DEPARTMENT OF CHEMISTY
MSC SYLLABUS

Paper No	Name of Paper	Credits	Marks
1st Semester			
CHE-PG-C101	Inorganic Chemistry I	4	100
CHE-PG-C102	Organic Chemistry I	4	100
CHE-PG-C103	Physical Chemistry I	4	100
CHE-PG-C104	Practicals I	4	100
		16	400
2nd Semester			
CHE-PG-C201	Inorganic Chemistry II	4	100
CHE-PG-C202	Organic Chemistry II	4	100
CHE-PG-O203	Mathematics	4	100
CHE-PG-C204	Practicals II	4	100
		16	400
3rd Semester			
CHE-PG-O301	Biochemistry	4	100
CHE-PG-C302	Physical Chemistry II	4	100
CHE-PG-C303	Instrumental Techniques	4	100
CHE-PG-C304	Practicals III	4	100
		16	400
4th Semester			
CHE-PG-E401	Elective I	4	100
CHE-PG-E402	Elective II	4	100
CHE-PG-O403	Environmental Chemistry	4	100
CHE-PG-C404	Project	4	100
		16	400
TOTAL	36	1600	

Semester I

CHE-PG-C101: Inorganic Chemistry I

Unit I: Valence Shell Electron Pair Repulsion (VSEPR) Model
Valence Shell Electron Pair Repulsion model, stereochemical rules and explanation of the shapes of molecules and ions of non-transition elements with 2-7 valence shell electron pairs.
Hard Soft Acid Base (HSAB) Theory: Classification of acids and bases as hard and soft; HSAB principle, theoretical basis of hardness and softness; Lewis-acid base reactivity approximation; donor and acceptor numbers, E and C equation; applications of HSAB concept.

Unit II: Symmetry of molecules
Symmetry operations and symmetry elements, point group classification and symmetry number.
Coupling: Russell-Saunders coupling for d^n states. Splitting of one-electron levels in an octahedral environment. Correlation diagram. The method of descending symmetry, selection rules. Spectral transition probability, vibronic coupling, non-centrosymmetric complexes, polarization of allowed transitions.

Unit III: Metal-Ligand Bonding in Transition Metal Complexes
Crystal field splitting diagrams in complexes of low symmetry; Spectrochemical and Nephelauxetic series; thermodynamic and structural effects; site selection in spinels, Jahn-Teller distortions; experimental evidence for metal-ligand orbital overlap; ligand field theory, molecular orbital theory of octahedral complexes, brief introduction to Angular Overlap Model.
Electronic spectra of Transition Metal Complexes: Spectroscopic ground states; Orgel energy level and Tanabe-Sugano diagrams for transition metal complexes; Charge transfer spectra; electronic spectra of octahedral and tetrahedral Co(II) and Ni(II) complexes and calculation of ligand-field parameters.

Unit IV: Chemistry of non-transition elements
Non-transition metal chemistry. Synthesis, Properties, Structure and Bonding: Nitrogen, Phosphorous, Sulfur, Pseudohalogen, Interhalogen and Xenon Compounds; Boranes, Carboranes, Metallocarboranes, Borazines, Phosphazenes, Sulfur-Nitrogen compounds, silicates, silicones. Iso- and Hetero- poly anions.

References

1. Cotton, F.A. and Wilkinson, G. 1999 Advanced Inorganic Chemistry, 6th Edn., John Wiley & Sons, New York.
2. Huheey, J. E., 1993 Inorganic Chemistry, 4th Ed., Addison-Wesley Pub. Co., New York.
3. Drago, R. S., 1971 Physical Methods in Inorganic Chemistry, International Edn., Affiliated East-West Press, New Delhi.
4. Shriver, D. F. and Atkins, P. W., 1999 Inorganic Chemistry, 3rd Edn., ELBS, London.
5. Cotton, F. A., Wilkinson, G. and Gaus, P.L., Basic Inorganic Chemistry, 3rd Edition, John Wiley & Sons, New York.
6. Greenhood, 1976, Spectroscopic properties of inorganic and organometallic compounds, Royal Society of Chemistry.
7. Lee, J. D. 1999 Concise Inorganic Chemistry, Blackwell Science.
8. Purcell K. F. and Kotz J. C., 1987 Inorganic Chemistry, W. B. Sauders Com. , Hong Kong.

CHE-PG-C102: Organic Chemistry I

Unit I: Aromaticity
Benzenoid and nonbenzenoid systems, antiaromaticity and non aromatic compounds.
Effects of Structure on Reactivity: Hammett equation, Linear free energy relationships (LFER) and substituent and reaction constants. Structure-activity relationship. Taft equation

Unit II: Aliphatic Nucleophilic Substitution at Saturated Carbon

Mechanism and Stereo-chemistry of S_N1, S_N2, S_Ni, S_N1' and S_N2' reactions. Neighboring group participation. Classical and non-classical carbocations. The reactivity effects of substrate structure, solvent effects, competition between S_N1 and S_N2 mechanisms. Phase transfer catalysis, ambident nucleophilicity, regioselectivity.

Unit III: Aromatic Electrophilic Substitution

The Arenium ion mechanism, orientation and reactivity in monosubstituted benzene rings, ortho/ para ratio. Ipso substitution. Effect of substrates, leaving groups and solvent polarity on the reaction.

Aromatic Nucleophilic substitution: Aromatic S_NAr, S_N1, S_N2 and benzyne mechanisms. Reactivtiy : effect of substrate structure, leaving group, and attacking nucleophile.

Unit IV: Addition to Carbon–Carbon Multiple Bonds

Electrophilic, free-radical and nucleophilic mechanisms-Mechanistic and Stereochemical aspects. Orientation and reactivity. Hydroboration and Michael reaction.

Elimination reactions: The E1, E2 and E1cB mechanisms, Orientation of the double bond. Hofmann versus Saytzeff elimination, Pyrolytic *syn*-elimination- Chugaev and Cope eliminations, Competition between substitution and elimination reactions.

Nucleophilic Addition to Carbonyl Compounds

Hard and soft nucleophiles, addition to conjugated carbonyls; Competition between 1,2 and 1,4 addition, Meerwin-Pondorf Reaction, Cannizaro reaction, stetter reaction, Aldol condensation, Grignard reagent, alkyl lithium, Perkin reaction, Benzoin condensation, Benzilic acid rearrangement, Wittig reaction,

References

1. Smith M. B. and March, J. 2001 March's Advanced Organic Chemistry, 6th Edn, John Wiley & Sons, New York.
2. Sykes, P. 1997 A Guide book to Mechanism in Organic Chemistry, 6th Edition, Orient Longman Ltd., New Delhi.
3. Fryhle, S. Organic Chemistry, 8th Edition, John Wiley & Sons, New York.
4. Clayden, J., Greeves, N. , Warren, S. and Wothers, P., 2000 Organic chemistry, Oxford University Press.
5. Bruice, Organic Chemistry, 5th Edition, Pearson Education
6. Carey F. A. and Sundburg R. J. 2007 Advance Organic Chemistry; 5th Ed. Springer
7. Mukherjee S. M. and Singh, S. P, 1990 Reaction Mechanism in Organic Chemistry, Ist Edition, Macmillan India Ltd., New Delhi.
8. Lowry T.H. and Richardson, K. S. 1998 Mechanism and Theory in Organic Chemistry, 3rd Edition, Addison – Wesley Longman Inc. (IS Edition)
9. Morrison R. T. and Boyd, R. N. 2003 Organic Chemistry, 6th Edition, Prentice- Hall of India, New Delhi.
10. Kalsi, P. S. 1996 Organic Reactions and Their Mechanisms, Ist Edition, New Age International Publication, New Delhi.

CHE-PG-C103: Physical Chemistry I

Unit I: Thermodynamics

Review of Laws of Thermodynamics. Entropy, free energy and chemical potential. Partial molar properties and their significance. Fugacity: its concept and determination. Properties of ideal solutions; non-ideal systems-deviations (negative and positive) from ideal behaviour, excess functions for non-ideal solutions, calculations of partial molar quantities, determination of partial molar volume and partial molar enthalpy.

Chemical Kinetics: Composite Reactions – types of composite mechanisms, rate equations for composite mechanisms, simultaneous and consecutive reactions, steady state treatment, rate-determining steps, microscopic reversibility and detailed balance, chain reactions (H_2-Br_2 reaction, decomposition of ethane and acetaldehyde) and oscillatory reactions (Belousov-Zhabotinskii reaction)

Unit II: Electrochemistry

Metal/Electrolyte interface**:** Outer Helmholtz Potential **(**OHP) and Inner Helmholtz Potential **(**IHP), potential profile across double layer region, potential difference across electrified interface; Structure of the double layer **:** Helmholtz-Perrin, Gouy-Chapman, and Stern models. Butler-Volmer equation under near equilibrium and non-equilibrium conditions, exchange current density, Tafel plot. Polarizable and non-polarizable interfaces. Electrochemical cells and Batteries.

Unit III: Surface Chemistry and Catalysis

Interphase region, curved surfaces. Thermodynamics of surfaces **:** Gibbs adsorption isotherm, heat and entropy of adsorption. Surface film on liquids, electro-kinetic phenomena. Catalytic activity at surfaces (volcano curve), Surface area determination (BET equation), transition state theory of surface reactions: rates of systematic ions and desorption, unimolecular and bimolecular surface reaction, comparison of homogeneous and heterogeneous reaction rates, surface heterogeneity, lateral interaction.

Unit IV: Micelles and Macromolecules

Surface active agents and their classification, micellization, hydrophobic interaction, critical micellar concentration (cmc), factors affecting cmc of surfactants, counter ion binding to micelles, thermodynamics of micellization-phase separation and mass action models, solubilization, micro emulsions, reverse micelles. Polymers-definition, types of polymers, liquid crystal polymers. Molecular mass-number and mass average molecular mass, determination of molecular mass (osmometry, viscosity, light scattering methods, Gel Permeation chromatography).

Colloids: Multimolecular, macromolecular and associated colloids. Stability of collids. The zeta potential. Kinetic, optical and electrical properties of colloids. Electrokinetic phenomena: Electrophoresis, electroosmosis, sedimentation potential and streaming potential. Donnan membrane equilibrium. Collodal quntum dots, Metal nanoparticles and magnetic nanoparticles. Size dependent optical and electrical properties. Supermagnetic limit.

Solid states: Crystal systems; Designation of crystal faces, lattice structures and unit cell; Bragg's law; X-ray diffraction by crystals; Close packing, radius ratio rules, calculation of some

limiting radius ratio values; Structures of NaCl, KCl, ZnS, CsCl and CaF2; Stoichiometric and nonstoichiometric defects, impurity defects, semi-conductors.

References

1. Bockris J.O'M., and Reddy, A. K. N. 1998 Modern Electrochemistry, Vol. 1 & Vol. 2 A & B, Second Edition, Plenum Press, New York.
2. Laidler, K. J. 1987, Chemical Kinetics, Third Edition, Harper & Row, New York.
3. Atkins, P. W. , 2002 Physical Chemistry, Seventh Edition, Oxford University Press, New York.
4. Levine, I. N. 2002 Physical Chemistry, 5th Edition, Tata McGraw Hill Pub. Co. Ltd., New Delhi.
5. Ram J. Raja and Kuriacose, J.C. 1993 Kinetics and Mechanism of Chemical Transformations, MacMillan Indian Ltd., New Delhi.
6. Barrow, G.M. Physical chemistry, 3rd edn., international student edition, McGraw-Hill
7. Glasstone. S. 1940, Text - book of physical 1940. Publisher: Van Nostrand.
8. Pilling M. J. and Seakins, P. W. 1995 Reaction Kinetics, Oxford University Press, 1995
9. Moore, W. J. 1972, Physical Chemistry, Prentice Hall College Div; 4th edition
10. Engel T. and Reid P., Physical Chemistry, Pearson Education

CHE-PG-C104: Practicals I

Inorganic Chemistry Experiments

A. Ore and Alloy Analysis: (Any two)

1. Determination of Silica and Manganese in pyrolusite
1. Determination of Copper and iron from chalcopyrite.
2. Determination of iron from hematite by complexometric titration.
3. Determination of tin & lead from solder.
4. Determination of iron & chromium from mild steel.
5. Determination of copper and nickel from cupronickel.
6. Determination of iron from hematite using UV-Vis spectrophotometer.
7. Determination of phosphoric acid in soft drinks

B. Preparation and Characterization of the following compounds (Any eight preparations are to be completed):

1. Tris (oxalate) manganese (III)
2. Tetrapyridinesilver (II) peroxidisulphate
3. Tris (acetylacetonato) iron (III)
4. Bis (N,N-diethyldithiocarbamato) nitrosyliron (I)
5. Optical isomers of tris (ethylenediamine) cobalt (III) chloride
6. Linkage isomers of nitro and nitritopentamminecobalt (III) chloride

7. Ferrocene or dibenzene chromium
8. Hydridochlorocarbonyl tris (triphenylphosphine) ruthenium (II)
9. Tris(2,2'-bipyridine)ruthenium (II) perchlorate
10. $[(p\text{-(cymene)}RuCl_2]_2$
11. Tris (acetylacetonato) manganese (III)
12. Copper(I) Thiourea complexes: $[Cu(Tu)_6]SO_4.\ H_2O$

Characterization includes microanalysis, magnetic susceptibility and conductance measurements and infrared, UV-Visible, NMR spectroscopy, XRD and cyclic voltammetry studies.

Books Recommended:

1. Elias, A. J., Collection of Interesting General Chemistry Experiments, Orient Longman.
2. A text book of Quantitative Inorganic Analysis – A. I. Vogel
3. Experimental Inorganic Chemistry - W. G. Palmer
4. Synthesis and Characterization of Inorganic Compounds, W.L. Jolly, Prentice Hall.
5. Chemistry experiments for Instrumental Methods by Donald T. Sawyer, William R. Heineman & Jalice M. Beebe , John Wiley & Sons ,1984.
6. Experimental Physical Chemistry by G. Peter Matthews, Clarendon Press, 1985.
7. Modern Experiments for Introductory Chemistry, compiled by Neidig and Strattom, 2nd Ed., Reprinted from Journal of Chemical Education,1990.
8. Handbook of Inorganic Synthesis: G. Brauer
9. Inorganic Synthesis: R. B. King
10. Synthesis and Technique in Inorganic Chemistry: A Laboratory Manual, Gregory S. Girolami, Thomas B. Rauchfuss and Robert J. Angelici. University Science Books.

Semester II

CHE-PG-C201: Inorganic Chemistry II

Unit I: Kinetics and Mechanism of Substitution Reactions

Nature of substitution reactions; prediction of reactivity of octahedral, tetrahedral and square-planar complexes in terms of crystal field activation energy and structure preference energy; rates of reactions; acid hydrolysis, base hydrolysis and anation reactions.

Electron Transfer Reactions: Mechanism and rate laws; various types of electron transfer reactions, Marcus-Husch theory, correlation between thermal and optical electron transfer reactions; identification of intervalence transfer bands in solution.

Unit II: Metal Carbonyls

Preparation, structure, and properties; bonding in metal carbonyls, variants of CO bridging, vibrational spectra of metal carbonyls, principal reaction types of metal carbonyls. Carbonyl metal halides.

Complexes of σ- donor π-acceptor ligands: metal nitrosyls; tertiary phosphines and arsines as ligands; cyanides, isocyanides, alkenyls, alkynyls, carbene and carbine complexes.

Unit III: π-Complexes of Unsaturated Molecules

Preparation, bonding and structures of alkene, alkyne, allyl, dienyl and trienyl complexes; reactions with special reference to organic synthesis.

Transition Metal Compounds in Catalysis: Homogeneous and heterogeneous catalysis, Hydrogenation, hydroformylation and polymerization; Waker process. Fluxional molecules. Heck Reaction, Suzuki Reaction, Buchwald-Hartwig Reaction and Metathesis reaction

Unit IV: Metal Clusters and Metal-Metal Bonds

Compounds with metal-metal multiple bonds, metal carbonyl and halide clusters. Isolobal concept (Hoffman) in organometallic and metal-cluster chemistry.

References

2. Cotton F. A. and Wilkinson, G. 1999 Advanced Inorganic Chemistry, 6th Edn., John-Wiley & Sons, New York.
1. Huheey, J. 1993 E. Inorganic Chemistry, 4th Edn., Addison Wesley Pub. Co., New York.
2. Crabtree, R.H. 1988 The Organometallic Chemistry of the Transition Metals, 1st Edn., John-Wiley & Sons, New York.
3. Shriver , D. F. and Atkins, P. W. 1999 Inorganic Chemistry, 3rd Edn., ELBS, London.
4. Greenhood, 1976 Spectroscopic properties of inorganic and organometallic compounds, Royal Society of Chemistry.
5. Cleydon, J. , Greeves, N. , Warren, S. and Wolthers, P. , 2001 Organic Chemistry: Oxford
6. Collman, J. P. , Hegedus, L. S. , Norton J. R and Finke, Richard G. 1987 Principles and Applications of Organotransition Metal Chemistry, 1st Edn., University Science Books, Mill Valley, California.
7. Elschenbroich, Ch. and. Salzer, A, 1991 Organometallics: A Cosize Introduction, 2nd Edn., VCH
8. Mehrotra, R. C. and Singh, A., 2004 Organometallic Chemistry: A Unified Approach, New age international limited, 2nd Edn.

CHE-PG-C202: Organic Chemistry II

Unit I: Pericyclic Reactions

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reaction; conrotatory and disrotatory motions 4n, 4n+2 and allyl systems. Cycloaddition; antrafacial and suprafacial addition, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions. Sigmatropic Rearrangements; suprafacial and antrafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3- and 5,5- sigmatropic rearrangements, Claisen, Cope and Aza-Cope rearrangements. Ene reaction.

Unit II: Reagents in Organic Synthesis

Use of the following reagents in organic synthesis and functional group transformations; complex metal hydrides, Gilman's reagent, lithium dimethylcuprate, lithium diisopropylamide (LDA), dicyclohexylcarbodiimide, 1,3-dithiane (reactivity Umpoloung), trimethylsilyl iodide, tri-n-butyltin hydride, Woodward and pervost hydroxylation, osmium tetroxide, DDQ, selenium dioxide, Phase transfer catalysts, crown ethers and Merrifield resin, Peterson's synthesis, Wilkinson's catalyst, Baker yeast.

Unit III: Heterocyclic Chemistry

Synthesis and reactivity of furan, thiophene, pyrrole, pyridine, quinoline, isoquinoline and indole; Skraup synthesis, Fisher indole synthesis.

Chemistry of Natural Products: Structure elucidation and biosyntheses of Alkaliods, Terpenoids, Steroids.

Unit IV: Esterification and Hydrolysis of Esters

Evidence for tetrahedral intermediate in BAc^2 and AAc^2 mechanisms, steric and electronic effects. The AAc^1 and other pathways involving alkylto-oxygen bond cleavage.

References

1. Fleming, I. 1976 Frontier Orbital and Organic Chemical Reactions John Wiley,.
2. Carruthers, W. 1990 Some modern Methods of Organic Synthesis Cambridge University Press.
3. Greene, T.W. 1999 Protective Groups in Organic Synthesis Wiley-VCH,.
4. Smith M.B. and March, J. 2001 March's Advanced Organic Chemistry, 5th Edition, John Wiley & Sons, New York.
5. Joule J. A. and Mills, K. Heterocyclic Chemistry: (4th Ed) Wiley-Blackwell
6. Cleydon, J. , Greeves, N. , Warren, S. and Wolthers, P. 2001 Organic Chemistry: Oxford (2001)
7. Paquette L. A. and Benjamin W. A. 1968 Modern Heterocyclic Chemistry by W.A., Inc.,
8. Finar I. L. 1968 Organic Chemistry Vol II, ELBS.
9. Gilchrist, T. R. 1989 Heterocyclic Chemistry.
10. Ward, 1999 Selectivity in Organic Synthesis, Wiley-VCH.
11. Kartritzky A. R. Advances in Heterocyclic Chemistry: Ed., Acad. Press

CHE-PG-O203: Mathematics

Unit I: Functions

Differential and integral calculus, limits, derivative, physical
significance, basic rules of differentiation, maxima and minima, applications in chemistry, exact and inexact differential, periodic function, Taylor and McLaurin series, curve sketching, partial differentiation, rules of integration, definite and indefinite integrals.

Unit II: Differential equations

Separation of variables, homogeneous, exact, linear equations, equations of second order, series solution method. Fourier series and analysis. Complex numbers. Laplace transformation.

Unit III: Permutations, combinations and theory of probability

Distributions.

Vectors, matrices and determinants: Vectors, dot, cross and triple products, introduction to matrix algebra, addition and multiplication of matrices, inverse, adjoint and transpose of matrices, unit and diagonal matrices. Complex Variables

Unit IV: Numerical Methods

Roots of Polynomials, Solution of Linear simultaneous equations, matrix multiplication and inversion. Numerical integration. Statistical treatment of data, variance and correlations, Least square curve fitting. Computer programming in FORTRAN. Computer application in Chemistry: Development of small computer codes involving simple formulae in chemistry

References

1. Steiner E. 1996The Chemical Maths Book, , Oxford University Press.
2. Daniels F. , 1972 Mathematical Preparation for Physical Chemistry, , McGraw Hill
3. Margenau, H and Murphy , G. M. 1956 The Mathematics of Chemistry and Physics- van Nostrand, Princeton, NJ.
4. Norris A. C. Computational Chemistry, John Wiley
5. Press, W. H. , Teukolsky, S. A. Vetterling, W. T. and Flannery B. P. 1996 Numerical Recipes in FORTRAN/C by, Cambridge University Press, 2nd Ed.
6. Xavier , C. 2002 Fortran 77 and Numerical Methods b, New Age International,
7. Boas, M. L. Mathematical Methods in the Physical Sciences, Wiley; 2nd edition

CHE-PG-C204: Practical II
Organic Chemistry Experiments

A. Extraction of Organic Compounds from Natural Source (Any three)

1. Isolation of caffeine, an alkaloid, from tea leaves.
2. Isolation of casein from milk (the students are required to try some typical colour reactions of proteins)
3. Isolation of lactose from milk (purity of sugar should be checked by TLC and PC and Rf value reported.)
4. Isolation of nicotine dipicrate from tobacco.
5. Isolation of cinchonine from cinchona bark.
6. Isolation of piperine from black pepper.
7. Isolation of lycopene from tomatoes.
8. Isolation of □-carotene from carrots.
9. Isolation of oleic acid from olive oil (involving the preparation of complex with urea and separation of linoleic acid.
10. Isolation of eugenol from cloves.
11. Isolation of limonine from citrus rinds.
12. Extraction and identification of DNA from green peas and onions

B. Spectro-photometric (UV/VIS) Estimations (Any Three)

1. Amino acids
2. Proteins
3. Carbohydrates
4. Cholesterol
5. Ascorbic acid
6. Aspirin
7. Caffeine

C. Synthesis of organic compounds, purification and characterization by chemical analysis, IR, UV-Vis, PL, NMR spectral analysis and mass spectral analysis: (Any three)

1. Synthesis of fluorescein, a classic fluorescent dye
2. Synthesis and chemiluminescence of luminol
3. Diels-Alder reaction of anthracene and maleic anhydride
4. Aspirin synthesis: Conventional and with microwave assistance
5. Sand Meyer's reaction: p-Chlorotoluene from p-chlorotoluidine.
6. Cannizzaro reaction using 4-chlorobenzaldehyde
7. Preparation of 1,3,5 tribromobenzene from analine
8. Acetoacetic ester condensation

Books Recommended:

1. Elias, A. J., Collection of Interesting General Chemistry Experiments, Orient Longman.
2. Addison Ault Techniques and Experiments for Organic Chemistry 6th Ed. University Science Books (1998).
3. Mann, F. G. & Saunders, B. C. Practical Organic Chemistry 4th Ed. Orient Longmans (1990).
4. Vogel, A. I. Vogel's Textbook of Practical Organic Chemistry 5th Ed. (revised by A.R. Tatchell et al.) Wiley (1989) ISBN 0582-46236-3

SEMESTER III

CHE-PG-O301: Biochemistry

Unit I: Carbohydrates

Glycosides, Oligosaccharides and polysaccharides. Role of sugar in molecular recognition.

Nucleic Acids: RNA, DNA, base-pairing, double helical structure of DNA, Gene regulatory protein- Zinc finger protein.

Aminoacids and Proteins: Aminoacids, peptide links and oligopeptides. Proteins: primary, secondary, tertiary, and quaternary structure of proteins. Structure, purification and denaturation of proteins.

Lipids and membranes: Lipids, fatty acids, Classification of lipids, self-association of lipids-micelles, reverse micelles and membranes, transport of cations through membranes.

Unit II: Metabolism and Energetics
Catabolic and anabolic processes, glycolysis, citric acid cycle and oxidative phosphorylation. Photosystems (PSI & PSII).

Unit III: Enzyme
Enzyme kinetics and applications of enzymes in organic synthesis. Enzyme inhibitors and co-enzymes in organics reactions. Drugs based on enzyme inhibition.

Unit IV: Metal ions in biological systems and their role in ion transport across the membranes (molecular mechanism)
Oxygen-uptake proteins, cytochromes and ferredoxins. Oxygen uptake proteins: Hemoglobin, Myoglobin, hemerythrin and hemocyanin. Metal complexes in medicine. Chemotherapy.

References

1. Stryer L., 2002 Biochemistry, 5th edition, Freeman & Co., New York.
2. Nelson D. L. and Cox M.M., 2002 Lehninger Principles of Biochemistry, 3rd edition McMillan North Publication.
3. Hughes M. N. , 1981 Inorganic Chemistry of Biological Processes, John Wiley.
4. Smith M.B., 1995 Organic Synthesis, McGraw Hill Inc., New York.
5. Ariga K. and Kunitake T. 2006 Supramolecular Chemistry – Fundamentals and Applications, Springer
6. Crabtree R. H., Organometallics in Organic synthesis Vol-II – Organometallics of Transition Metals in Organic Synthesis
7. Voet D., Voet J.G and Pratt C. W., 1999 Fundamentals of Biochemistry, John Wiley & Sons, New York

CHE-PG-C302: Physical Chemistry II

Unit I: Statistical Thermodynamics
Concepts of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging. Canonical and microcanonical ensembles, Boltzmann distribution of particles.
Partition function: translational, rotational and vibrational partition functions, thermodynamic properties of ideal gases in terms of partition function.

Unit II: Quantum Mechanics
Fundamentals: Review of essential mathematical concepts. Origin of the quantum theory. Postulates of quantum mechanics and Schrödinger equation; its application on some model systems viz., free-particle and particle in a box, tunneling, the harmonic oscillator, the rigid rotator, and the hydrogen atom. The variation theorem; linear variation principle;

Approximation Methods: Stationary perturbation theory for non-degenerate and degenerate systems with examples. Variation method. Ground state of He atom. Time-dependent perturbation theory. Radiative transitions. Einstein coefficients.
Atomic Structure: Many electron wave functions. Pauli Exclusion principle. Helium atom. Atomic term symbols. The self-consistent field method. Slater-type orbitals.
Quantum dots, wires and wells. Quantum Confinement effect.

Unit III: Rotation and Vibration of Diatomic Molecules
Selection rules. A review of MW and IR spectroscopy. Symmetry properties and nuclear spin effects. Raman effect: Rotational and vibration-rotational transitions. Polarization of Raman lines. Vibration of polyatomic molecules– normal coordinates.
Electronic Spectroscopy: Absorption and Emission of radiation. Selection rules. Line shapes and widths. Electronic spectroscopy of diatomic molecules. Franck-Condon factor. Dissociation and pre-dissociation. Rotational fine structure. Lasers and Laser spectroscopy.

Unit IV: Chemical Equilibrium
General treatment of equilibria in aqueous medium involving monoprotic weak acid and weak base, and salts of weak acids and weak bases. Activity and concentration, Effect of electrolytes on chemical equilibria, Complexation equilibria and complexometric titrations, Redox equilibria and redox titration, Theory of redox indicators, Precipitation reaction and precipitation titrations and theory of adsorption indicators.
Chemical dynamics: Methods of determining rate laws, collision theory of reaction rates, Arrhenius equation and activated complex theory. Potential energy surfaces. Unimolecular reactions and their treatments (Lindemann-Hinshelwood and Rice-Ramsperger-Kassel-Marcus [RRKM] theory)
Experimental Methods: Enzyme kinetics, studies of fast reactions by flow method, relaxation method, flash photolysis and NMR.

References

1. Atkins, P. W. 2002 Physical Chemistry, 7th Edition, Oxford University Press, New York.
2. Maczek, A. Statistical Thermodynamics, Oxford University Press Inc., New
3. Reif, F. , 1985 Fundamental of Statistical and Thermal Physics McGraw Hill, International edition.
4. Barrow, G. M. Introduction to Molecular Spectroscopy McGraw Hill
5. Pilar, F. L. 1990 Elementary Quantum Chemistry 2nd Edition, McGraw - Hill Publishing Company.
6. Atkins P. W. and Friedman, R. S, 1997, Molecular Quantum Mechanics 3rd Edition, Oxford Univ. Press.
7. Laidler, K. 1995 Chemical Kinetics Harper and Row.
8. Levine, I. N. 2002 Physical Chemistry, 5th Edition, Tata McGraw Hill Pub. Co. Ltd., New Delhi.
9. Brouard, M. 1998 Reaction Dynamics, Oxford University Press, Oxford.
10. Levine R.D. and Bernstein, R.B. 1987 Molecular Reaction Dynamics and Chemical Reactivity, Oxford University Press, Oxford.

CHE-PG-C303: Instrumental Techniques

Unit I: Chemical Instrumentation

Elementary Electronics, Simple integrated circuit, Semiconductor, Power supply, transformer, operational amplifier, Lock-in amplifiers, Detectors (Oscilloscope and recorders), transducers, Rectifiers, Signal to noise ratio, Electronic components (Resistors, capacitors, inductors, transistors), Measuring instruments for pressure, temperature, pH, speed, flow, current and voltage. Fourier transformation.

Errors in Chemical Analysis and Statistical Evaluation of Data: Systematic and random errors, accuracy and precision, the correlation coefficient, Mean, Median and Modes, variance, standard deviation and significant figures.

Separation Methods: Principle of chromatography, Classifications of chromatography, Techniques of planar and column chromatography, Gas chromatography, High-performance liquid chromatography.

Unit II: UV-Visible Spectroscopy

Principles and Applications: dienes, polyenes, carbonyl compounds and α, β-unsaturated carbonyl compounds. Woodward Hoffman rule and its application in aromatic compounds.

Infrared Spectroscopy: Vibration modes. Absorption frequency of common functional groups, electronic and steric effects, effects of Hydrogen bonding. Interpretation of IR spectra.

Raman Spectroscopy: Principles of Raman Spectroscopy and its comparison with IR spectroscopy. Applications of vibrational spectroscopy: Symmetry and shapes of AB_2, AB_3, AB_4, modes of bonding in ambidentate ligands.

Emission Spectroscopy: Principle and application of Fluorescence, phosphorescence, chemi-luminescence

Mössbauer Spectroscopy: Basic principle, conditions for Mössbauer spectroscopy, Spectral parameters (Isomer shift, electric quadrupole interactions, magnetic interactions), temperature-dependent effects, structural deductions for iron and tin complexes, miscellaneous applications.

Unit III: NMR Spectroscopy

Principle, instrumentation and different techniques (continuous wave and Fourier transformed) of NMR spectroscopy, factors influencing chemical shifts of the spectra, anisotropy, spin-spin interactions, coupling constant (J), spin-decoupling, Nuclear Overhauser Effect (NOE), classification of AB, ABC, AMX and A_2B_2 type couplings, First order spectra, lanthanides shift reagent, spin-spin and spin lattice relaxation processes. Applications. Introduction to ^{13}C NMR, principles of decoupling, Application of DEPT. ^{1}H-^{1}H COSY, HETCOR, NOESY, ROESY. Basic introduction to ^{19}F and ^{31}P NMR and heteronuclear coupling. Solid-state NMR: Basic principles and applications. MRI basics. MRI Contrast agents.

Electron Spin Resonance Spectroscopy: Basic principle, Hyperfine splittings (isotropic systems); the *g*-value and the factors affecting thereof; interactions affecting electron energies in paramagnetic complexes (Zero-field splitting and Kramer's degeneracy); Anisotropic effects (the *g*-value and the hyperfine couplings); The EPR of triplet states; Structural applications to transition metal complexes.

Unit IV: Basic principle and data analysis

UV photoelectron spectroscopy, X-ray photoelectron spectroscopy, ESCA and Auger, EDX. Scanning electron microscopy (SEM), Transmission electron microscopy (TEM), Scanning tunnelling microscopy (STM) and Atomic force microscopy (AFM). Cyclic Voltammetry, Inductively coupled plasma emission spectroscopy (ICPE), TGA, DSC, DTA and thermometric titration.

Mass Spectrometry: Introduction, ion production, fragmentation, factors influencing ion abundance, single and multiple bond cleavage, rearrangements, cleavage associated with common functional groups, molecular ion peak, metastable ion peak, Nitrogen rule and interpretation of mass spectra, effect of isotopes on the appearance of mass spectrum, recognition of the molecular ion peak; Ionization techniques (EI and FAB).

Optical Rotatory Dispersion and Circular Dichroism. Linearly and circularly polarized lights; optical rotatory power and circular birefringence, elipticity and circular dichroism; ORD and Cotton effect, Faraday and Kerr effects

References

1. Strobel, H.A. 1973 Chemical Instrumentation - A Systematic Approach, 2nd Edition, Addison Wesley, Mass.
2. Skoog D.A., Holler F.J. and Nieman, T.A. , 1998 Principles of Instrumental Analysis, 5th Edition, Harcourt Brace & Company, Florida.
3. Hollas, J. M. 2004 Modern Spectroscopy, 4th edition, John Wiley & Sons, Ltd., Chichester.
4. Harris, R. K. 1986 Nuclear magnetic resonance spectroscopy John Wiley and Sons Inc.,New York, NY .
5. R.J. Abraham and J. Fishe and P. Loftus, 1994, Introduction to NMR Spectroscopy John Wiley & Sons.
6. Ladd M. F. C. and Palmer, R. A. 1985 Structure Determination by X-Ray Crystallography Plenum, NY, 2nd Ed.
7. Williams, D B. Carter, C. B. 2008 Transmission Electron Microscopy: A Textbook for Materials Science Springer.
8. Sarid, D. 1991 Scanning Force Microscopy With Applications to Electric, Magnetic and Atomic Forces New York, Oxford University Press
9. Chary, K. V. R. and Govil, G. 2008 NMR in biological systems: from molecules to human, Springer
10. Pecsok, R. P., Shields, L. D. , Cairns T. and William, L.C. Mc, 1976, 2nd Edition, John Wiley, New York.

CHE-PG-C304: Practical III
Physical Chemistry Experiments

A. Electrochemistry and Kinetics: (Any three)

1 Analysis of halide mixture by differential potentiometry.
2. Degree of hydrolysis of urea hydrochloride by kinetics method.
3. Equilibrium constant of $KI + I_2 \leftrightarrow KI_3$ by distribution method.
4. Kinetics of the iodide-hydrogen peroxide clock reaction
5. An experiment to determine the energy of activation, Ea
6. Determination of the amount of calcium in milk powder by EDTA complexometry
7. Estimation of iodine in iodized common salt using iodometry
8. Determination of phosphoric acid in soft drinks
9. Antioxidant property of Tea (DPPH method)

B. Physical and Analytical methods: (Any seven)

Experiments based on

1 UV - Visible spectroscopy with application
2 Fluorescence Spectroscopy with application
3 Infrared Spectroscopy
4 EPR Spectroscopy
5 NMR Spectroscopy
6 Solvents effects in spectra
7 Differential Scanning Calorimetry
8 High Pressure Liquid Chromatography
9 Spectroscopy Instrumentation
10 Cyclic voltametry
11 Enzymetic reaction
12 Semiconductor materials (Quantum dots)
13 Metal Nanoparticles
14 Polymer
15 Magnetic nanoparticles
16 Ionic liquids
17 Liquid crystals
18 Optical materials
19 Carbon based nanomaterials
20 Paper and column chromatography of plant pigments
21 Acetylation of ferrocene and its purification by column chromatography
22 Ternary phase diagram
23 Determination of surface tension by differential capillary method.
24 Determination of molecular weight of a macromolecule by viscometry.
25 Determination of molecular weight by Victor Meyer's method.
26 Cryoscopy and determination of degree of dissociation.
27 Determination of g-value by ESR method.
28 Analysis of a UV spectrum, Raman spectrum, IR spectrum, NMR spectrum and EPR spectrum. Calculation of oscillator strength and transition moment.
29 Potentiometric titrations using the pH meter and determination of pI
30 Conductometric titrations and determination of dissociation constant
31 Determination of Phosphoric acid in soft drinks

Books Recommended:

1. Elias, A. J., Collection of Interesting General Chemistry Experiments, Orient Longman.
2. Daniels, F., Williams, J. W., Bender, P., Alberty, R. A., Cornwell, C. D. & Harriman, J. E. Experimental Physical Chemistry, McGraw-Hill (1962).
3. Das & R. C. & Behera, B., Experimental Physical Chemistry, Tata McGraw-Hill Publishing Co. Pvt. Ltd. (1993).
4. Shoemaker, D. P., Garland, C. W. & Nibler, J. W. Experiments in Physical Chemistry, McGraw-Hill: New York (1996).
5. Day, R. A., Jr. & Underwood, A. L. Quantitative Analysis 3rd Ed. Prentice-Hall India Pvt. Ltd.: New Delhi (1977).
6. Burns, D. T. & Rattenbury, E. M. Introductory Practical Physical Chemistry Pergamon Press (1966)
7. Harris, D. C. Quantitative Chemical Analysis 6th Ed. W. H. Freeman & Co. (2002).
8. Willard, H. H., Merritt, L. L., Dean, J. A. & Settle, F. A. (Eds.) Instrumental Methods of Analysis - 7th Ed., Wadsworth Publishing (February 1988) ISBN 0534081428
9. EDTA Titrations –F.Laschka
10. Experimental Physical Chemistry by A.M. Halpern, 2nd Ed., Prentice Hall, 1997.

SEMESTER IV
Elective I

CHE-PG-E401: Chemistry of Inorganic Materials

Inorganic Chemistry Elective I

Unit I: Isopoly and Heteropoly Acids and Salts

Synthesis, structural principles and application of V, Nb, Ta, Cr, Mo and W polyacids.

Unit II: Supramolecular systems

Macrocyclic Complexes: Types of macrocyclic ligands – design and template synthesis of di- and poly-nuclear macrocyclic complexes and their applications.

Supramolecular Chemistry: Concept of supramolecular chemistry, molecular recognition, supramolecular reactivity and catalysis, molecular recognition, nomenclature, design of supramolecules through non-covalent interactions. Some examples of self-assembly in supra molecular chemistry. Design and synthesis of different types of receptors and co-receptors and multiple recognition, carrier design and transport processes. Supramolecular devices- electronic and ionic switches, supramolecular photochemistry.

Unit III: Molecular Magnetic Materials

Basic concepts of molecular magnetism, types of magnetic interactions, recent techniques of magnetic susceptibility measurements, inorganic and organic ferro-magnetic materials, low-spin

– high-spin transitions, isotropic interactions in dinuclear compounds (dipolar, anisotropic and anti-symmetric interactions), trinuclear compounds and compounds of high nuclearity, magnetic chain compounds, magnetic long-range ordering in molecular compounds: design of molecular magnets, physical investigations and applications.

Unit IV: Metallomesogens

Basic concepts, types of meso-phases, synthetic strategies, characterization and applications.

Inorganic Polymers: Classification, Types of Inorganic Polymerization, Comparison with organic polymers, Boron-oxygen and boron-nitrogen polymers, silicones, coordination polymers, sulfur-nitrogen, sulfur-nitrogen-fluorine compounds, chalcogenide clusters – binary and multi-component systems, homolytic inorganic systems.

References

1. Greenwood N. N. and. Earnshaw, A. 1997 Chemistry of the Elements, 2nd Edn., Butterworth Heinemann, London.
2. Lehn J. M., 1995 Supramolecular Chemistry, VCH, Weinheim.
3. Kahn O., 1993 Molecular Magnetism, VCH, Weinheim.
4. Cotton, F. A., Wilkinson, G., Murillo C. A. and Bochmann, M. , 2003, Advanced Inorganic Chemistry, 6th Edn., John Wiley & Sons (Asia), Singapore.
5. Mark, J. E., Allcock, H. R. and West, |R. 2004 Inorganic Polymers, 2nd Edn., Oxford University Press.
6. Huheey, J. 1993 Inorganic Chemistry, 4th Edn., Addison Wesley Pub. Co., New York
7. Miessler G. L. and Tarr, D. A. 1999 Inorganic Chemistry, 2nd Edn., Prentice Hall International Inc., London.
8. Serrano, J. L. 1996 Metallomesogens, VCH, Weinheim.

CHE-PG-E411: Chemistry of Organic Materials

Organic Chemistry Elective I

Unit: Stereochemistry

Basic stereochemistry, general consideration of molecular asymmetry and dissymmetry.

Configuration: absolute and relative, methods of determination, chemical transformation, asymmetric synthesis using chiral auxiliaries, reagents and catalysts, quasiracemates, dynamic stereochemistry , atropisomerism of biphenyls.

Conformation: conformational analysis based on physical properties and chemical reactivity, shape of six membered ring, conformation and reactivity in cyclohexanes and decalins.

Unit II: Molecular Rearrangements

Sommelet-Hauser, Favorskii, Fries and Benzilic acid rearrangements. Hofmann-Loffler-Freytag reaction, Barton reaction and Shapiro reaction. Sharpless epoxidation

Unit III: Synthesis and characterization of materials

Preparative techniques: Pyrolytic methods; chemical strategies, chemical vapour deposition; preparation of nanomaterials, Langmuir- Blodgett Films. Fabrication of ordered nanostructuress. Composition and purity of materials.

Organic Materials: Conducting organics - Metals from molecules, charge transfer materials and conducting polymers. Organic superconductors. Fullerenes, Carbon nanotubes and graphene. Molecular ferromagnets and ferroelectrics. Liquid crystals: mesomorphic behaviour, optical properties of liquid crystals, display devices. Organic light emitting diodes.

Unit IV: Green Chemistry and solid phase reactions

Green Chemistry: Overview. Set of principles of green chemistry, green synthetic methods, catalysis, organics reactions in aqueous media, ionic liquids, supercritical fluids and under microwave radiations. Solvent from organics reactions, solid phase organics reaction and catalysis.

References:

1. Joule J. A. and Mills K. Heterocyclic Chemistry: (4th Ed) Wiley-Blackwell
2. Cleydon, J., Greeves, N., Warren, S. and Wolthers, P. 2001 Organic Chemistry: Oxford.
3. Anastas, P. A. and Warner, J. C. 1998 Green Chemistry: Theory and Practice, Oxford Univ. Press
4. Smith M.B. and March, J. 2001 March's Advanced Organic Chemistry-Reactions, Mechanisms and Structure, 5th Edition , John Wiley & Sons, New York.
5. Eliel E.L. and Wilen, S.H. 1994 Stereochemistry of Organic Compounds, Wiley Interscience, New York.
6. Rajappa, S. 2000 Eco-friendly Alternatives for the Fine Chemical Industry:, Sevak Publications.
7. Lancaster , M. 2002 Green Chemistry: An Introductory Text:, Royal Society of Chemistry
8. Loupy A. Microwaves in Organic Synthesis: Wiley-VCH
9. Herkes F. E. 1998 Catalysis of Organic Reactions: (Ed.)Marcel Dekker Inc .

CHE-PG-E421: Advanced Physical Chemistry

Physical Chemistry Elective I

Unit I: Group Theory

Group Theory: Definition of group, symmetry, point groups, representation of group, orthogonality theorem, irreducible representation, character table, direct sum, direct product, derivation of projection operator.

Unit II: Advanced Quantum Chemistry

Tunneling Phenomena: Principles and selected problems.

Ab initio and Semi-empirical Methods for Closed Shell Systems:

The Hartree-Fock Self-Consistent Field Method: The generation of Optimized orbitals, Koopman's Theorem (The Physical Significance of Orbital Energies), The electron correlation

energy, Density matrix analysis of the Hartree-Fock Approximation, Natural orbitals, The matrix solution of the Hartree- Fock Equations (Roothaan's equations). Density functional theory.

Semiempirical Molecular Orbital Methods I - PI Electron Systems: The Hückel Approximation for Conjugated Hydrocarbons, The Pariser-Parr-Pople Method.Semiempirical Molecular Orbital Methods II - All valence - Electron systems: The Extended Hückel Method, The CNDO Method.

Unit III: Electronic Structure of Linear and non linear Molecule

The MO - LCAO Approximation, The Hydrogen Molecule Ion, H^{+}_{2} , The Hydrogen molecule, Molecular Configuration - Interactions, The Valence Bond Method, Molecular Perturbation Calculations. Electronic Structure of AH_n molecule: Methane, Ammonia and Water, Hybrid Orbitals: The Ethylene and Benzene Molecules.

Unit IV: Fast Reaction

Techniques: Flow techniques, relaxation methods, flash photolysis and NMR methods.

General consideration of gas and solution phase fast reactions: Gas phase and solution phase reactions, Reactions at microsecond and nanosecond scale, ultrafast reactions: reactions at picoseconds and femtoseconds scale.

References

1. Cotton, F.A., 1990 Chemical Applications of Group Theory Wiley Interscience, 3rd Ed.
2. Levine, I.N. 2000 Quantum Chemistry, 5th edition, Pearson Educ., Inc. New Delhi.
3. Karplus M. and Porter, R. N., 1970 Atoms and Molecules, Benjamin, London.
4. Atkins P.W. and Friedman, R.S., 1997 Molecular Quantum Mechanics, 3rd edition, Oxford University Press. Oxford.
5. Pilar, Frank L. 1990 Elementary Quantum Chemistry 2nd Edition, McGraw - Hill Publishing Company.
6. Zewail, Ahmed H. 1994 Femtochemistry: ultrafast dynamics of the chemical bond, World Scientific Publications.
7. Mc Quarrie D.A. and Simon, J.D. , 1998, Physical Chemistry: A Molecular Approach, Viva Books, New Delhi.
8. Murrell, J.N. ,. Kettle S.F.A and Tedder, J. M. , 1965, Valence Theory,2nd edition, John Viley, New York.
9. Chandra, A.K. , 1994 Introductory Quantum Chemistry, 4th edition, Tata McGraw Hill, New Delhi.
10. Pualing L. and Wilson, E. B. , 1935 Introduction to Quantum Mechanics with Applications to Chemistry, McGraw Hill, New York.

Elective II

CHE-PG-E402: Bio-inorganic chemistry

Inorganic Chemistry Elective II

Unit I: Role of alkali and alkaline earth metal ions in biological systems

A. Role of alkali metal ions: Na^+-K^+ Pump, ionophores and crown ethers. Transport of Na^+-K^+ through membranes
B. Catalysis of phosphate transfer by Mg^{2+} ion,
C. Regulatory role of Ca^{2+} - muscle contraction

Unit II: Heme Proteins
Hemoglobin, myoglobin, hemerythrin, hemocyanin Oxygen activation: Cytochrome P450, Cytochrome c oxidase.
Non-heme proteins: Copper Proteins: Type I, II and III. Copper in cytochrome c oxidase and in respiratory chain, blue copper proteins

Unit III: Proteins with reference to their oxygenation and oxidase activity
Anti-oxidative functions, Nitrate and nitrite reduction (NO_3^- and NO_2^- reductase), Synthetic models of iron-sulfur proteins, molybdo-enzymes – molybdenum cofactors (molybdenum-pterin complexes, nitrogen fixation through metal complexation, nitrogenase, Photosynthesis (PS-I and PS-II).

Unit IV: Metalloenzymes
Zinc enzymes- carboxypeptidase and carbonic anhydrase. Iron enzyme - catalyses, peroxidase and cytochrome P-450. Copper enzyme-superoxide dismutase. Molybdenum oxo-transferase enzyme- xanthine oxidase. Urease and hydrogenase, and cyanocobalamine.
Metal ion storage and transport: Ferritin, transferritin, siderophores and metallothionein and hemosiderin.
Chemotherapeutic applications of metal complexes: Pt(II), Pt(IV) complexes and Ru(II), Ru(III) complexes as anticancer drugs, Au complexes as antiarthritis drugs

References
1. Hughes M. N., 1981 Inorganic Chemistry of Biological Processes, 2nd Ed., John-Wiley & Sons, New York.
2. Kaim W. and Schwederski B., 1995 Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, An Introduction and Guide, Wiley, New York.
3. Lippard S. J. and Berg J. M., Principles of Bioinorganic Chemistry, University Science Books.
4. Bertini, I. , Grey H. B., Lippard S. J. and Valentine, J. S. , 1998 Bioinorganic Chemistry, Viva Books Pvt. Ltd., New Delhi.

CHE-PG-E412: Natural Products and Bio-Organic chemistry

Organic Chemistry Elective II

Unit I: Natural Products
Isoprene Rule, biogenesis and biosynthesis of representative examples. Retrosynthetic analysis of some typical natural products.
Alkaloids: Structure, synthesis, and stereochemistry of Narcotine and Quinine; synthesis and stereochemistry of Morphine, Lysergic acid and Reserpine.
Terpenoids: Camphor, Longifolene, Abietic acid, and Taxol.
Steroids: Cholesterol, Aldosterone and Cortisone.

Prostaglandins and Thromboxanes: Introduction, nomenclature of prostaglandins and thromboxanes; approaches to prostaglandin synthesis; cyclohexane precurors (Woodward synthesis of PGF2a), bicycloheptane precursors (Corey's synthesis of prostaglandins E and F)
Oxygen Hetrocycles: Flavonoids, isoflavonoids and biosynthetic pathways. Antioxidant properties of flavonoids.

Unit II: The Chemistry of:

(i) Three-membered rings-Aziridines,
(ii) Four-membered rings- Azetidines and their 2-Oxo derivatives,
(iii) Condensed pyrroles- Indoles,
(iv) Azoles- Oxazoles, isoxazoles, pyrazoles, imidazoles and thiazoles,
(v) Six-membered rings- Pyrimidines and purines.
(vi) Structure and synthesis of Caffeine.
(vii) Structure of penicillins. Synthesis of paracetamol, phenobarbital, diazepam, sulfamethoxazole, benzyl penicillin and chloramphenicol.

Vitamins: Structure and synthesis of Vitamins A, C, Thiamine (B_1), Riboflavin (B_2), Pyridoxine (B_6), Cobalamin (B_{12}) and Vitamin D, Vitamin E, Biotin (H) and Vitamin K.

Unit III: Enzymes and Mechanism of Enzyme Action

Classification, isolation and purification. Methods of Enzyme analysis. Two substrate reactions; Enzyme inhibition. Mechanism of action of chymotrypsin, aldolase, alcohol dehydrogenase, and lysozyme.

Co-enzyme Chemistry: Cofactors as derived from vitamins; coenzymes, prosthetic groups, and apoenzymes. Structure and biological functions of coenzyme A, thiamine Pyrophosphate, Pyridoxal phosphate, NAD^+, $NADP^+$, FMN, FAD, lipoic acid, and vitamin B_{12}. Mechanisms of reactions catalyzed by the above cofactors.

Unit IV: Biotechnological Applications of Enzymes

Techniques and methods of immobilization of enzymes, effect of immobilization on enzyme activity, application of immobilized enzymes, use of enzymes in food and drink industry-Brewing and cheese-making, syrups from corn starch, enzymes as targets for drug design.

References

1. Bruice T.C. and Bentkovic, S. , 1996, Bioorganic Mechanisms, Vol. I & II, W. A. Benjamin, New York.
2. Voet D., Voet J.G. and Pratt CW, 1999 Fundamentals of Biochemistry, John Wiley & Sons, New York .
3. Dugas H. and Penney C., 1981, Bioorganic Chemistry: A Chemical Approach to Enzyme Action, Springer- Verlag, New York.
4. Apsimon J.W., Total Synthesis of Natural Products, Vol. 1-6, Wiley-Interscience Publications, New York.
5. Clayden J. , Greeves N., Warren S., and Wothers P., 2001 Organic Chemistry, Chapter 30, Oxford University Press, Oxford.
6. Burger's Medicinal Chemistry and Drug Discovery, 2003 6th Edn. Donald J. Abraham (Editor), Wiley Interscience

7. Smith M. B., March J., 2000 March's Advanced Organic Chemistry. Reactions, Mechanisms, and Structure 5th Edn, Wiley-Interscience
8. Finar I.L., 1975 Organic Chemistry, Vol. II, 5th Edition Reprinted in 1996, ELBS and Longman Ltd., New Delhi.
9. Lehninger A.L., 1992 Principles of Biochemistry, CBS Publishers, Delhi
10. Mahler H.R. and Cordes E.H., 1971 Biological Chemistry, 2nd Edition, Harper and Row Pub., New York.

CHE-PG-E422: Solid-State Chemistry

Physical Chemistry Major Elective II

Unit I: Solid state Chemistry

Basic Principles and applications

Solid State Reactions: General Principles, Experimental procedure, Kinetics of solid-state reactions, Crystallization of solutions, melts, glasses and gels. Growth of single crystals: Czochralski method, Bridgman and Stockbarger methods. Zone Melting. Reactions at solid surfaces.

Unit II: Phase transitions, electronic and magnetic properties

Phase Transitions: Thermodynamic and Burger's classification of phase transition, Kinetics of phase transition- nucleation and growth, T-T-T diagrams, Factors that influence kinetics of phase transition, Martensitic and order-disorder transitions.

Electronic Properties and Band Theory: Electronic structure of solids- band theory, Refinement to simple band theory- k-space and Brillouin Zones, Band structure of metals, insulators and semiconductors, Intrinsic and extrinsic semiconductors, Doped semiconductors, p-n junctions.

Magnetic Properties: Classification of materials. Magnetism: Types, determination of magnetic susceptibility. Quantum theory of paramagnetism. Cooperative phenomena. Magnetic domains. Hysteresis.

Unit III: Diffractions Techniques

X-ray Diffraction: Diffraction of X-rays by crystals: The Laue equations and Bragg's law, Definitions related to crystal structure. X-ray diffraction experiments: The powder method and the single crystal method. Reciprocal lattice. Structure factor. Structure factor and intensity. Electron density maps.

Electron diffraction: Scattering intensity versus scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules. Low energy electron diffraction and structure of surfaces.

Neutron diffraction: Scattering of neutrons by solids and liquids, magnetic scattering, measurement techniques. Elucidation of structure of magnetically ordered unit cells.

Unit IV: High-Tc Oxide Superconductors

Structural features of cuprate superconductors. 1-2-3 and 2-1-4 cuprates; structure. Normal state properties: anisotropy and temperature dependence of electrical resistance. Superconducting

state: heat capacity, coherence length, relation between Tc and hole concentration in cuprates; mechanism of superconductivity in cuprates. Applications of high Tc-cuprates.

Non-linear materials: Second and third order non-linear effects; molecular rectifiers and frequency doublers; unimolecular electronic devices. Photochromic materials; optical data storage, memory and switches.

References

1. West A.R. 2003 Solid State Chemistry and its Applications, John Wiley and Sons, Singapore.
2. Azaroff L. V. 1977, Introduction to Solids, Tata McGraw-Hill, New Delhi
3. Massa, W. 2004 Crystal Structure Determination 2nd Ed. Springer.
4. Warren, B. E., 1990 X-Ray Diffraction 1st Ed. Dover Publications (1990).
5. Sands, D. E. 1994 Introduction to Crystallography, Reprint Dover Publications.
6. Tinkham Michael, 2004 Introduction to Superconductivity 2nd Edn, Courier Dover Publications.
7. Rammakrishnan, T.V. and Rao C.N.R. 1999 Superconductivity Today Orient Blackswan.
8. Ashcroft N. W. and Mermin N. D., 1976 Solid State Physics, Brooks Cole; 1st edition
9. Keer H. V. 1993 Principles of the Solid State, New Age International.
10. Chakrabarty D.K., 2010 Solid State Chemistry, New Age Science ltd; 2nd Revised edition.

CHE-PG-O403: Environmental Chemistry

Unit I: Introduction to Environmental Chemistry

Concept and scope of environmental chemistry, Environmental terminology and nomenclatures, Environmental segments, The natural cycles of environment (Hydrological, Oxygen, Nitrogen, Phosphorous and Sulphur cycles).

Air Pollution: Air pollutants (sources, classification, sampling and monitoring): Particulates, Aerosols, SO_x, NO_x, CO_x and hydrocarbon emission, Photochemical smog, Auto-exhausts, Acid rains, Air-quality standards.

Water Pollution: Water pollutants (sources, sampling and monitoring), Water-quality parameters and standards: physical and chemical parameters (colour, odour, taste and turbidity), Dissolved oxygen, BOD, COD, Total organic carbon, Total nitrogen, Total sulfur, Total phosphorus and Chlorine, Chemical speciation.

Unit II: Atmosphere

Regions of the atmosphere, Reactions in atmospheric chemistry, Earth's radiation balance, Particles, ion and radicals in the atmosphere, stratospheric chemistry: The chemistry of ozone layer, The role of chemicals in ozone destruction, The green-house effect and Global warming, El-Nino phenomenon.

Hydrosphere: Complexation in natural water and waste-water, Micro-organism in aquatic chemical reactions, Eutrophication, Re-cycle of waste-water in process industry, Treatment of

sewage and reuse of water in industry and agriculture, Microbiology mediated redox reactions and Nitrogen transformation by bacteria.

Lithosphere : The terrestrial environment, Soil formations, Soil properties (physical/chemical), inorganic and organic components in soil, acid-base and ion-exchange reactions in soil, micro and macro nutrients, nitrogen pathways and NPK in soil, waste and pollutants in soil, waste classification and disposal.

Unit III: Chemical Toxicology

Toxic chemicals in the environments, Impact of toxic chemicals on enzymes, Biochemical effects of arsenic, cadmium (Itai-itai disease), lead, mercury (Minamata disease), copper (Wilson's disease), carbon mono-oxide, nitrogen oxides, sulphur oxides, ozone, PAN, cyanide, pesticides, insecticides and carcinogens.

Unit IV: Environmental Management

Methods of environmental management, Radioactive waste management, Environmental impact assessment, Natural resources of energy-consumptions and conservation.

Region inspired environmental chemistry: Local drug plants, soil chemistry, mineral formation and water chemistry.

References

1. Vanloon G.W. , Duffer S.J. , 2000 Environmental Chemistry - A Global Perspective, Oxford University Press
2. Fifield F.W. and Hairens W.P.J., 2000 Environmental Analytical Chemistry, 2nd Edition Black Well Science Ltd.
3. Baird Colin, 1995 Environmental Chemistry, W.H. Freeman and Company, New York.
4. De A.K., 2000 Environmental Chemistry, 4th Edition, New Age International Private Ltd., New Delhi.
5. Warner Peter O. , 1996 Analysis of Air Pollutants,1st Edition , John Wiley, New York.
6. Khopkar S.M , 1993 Environmental Pollution Analysis, 1st Edition, Wiley Estern Ltd., New Delhi.
7. Banerji S.K., 1993 Environmental Chemistry, 1st Edition, Prentice-Hall of India, New Delhi.

CHE-PG-C404: Project for M.Sc. Thesis

Each student has to carry out innovative research on a topic chosen by the student.

Course Objectives:

a) Identification of the problem.
b) Literature review.
c) Exposure to analytical techniques/software
d) Communication skills: Scientific writing, presentation
a) Scientific ethics