precipitative methods - reactive methods in high boiling point solvent - hydrothermal and solvothermal methods - gas phase synthesis of semiconductor nano- particles – water based gold nanoparticle synthesis - organic solution based synthesis-sonochemical methods and microwave methods. CNTs and CNFs

Properties of nanomaterials : Electronic Structure of Nanoparticles. Electronic properties and thermal properties. Melting point and phase transition processes- quantum-size-effect (QSE). Size-induced metal-insulator-transition (SIMIT)- nano-scale magnets, transparent magnetic materials, and ultrahigh-density magnetic recording materials-chemical physics of atomic and molecular clusters.

Chemistry Aspects Photochemistry; Photoconductivity; Electrochemistry of Nanomaterials-Diffusion in Nanomaterials; Nanoscale Heat Transfer; Transport in Semiconductor Nanostructures; Transition Metal Atoms on Nanocarbon Surfaces; Nanodeposition of Soft Materials; Nanocatalysis, Catalysis by gold and silver Nanoparticles;

Nanostructures- Kinetics in Nanostructured Materials- Zero dimensional, one-dimensional and two dimensional nanostructures- clusters of metals and semiconductors, nanowires, nanostructured beams, and nanocomposites-artificial atomic clusters-Size dependent properties size dependent absorption spectra-phonons in nanostructures.

Text Books

1. T. Pradeep, Nano: The Essentials, Tata McGraw-Hill, New Delhi, 2007.

References

1. G. Cao, Nanostructures and Nanomaterials – Synthesis, Properties and Applications, Imperial College Press, London, 2004, chapters 3, 4 and 5.
2. C. N. R.Rao, A. Muller and A. K. Cheetham, The Chemistry of Nanomaterials, Volume 1, Wiley –VCH Verlag GmbH & Co. KgaA, Weinheim, 2004,c Chapter 4.

CHE 626- Computational Methods in Chemistry

C – Syntax : Character set-constants and variables, data types and sizes, declarations, operators – Expressions – Conditional expressions, precedence and order of evaluation, Statements and blocks, if-else, if-else-if and switch statements, while, for and Do – while loops, break and continue statements, Goto and labels, basics of functions and types, header files, recursion, Arrays – 1D and 2D, file handling concepts.

Kinetics – Solving rate equations, thermodynamics – Heats of reactions, heat capacity, entropy, spectroscopy – Moment of inertia, wave numbers of stokes and anti-stokes Raman lines, masses of isotopes from rotational and vibrational spectroscopic data – Group theory – Huckel MO calculations of delocalisation energy, hybridisation schemes and symmetries of

vibrations in non – linear molecules. Crystallography – d spacings for an orthorhombic crystal, Fourier synthesis of electron density using structure factor, axial angles of a triclinic crystal.

Solving polynomial equations – Newton – Raphson method, solutions of simultaneous equations – Gauss elimination, Jacobi iteration and matrix diagonalisation, numerical differentiation and integration – Simpson’s rule, trapezoidal rule- determination of entropy, solution of differential equations – Runge-Kutta method- theory and application to thermodynamics, linear and nonlinear curve fitting.

Force field methods-force field energy and parameterization, Electronic structure methods-SCF techniques, semi-empirical methods, Basis sets and their classification, density functional theory and methods.

Geometry convergence, energy convergence, dipole moment convergence, vibrational frequencies convergence, bond dissociation curve, angle bending curve, transition state modeling using Chemoffice and Gaussian software.

Text Books

1. K. V. Raman, ‘Computers in Chemistry’, Tata McGraw Hill, 1993.
2. F. Jensen, ‘Introduction to Computational Chemistry’, John Wiley & Sons, 2003.

References

1. C. Balagurusamy, ‘Programming in C’, Tata McGraw Hill, 1997.
2. M. K. Jain, ‘Numerical Methods for Scientific and Engineering Computation’, Wiley Eastern Ltd, 1995.
3. User manuals of Gaussian03, Chemoffice Ultra and Gauss View.

CHE 628 – Unit Operations and Processes

Material balances, Different types of Evaporators, Different feed, Single and Multiple effects, multistage, Capacity and Economy.

Material balance, Yield, Super Saturation Theory, Nucleation, Miers Theory, Different Types of crystallisers. Extraction - Principles of Solid-liquid extraction, leaching, equipments.

Material balances, Various types of distillation, Vacuum distillation, Rectification, Stripping, McCabe-Tiele Diagram, Reflux, Murphree Plate efficiency.

Humidifications - Definitions, Psychrometric charts, Cooling towers. Drying: Principles of drying, Rate curves, theories of drying, Effect of flow rate, temp. humidity on drying rates, classification of dryers, Equipments. Filtration - Principle involved only.

Basic principles of unit processes and industrial applications of Nitration, Hydrogenation, oxidation, sulfonation and alkylation.

Text books

1. I. W.L. McCabe. and J.C. Smith, ‘ Unit Operation in Chemical Engineering’, 5th Edn., McGraw Hill ,1994.
2. Groggins, Unit Processes of Organic Synthesis.