M.Sc. (CHEMISTRY)

(Semester Pattern)

[Placed before the Academic Council and Approval sought for implementation from the Academic year 2009 – 2010 onwards]

COURSE STRUCTURE, SYLLABUS AND SCHEME OF EXAMINATION

SEMESTER-I						
Subject code	**Title of the paper**	**Hours per week**	**Duration of semester exam**	**Marks**		**Total marks**
				Internal	**External**	
PGCH09IC1	INORGANIC CHEMISTRY-I	5	3	25	75	100
PGCH09OC1	ORGANIC CHEMISTRY-I	5	3	25	75	100
PGCH09PC1	PHYSICAL CHEMISTRY-I	5	3	25	75	100
PGCH09AC1	ANALYTICAL CHEMISTRY-I	5	3	25	75	100
PGCH09IP1	INORGANIC PRACTICAL-I	6	To be continued in semester II			
PGCH09OP1	ORGANIC PRACTICAL -I	6	To be continued in semester II			
PGCH09PP1	PHYSICAL PRACTICAL -I	6	To be continued in semester II			
Distribution of working hours / Week	**Theory 20 Hours**		**Practical- 18 Hours**		**Seminar 2 Hours**	
SEMESTER -II						
PGCH09IC2	INORGANIC CHEMISTRY-II	5	3	25	75	100
PGCH09OC2	ORGANIC CHEMISTRY-II	5	3	25	75	100
PGCH09PC2	PHYSICAL CHEMISTRY-II	5	3	25	75	100
PGCH09AC2	ANALYTICAL CHEMISTRY-II	5	3	25	75	100
PGCH09IP1	INORGANIC PRACTICAL-I	6	6	25	75	100
PGCH09OP1	ORGANIC PRACTICAL -I	6	6	25	75	100
PGCH09PP1	PHYSICAL PRACTICAL -I	6	6	25	75	100
Distribution of working hours / Week	**Theory 20 Hours**		**Practical- 18 Hours**		**Seminar 2 Hours**	
SEMESTER-III						
PGCH09OC3	ORGANIC CHEMISTRY -III	5	3	25	75	100
PGCH093IA	INSTRUMENTATION ANALYSIS	5	3	25	75	100
PGCH093MC	MATERIAL CHEMISTRY	5	3	25	75	100
PGCH093EC	ENVIRONMENTAL CHEMISTRY	5	3	25	75	100
PGCH093PO	POLYMER CHEMISTRY	5	3	25	75	100
PGCH09IL	INSTRUMENTATION LAB	6	6	25	75	100
Distribution	**Theory 25 Hours**	**Practical- 6 Hours**	**Seminar 4 Hours**		**Pre project 5 Hours**	
SEMESTER-IV						
PGCH09CA	PROGRAMMING IN C AND C++	5	3	25	75	100
PGCH09ICQ	INDUSTRIAL CHEMICAL ANALYSIS AND QUALITY CONTROL	5	3	25	75	100
PGCH09SEM	SEMINAR	4	-	-	-	100
PGCH09PRO	PROJECT WORK AND VIVA VOCE	-	-	-	200	200
Distribution of working hours / Week	**Theory 20 Hours**		**Seminar 2 Hours**		**Project 5 Hours**	

SEMESTER I

PGCH0911- INORGANIC CHEMISTRY-I ***Total 90 hours***

Unit I Main Group and Transition Elements

Noble gas compounds: Preparation- properties- structure and bonding. Interhalogen compounds - Preparation - properties – structure – bonding - uses - Pseudo halogens: Preparation – properties- structure- bonding - Polyhalide ions – chemistry of Astatine.

Transition elements- general characteristics - electronic configuration- oxidation states – study of vanadium, chromium and manganese groups and their compounds including metal clusters with **δ-** bonds and polyoxo mettalates.

Unit II Theories of Metal Complexes

Co-ordination compounds introduction- nomenclature- detection of complex formation (photometric and potentiometric methods)- Isomerism in complexes-Theories of bonding in complexes-Valence bond theory - limitations-Crystal field theory - Splitting of d orbitals in different ligand fields - Cryatal field stabilization energy (CFSE) calculations- evidences of splitting of d-orbital effects of CFSE - Factors affecting splitting – Spectrochemical series. Jahn-Teller distortion – limitations of CFT.MO theory - **σ** and **π-** bonding in metal complexes – evidences for **π-** bonding in complexes. MO diagrams of complexes- effect of **π-** donors and **π-**acceptors- nephelauxetic effect and series – Ligand field theory- comparison of the three theories as applied to metal complexes.

Unit III Reactions of Metal Complexes

Stability of complexes – formation constants- Stepwise and overall formation constants- relation between them –factors affecting the stability of complexes- statistical effects-Irwing-William order of stability- Chelate effect. Kinetics and mechanism of reactions involving complexes in solution - Inert and labile complexes - substitution reactions in octahedral and square planar complexes- acid and base hydrolysis- Anation reactions-substitutions without breaking bonds – factors affecting reactivity of complexes- the trans effect - Redox reactions- complementary and non-complementary- outer sphere and inner sphere mechanisms – Marcus theory.

Unit IV Organometallic Compounds

Complexes with **π-**donor ligands - types –metal-olefin, metal –acetylene complexes- complexes with dienes and allyl systems.Complexes with cyclic π-donors- Cyclopentadiene- ferrocne synthesis and reactions - benzene, cycloheptatriene and cyclooctatetraene complexes, structure and bonding-Fluxional molecules. Catalysis by organometallic compounds: Hydrogenation-hydroformylation – oligomerization - polymerization reactions..

Unit V Nuclear Chemistry

Nuclear structure- properties of nucleus- mass-charge- nuclear moment - Binding energy. Semi empirical mass equation- Stability rules- Magic numbers-Nuclear models -Shell, Liquid drop - Fermi gas - Collective and Optical models. Radio active decay – Kinetics growth- Half life- average life -Radioactive equilibrium types - Transient and secular equlibria -Nuclear reactions -energetics of nuclear reactions.- types of nuclear reactions - Spontaneous and reduced fission - Neutron capture cross section and critical size - nuclear power plants- Breeder reactor.-nuclear fusions. Detection and measurement of radioactivity- - Principles of working of - Wilson cloud chamber- bubble chamber – Geiger-Muller, Proportional, Ionization and Scintillation counters. Applications of radioactivity

References

1. F.A.Cotton and G.Wilkinson, “Advanced Inorganic Chemistry”, 6th edition (1999)
2. John Wiley & Sons
3. J.E.Huheey, “Inorganic Chemistry – Principles of Structure and Reactivity”, 4th edition(1993) - Harper Collins College Publishers.
4. Concise inorganic chemistry – J.D.Lee ,(1995) ELBS .
5. C.J.Mooday and J.D.R.Tanas, “Noble Gases and Their Compounds”, Pergamon Press
6. J.H.Hollaway, “Noble Gas Chemistry”, Methuen, New York
7. H.R.Alcock, “Phosphorus-Nitrogen Compounds”, Academic Press
8. K.F.Purcell and J.C.Kotz, “Inorganic Chemistry”, Saunders
9. A.I.Vogel, “A Text Book of Quantitative Inorganic Anaysis”, Longman
10. D.A.Skoog, D.M.West and F.J.Holler, “Fundamentals of Analytical Chemistry”, Saunders College Publishing.
11. W.W.Wendlandt, “Thermal Methods of Analysis”, John Wiley & Sons
12. G.Friedlander and J.W.Kennady, “Introduction to Radiochemistry”, John Wiley & Sons
13. S.Glasstone, “Source Book on Atomic Energy”, Associated East-West Press
14. H.J.Arnikar, “Essentials of Nuclear Chemistry” 4 th Edition, New Age International, New Delhi

PGCH0912 – ORGANIC CHEMISTRY-I ***Total 90 hours***

Unit I Stereochemistry of Organic Compounds

Molecular chirality -terminology in stereo chemistry- conformation – configuration -priority rules -R,S notation – atropisomerism - stereo chemistry of cyclophanes –ansa compounds-helicity – Racemisation –resolution--

enantiomeric excess – prochirality – stereotopicity - Non-carbon chiral centres. chirotropical properties – Cotton effect - ORD, CD – application- Octant rule - axial haloketone rule. Conformational analysis of cyclopentane –cyclohexane and cyclooctatetraene –decalins.

Unit II Structure, Reactivity and Intermediates

Electronic effects - inductive effect- Influence on acidity, basicty and reactivity. Electromeric effect -resonance -hyper conjugation.

Generation-structure, stability and reactions of carbocations- carbanions – carbenes -carbenoids nirenes- arynes- effects of substituents on the substitution reactions in aromatic systems

Unit III Elucidation of organic reaction mechanisms

Mechanism-types of reactions in organic chemistry-concept of intermediates and transition state-potential energy profiles-Hammond's postulate-Microscopic reversibility- kinetic and thermodynamic requirements of a reaction-kinetic and thermodynamic control-Marcus relation-Methods of elucidating reaction mechanism-kinetic and non-kinetic methods-stereo chemical evidences –cross over experiments-Isotopic effects.

Linear free energy relation-Hammett equation-significance of σ and ρ -Taft equation-effect of solvents - Swain-Scot equation- Winstein-Grunwald equation

Unit IV Substitution and Elimination Reactions

Substitution reactions – types- nucleosphilic substitution at sp^3 carbon -stereochemical aspects - effect of solvent, leaving group and substrate structure -Neighbouring group participation - Non-classical carbocations - allylic substitutions.

Elimination reactions – E1-E2 –E1CB mechanisms-factors affecting eliminations- Stereo aspects of C=C bond formation - Hoffman and Saytzeff rules – thermal eliminations - Chugave reaction-pyrolysis of acetates

Unit V Reactivity of Unsaturated Systems

Additions to C=C bond – addition of X_2, HX, boranes, and hindered boranes..- hydroxylations - Cis and trans Hydroxylations - Nucleophilic and free radical additions to C=C systems- addition to C=O systems. Cram's rule - Michael addition.-mechanism,evidences and application of Aldol (normal, crossed and directed) Robinson's annulation – Perkin - Stobbe – Knovenagel - Darzen - Reformatsky and Benzoin condensation - Grignard - Cannizzaro - Wittig and Witting-Horner reactions- Mechanism of esterification and ester hydrolysis.

Reference

1. D.Nasipuri, "Stereochemistry of Organic Compounds", Wiley Eastern
2. I.L.Finar, "Organic Chemistry",Vol 2, Longman
3. P.Sykes, "A Guidebook to Mechanisms in Organic Chemistry", Longman
4. S.N.Issacs, "Physical Organic Chemistry", Longman
5. J.March, "Advanced Organic Chemistry", Wiley
6. C.J.Moody and W.H.Whitham, "Reactive Intermediates", Oxford University Press.
7. Rodert D. Mayo , " Molecular Rearrangement",
8. Mukharjee and Singh "Organic reaction Mechanism"
9. Ernest Eliel " Stereo chemistry of carbon compounds" Wiley and sons.

PHYSICAL CHEMISTRY-I

Total 90 hours

Unit I Development of Quantum Mechanics

Classical Mechanics - Newtonian Mechanics - Lagrange and Hamiltonian equations - Conservation of angular momentum - Hamiltonian function and energy - Classical wave equation – inadequacies of classical mechanics -

Blackbody radiation - photoelectric effect - Compton effect - atomic spectra – explanation of the above on the basis of quantum theory –Planck's equation – value of h (Planck's constant)

Formulation of quantum mechanics - wave nature of microscopic bodies - de Broglie relation –Davisson-Germar experiment - Group velocity and phase velocity - uncertainty principle - consequences. The postulates of quantum mechanics –Operators –introduction – operator algebra - Angular momentum operators and their properties – Commutator - Eigen function and eigen values - wave functions - Physical interpretation of wave function - Orthogonality theorem -Orthonormality - Boundary conditions and well-behaved solutions -. Schrodinger wave equation – different forms - Solutions of Schrodinger wave equation for a free particle - particle on a ring - particle in 1D box – particle in 3D box –normalization of wave functions.

Unit II Molecular Symmetry and Basics of Spectroscopy

Symmetry - symmetry elements -symmetry operations - Point groups - Multiplication of operations –theory of groups – types of groups - group multiplication table - Similarity transformation - classification of symmetry operations - Matrix representation of an operation –representation of a point group - reducible and irreducible representations - Character of a matrix – The Great Orthogonality theorem -Rules derived from Orthogonality theorem (proof not required) - Setting up of the character tables of simple groups such as C_{2v} and C_{3v} – four columns of the character table and their uses.

Basics of molecular spectroscopy - origin of spectra – types of spectra- parameters for a spectral line- position – width –intensity –factors affecting these parameters - Energy levels in molecules – theory of rotational - vibrational – electronic - Raman spectra - selection rules -Basic elements of practical spectroscopy - Born-Oppenheimer approximation.

Unit III Electrochemistry

Ionics: Ions in solution. Deviation from ideal behaviour. Ionic activity. Ion-solvent interaction. Born equation. Ion ion interaction. Activity coefficient and its determination. Debye-Huckel limiting law. Equation for appreciable concentration. Osmotic coefficient. Acivities is concentrated solutions. Robinson-Stoke theory. Ion association. Strong electrolytes. Ion transport, Debye-Huckel treatment. Onsager equation. Limitation of the model. Conductance of high frequencies and high potentials.

Electrodics: Different types of elctrodes. Electrochemical cells. Concentration cell and activity coefficient determination. Origin of electrode potential. Liquid junction potential. Evaluation of thermodynamic proeprties. The electrode double layer: Electrode-electrolyte interface. Theory of multiple layer capacity. Electrocapillary. Lippmann potential. Membrane potential. Elecrokinetic phenomena. Mechanism of charge transfer at electrode-electrolyte interface. Electrolysis. Current-potential curves. Dissolution, deposition and decomposition potentials. Energy barriers at metal-electrolyte interface. Different types of over potentials. Butter-Volmer equation. Tafel and Nernst equation. Rate determining step in electrode kinetics. The hydrogen over voltage. The oxygen over voltage. Theories of over voltage.

Unit IV Gases, Liquids and Liquid Crystals

Random movement of molecules. Brownian movement and determination of Avogadro number. The distribution of molecular velocities. Deviation and discussion of Maxwells equation. Gamma function. Deviation of average and most probable velocities from Maxwells equation. Influence of temperature on molecular velocities. Molecular collisions and mean free path. Homogeneous and heterogeneous collisions. Molecular collisions and mean free path. Homogeneous and heterogenesous collisions. Collision of molecules with a surface and effusion. Effect of molecular interaction on collision. Transport properties: Viscosity, thermal conductivity and diffusion. Determination of viscosity of gases. Influence of temperature and pressure on transport properties.

Liquid State: X-ray diffraction study of simple liquids and their structure. Theories of liquid state. Oscillator, free space and van der Waals theories. Lennard-Jones theory of melting. Specific heat of liquids.

Liquid crystals: Mesomorphic state, types, examples and application of liquid crystals. Theories of liquid crystals. Chiral thermotropic liquid crystal polymers. Nematic liquid crystals fromed from flexible molecules. Molecular field theory. Order and odd-even effects in thermotropic nematic polyesters. Photoconducting liquid crystals. Electro-optic effects in smectogenic polysiloxane side chain liquid crystal polymer.

Unit V Surface chemistry, Colloids and Catalysis

Different types of surfaces. Examination of surfaces using ESCA, Auger, SEM and STM. Properties of surface phase. Thermodynamics of surface. Surface tension of solutions. Gibbs' adsorption equation and its verification. Surfactants and miscelles. Surface films: Different types Surface pressure and surface potential, and their measurements and interpretation.

The gas-solid inter phase: Types of adsorption. Heat of adosrption. The Langmuir theory-kinetic and statistical derivation. Multilayer adsorption- the BET theory and Harkins-Jura theory. Adsorption from solutions on

solids. Langumuir and classical isotherms. Chemisorption-differences with physical adsorption. Adsorpiton isotherms. Adsorption with dissociation. Adsorption with interaction between adsorbate molecules. Measurement of surface area of solids: Harkins-Jura absolute method, entropy method, and the point B method. Use of Langmuir, BET and Harkins-Jura isotherms for surface area determination.

The colloidal state: Multimolecular, macromolecular and associated colloids. Stability of colloids. The zeta potential. Kinetic, optical and electrical properties of colloids. Electrokinetic phenomena: Electrophoresis, electroosmosis, sedimentation potential and streaming potential. Donnan membrane equilibrium.

Catalysis: Mechanism and theories of homogeneous and heterogeneous catalysis. Acid-base and enzyme catalysis. Bimolecular surface reactions. Langmuir-Hinshelwood mechanism.

References

1. M.W.Hanna, "Quantum Mechanics in Chemistry" Benjamin
2. M.C.Day and J.Selbin, "Theoretical Inorganic Chemistry", Affiliated East West Press
3. I.N.Levine, "Quantum Chemistry", Prentice Hall
4. Manas Chanda, "Atomic Structure and Chemical Bond including Molecular Spectroscopu", Tata McGraw-Hill
5. Donald A McQuarrie, "Physical Chemistry-A Molecular Apprach", Viva Low Priced Edition
6. C.A.Coulson, "Valence", Oxford University Press
7. G.W.Castellan, "Physical Chemistry", Narosa Publishing House
8. S.Glasstone and H.S.Taylor, "Treatise on Physical Chemistry", D. van Nostrand
9. A.A.Frost and Pearson: "Kinetics and Mechanism", John Wiely and sons
10. K.J.Laidler: "Chemical Kinetics", McGraw-Hill
11. S.Glasstone, k.J.Laidler and H.Eyring: "The theory of Rate Process", McGraw Hill
12. P.H.Emmet, "Catalysis – Vol I – Fundamental Principles", John Wiley Ssons
13. A.E.Alexander and P.Johnson: "Colloid Science", Oxford University Press
14. J.N.Gurtu and H.Snehi: "Advanced Physical Chemistry", Pragati Prakash
15. A.W.Adamson: "The Physics and Chemistry of Surfaces", Interscience
16. S.J.Gegg: "The Surface Chemistry of Solids", Chapman and Hall
17. N.K.Adam: "The Physics and Chemistry of Surfaces", Oxford University Press

PGCH09AC1- ANALYTICAL CHEMISTRY-I **90 hours**

Unit I Basics of analysis and validation - analytical methods -Classification – selection of a method –- Steps in a quantitative analysis - Quantitative range (bispartite classification) –Sample preparation – processing - Data organization - Analytical validations - Limit of detection and limit of quantitations- good lab practices.

Unit II Errors in Chemical Analysis and Statistical Evaluation of Data –Errors -its types - Systematic random errors - Accuracy - precision - Ways of expressing accuracy and precision - Normal error curve - its equation - Propagation of error - statistical tests - test of significance - **F** test - student '**t**' test -the χ-test, - correlation coefficient - confidence limit of the mean - comparison of two standard values - comparison of standard deviation with average deviation - comparison of mean with true values -significant figures, regression analysis (least-square method for linear plots) - statistics of sampling and detection limit evaluation.

Unit III Concept of Equilibrium Solvents and solutions - general treatment of equilibria in aqueous medium involving monoprotic weak acid and weak base, and salts of weak acids and weak bases -Activity -concentration - Effect of electrolytes on chemical equilibria - Calculation of pH – Construction of titration curves from charge balance and mass balance equations-Acid-base – complexometric –redox –precipitation titrations –theory of the corresponding indicators.

Unit IV Spectrophotometric Determination of Stoichiometry of Complexes Job's method of continuous variation, mole ratio and slope ratio analysis, Advantages and limitations, Typical examples.

Unit V Automation in the Laboratory Principles of automation, Process control through automated instruments, Autoanalyzers (single channel and multi-channel), Basic sequences of multi-fold operational analyzers in segmented and non-segmented flows.

References

1. R. L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William, Modern Methods of Chemical Analysis, 2nd Edition (1976), John Wiley, New York.
2. G. D. Christian, Analytical Chemistry, Edition (1994), John Wiley & Sons, New York.
3. D. A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Analytical Chemistry - An Introduction, 7th Edition (2000), Saunders College Publishing, Philadelphia, London.
4. J. H. Kennedy, Analytical Chemistry: Principles, Edition (1990), Saunders Holt, London.

SEMESTER II

PGCH0921- INORGANIC CHEMISTRY-II ***Total 90 hours***

Unit I Crystalline State

Structure in solid state- lattice-lattice planes- symmetry in crystals-point groups and space groups- Bravais lattices. Miller indices. Close packed structures-limiting radius ratios – BCC-FCC-HCP- examples for AX, AX_2 and layered structures-Molecular, covalent, metallic and hydrogen-bonded crystals.

X-Ray diffraction – Functions of crystals- Transmission and reflection gratings.- Bragg's equation - diffraction methods. Powder, rotation crystal, oscillation and Weisenberg methods Indexing and determination of lattice type – reciprocal lattice- unit cell dimensions of cubic crystals. Structure factor.

Unit II Solid State Chemistry

Electronic structure of solids - Band theory – refinement - k space- Brillouin zones Conductors- insulators – semiconductors - band structure and applications.

Crystal defects-types of defects-point, line and plane defects - thermodynamics of Schottky and Frenkel defects. Colour centers-defect clusters - extended defects-crystallographic shear structure and stacking faults. .

Unit III Electrical and Magnetic Properties of Solids

Electrical properties of solids- Conductivity of pure metals – superconductivity - photoconductivity - photovoltaic effect.-dielectric properties - dielectric materials. Ferroelectricity - pyroelecricity and pizoelectricty- Applications of ferro, piezo and pyroelectrics.

Magnetic properties of solids- Types of magnetic materials – cooperative magnetism- effect of temperature- Curie and Curie-Weiss laws - calculation of magnetic moments.-super exchange-Lasers and their applications.

Unit IV Lanthanides and Actinides

Lanthanides - chemistry of beach sands of Kerala and their components monozite, ilmenite, zirconand siliminite – extraction of lanthanides and actinides-general properties- lathanide contraction and its consequences - oxidation states.- -spectral and magnetic properties-shapes of f - orbitals and their splitting in cubic ligand field - Actinides: Occurrence and general properties. Electronic configuration-Oxidation states - spectral and magnetic properties. . Trans-uranium elements and their stabilities. Applications of lanthanide and actinide compounds. .

Unit V Bioinorganic Chemistry

Metalloporphyrins -Chlorophyll – synthetic model for photosynthesis-Cytochromes: Biological importance of iron. Availability and transport of iron. Hemoglobin and myoglobin. Synthetic oxygen carriers(Vaska's complex)- iron in enzymes-Catalytic functions of metalloenzymes in biological processes - Cobaltamine in amino acid catabolism - Synthetic model of enzyme action - Inhibition and poisoning by metal ions - Copper in cytochrome oxidase and in respiratory chain- Na and K in blood, in urine, transport in kidney and in intracellular fluid –role of Zn in aldolase activity - Nitrogen fixation and nitrogenases.

References

1. L.V.Azaroff, "Introduction to Solids", McGraw-Hill
2. N.B.Hannay, "Solid State Chemistry", Prentice Hall.
3. F.C.Phillips, "An Introduction to Crystallography", Longman
4. C.Kittel, "Introduction to Solid State Physics", John Wiley & Sons
5. T.Moeller, "The Chemistry of the Lanthanides", Reinhold.
6. G.T.Seaborg. J.J.Katz and W.M.Manning, "The Transuranium Elements", McGraw-Hill
7. G.T.Seaborg, "Manmade Transuranium Elements", Prentice Hall
8. Simon Cotton, "Lanthanides and Actinides", Macmillan

PGCH0922 - ORGANIC CHEMISTRY-II **Total 90 hours**

Unit I Molecular Rearrangements

Rearrangements- terminology used - types of rearrangements – inter - intra molecular - Mechanism –evidences and applications of Wagner – Meerwein – Pinacol-Pinacolone – Demjanov – Hofmann – Curtius- Schmidt – Lossen - Beckmann –Wolff – Fries - Arylozo - Fischer-Hepp - Hofmann-Martius - von Richeter – Orton - Bamberger, -Smiles - Dienone-Phenol - Benzilic acid – Benzidine – Favorskii – Stevens – Wittig - Sommelet-Hauser - Baeyer-Villiger – Hydroperoxide rearrangements.

Unit II Aromaticity and Symmetry Controlled Reactions

Aromaticity – cosequences of Aromaticity – Huckle's rule- Craig's rule- alternant and non-alternant hydro carbons- antiaromaticity and homoaromaticity – non-benzenoid aromatic systems. Aromaticity of annulenes - mesoionic compounds.

Pericyclic reactions – definition - Classification – electrocyclic reactions - cycloadditions -sigma tropic reactions – conclusions on the basis of correlation diagram, FMO and PMO methods- Woodward-Hoffmann rules - Claisen rearrangement. Stereo aspects of Diels-Alder reaction and Cope rearrangement - Retro Diels-Alder – Ene - Cheletropic and cis elimination reactions. Synthetic applications.

Unit III Organic Photochemistry

Excitation – fate of the excited molecule - energy transfer, sensitization and quenching - Singlet and triplet states - differences between thermal and photochemical reactions - Photo reduction - photo oxidations-singlet oxygen - Photoreactions of carbonyl compounds – NorrishI and II reactions –
Paterno-Buchi – photo reactions of enes – dienes - arenes. tones. , Barton reaction - photo-Fries -
Di-π methane rearrangement – Photoreactions of Vitamin D - photo isomerisation of alkenic systems -. Photochemistry of vision

Unit IV Chemistry of natural products

Structure and synthesis of alpha-Pinene, Camphor, Cadenine and Caryophyllene. Hofmann, Emde and von Braun degradation in alkaloid chemistry. Structure elucidation of Papaverine, Quinine and Morphine. Synthesis of Quinine and Papaverine. Structure and synthesis of beta-Carotene, Flavone, Iosflavone, Cyanin and Quercetin. Biosynthesis of terpenes and alkaloids. Classification and structure of lipids and their biofunctions. Nomenclature, structure (not elucidation) and biosynthesis of Prostaglandins PGE_2, and PGF_{1v}.

Unit V Chemistry of Biomolecules

Nomenclature, reactivity and stereochemistry of steroidal systems. Stereochemistry and structure elucidation of cholesterol (no synthesis). Synthesis of Testosterone, Andestrone, Estrone and Progesterone. Steroid biosynthesis. Structure and synthesis of vitamins A, C M1 and Biotin. Structure of penicillins. Synthesis of paracetamol, phenobarbital, diazepam, sulfamethoxazole, benzyl penicillin and chloramphenicol.

Reference

1. L.M.Harwood, "Polar Rearrangements", Oxford University
2. J.March, "Advanced Organic Chemistry", Wiley
3. S.N.Issacs, "Physical Organic Chemistry", Longman
4. P.Y.Bruice, "Organic Chemistry", Prentice Hall
5. H.Arora, "Organic Photochemistry and Pericyclic Reactions"
6. C.H.Dupuoy, and O.L.Chapman, "Molecular Reactions and Photochemistry", Prentice Hall
7. J.M.Cozon and B.Holton, "Organic Photochemistry", Cambridge University Press
8. S.H.Pine, "Organic Chemistry", McGraw-Hill
9. I.L.Finar, "Organic Chemistry" Vol w, Longman
10. R.P.Wayne, "Principles and Applications of Photochemistry", Oxford University Press
11. J.Kagan, "Organic Photochemistry", Academic Press
12. R.J.Simmonds, "Chemistry of Biomolecules", Royal Society of Chemistry
13. J.Mann and others, "Natural Products – Their Chemistry and biological significance", Longman
14. I.L.Finar, "Organic Chemistry" Vol 2, Longman

PHYSICAL CHEMISTRY-II

Total 90 hours

Unit I Chemical Kinetics

Complex reactions: Reversible, consecutive, concurrent and branching reactions. Free radical and chain reactions. Steady state treatment. Reactions like H_2-Cl_2, H_2-Br_2, and decompositions of ethane, acetaldehyde and N_2O_5. Rice-Herzfelf mechanism. Unimolecular reaction. Lindemann treatment. Semenoff-Hinshelwood mechanism of chain reactions and explosion. Kinetics of fast reactions: Relaxation method, relaxation spectrometry, flow method, shock method, fast mixing method, field jump method and pulse method.

Theories of reaction rate: Influence of temperature on reaction rate. Arrhenius equation and its likitations, activation energy. Collision theory and absolute reaction rate theory. Free energy of activation and volume of activation. Thermodynamic formulation of reaction rate. Effects of pressure and volume on the velocity of gas reaction.

Reactions in solution: comparison between reactions in gas phase and in solution. Factors determining reaction rates in solution. Reaction between ions and influence of ionic strength. Primary and secondary kinetic salt effects. Influence of solvent on reaction rate. Significance of volume of activation. Hammet and Tafel equation.

Photochemistry: Effect of radiation on the rate of reaction. Law of photochemistry. Quantum yield. Radiative and non-radiative transitions. Fluorescence and quenching of fluorescence. Photosensitization. Flash photolysis. Photochemical reactions of H_2-Cl_2 and H_2-Br_2. Photostationary state. Chemiluminescence.

Unit II Basics of Chemical Thermodynamics

Thermodynamic properties: State and path properties. Intensive and extensive properties. Exact differentials. Intrinsic energy, enthalpy, entropy, free energy and their relations and significances. Eulers relation. Jacobians. Maxwell relations. Theromodynamic equations of state. Joule-Thomson effect. Joule-Thomson coefficient for van der Waals' gas. The third law of thermodynamics. Need for the third law. Nernst heat theorem. Apparent exceptions to third law. Applications of third law.

Properties of solutions: Thermodynamics of ideal solutions. Partial molar quantities. Chemical potentials. Duhem-Margules equation. Nonideal solutions. Excess thermodynamic functions. Determination of partial molar properties. Fugacity and activity: Fugacity of gases. Determination. Variation of fugacity with temperature and pressure. Fugacity of liquids and solids. Fugacity of mixtures of gases. Lewis-Randall rule. Fugacity in liquid mixtures. Activity and activity coefficients. Standard states. Determination of activity and activity coefficients of electrolytes and nonelectrolytes.

Unit III Application of Thermodynamics

Chemical equilibrium: Equilibrium constant in real systems. Equilibrium in homogeneous and heterogeneous systems. Reaction quotient. Reaction isotherm and spontaneity of reaction. Variation of equilibrium constant with temperature and pressure. Variation of standard free energy with temperature. Simultaneous equilibria and addition of free energies. Standard free energy of formation and its determination. Free energy functions.

Phase equilibria: Criteria of equilibrium. Derivation of phase rule. Discussion of two component systems formign solid solutions with and without maximum or minimum in freezing point curve. Systems with partially miscible solid phases. Three component systems: Graphical representation. Three component liquid systems with one pair of partially miscible liquids. Influence of temperature. Systems with two pairs and three pairs of partially miscible liquids. Two salts and water systems. Isothermal evaporation. Transition point and double salt formation.

Thermodynamics of irreversible processes: Simple examples of irreversible processes. General theory of near equilibrium processes. Entropy production from heat flow. Matter flow and current flow. Generalized equation for entropy production. The phenomenological relations. Onsager reciprocal relation. Application of irreversible thermodynamics to diffusion. Thermal diffusion. Thermoosmosis and thermomolecular pressure difference. The Glansdorf-Prigogine theorem. Quantitative introduction to treatment of far from equilibrium states.

Unit IV Statistical Thermodynamics

Statistical thermodynamics: Mechanical description of molecular systems. Termodynamic property and entropy. Microstates. Canonical and grand canonical ensembles. Equation of state of ideal quantum gases. Maxwell-Boltzman distribution. The partition functions. Partition function for free linear motion, for free motion in a shared space, for linear harmonic vibration. Complkex partition functions and partition functions for particles in different force fields.

Langevins partition function and its use for the determination of dipole moments. Electrostatic energies. Molecular partition functions. Trnslational, rotational, vibrational and electronic partition functions. Total partition functions. Partition functions ant thermodynamic properties.

Unit V-Quantum Statistics and Heat Capacity

Quantum Statistics-Bose-Einsein statistics. Bose-Einstein distribution, Thermodynamic probability, Bose Einstein Distribution Function, Examples of particles. Theory of paramagnetism. Bose-Einstein condensation. Liquid helium. Supercooled liquid. Fermi-Dirac statistics. Fermi-Dirac Distribution, Examples of particles. Fermi-Dirac Distribution Function, Thermionic emission. Relations between Maxwell-Boltzman, Bose-Einstein and Fermi-Dirac statistics.

Heat capacity of gases. Equipartition principle and quantum theory of heat capacity. Calculation of Heat Capacity of gases-Limitation of the Method. Heat capacity of solids. Dulong and Petit's law, Kopp's law, Classical theory and its limitation. The vibrational properties of solids. Einstein theory of heat capacity. The spectrum of normal modes. Limitation of Einstein theory. The Debye Theory. The electronic specific heat.

References:

1. A.A.Frost and Pearson: "Kinetics and Mechanism", John Wiely and sons
2. K.J.Laidler: "Chemical Kinetics", McGraw-Hill
3. S.Glasstone, k.J.Laidler and H.Eyring: "The theory of Rate Process", McGraw Hill
4. S.Glasstone: "Theormodynamics for Chemists", Affiliated East West Publishers.
5. S.Glasstone and H.S.Taylor, "Treatise of Physical Chemistry", D van Nostrand
6. I.Pregogine, "Introduction to Thermodynamics of Irreversible Processes", Inter science
7. M.C.Gupta, "Elements of Statistical Thermodynamics", New Age International (P) Ltd.
8. L.K>Nash, "Elements of Statistical Thermodynamics", Addison Wesley Publishing Co.
9. Kesting and Dofman, "Statistical thermodynamics"

PGCH09AC2 - ANALYTICAL CHEMISTRY-I

Unit I Polarography Origin of polargraphy, Current-voltage relationship, Theory of polarographic waves (DC and sampled DC (tast) polarograms), Instrumentation, Ilkoviè equation, Qualitative and quantitative applications.

Unit II Atomic Spectroscopy Theory, Instrumentation and applications of X-rays (emission, absorption, diffraction and fluorescence methods), Atomic absorption Spectroscopy, Atomic fluorescence spectrometry, Atomic emission spectrometry.

Unit III Molecular Spectroscopy UV-visible molecular absorption spectrometry (instrumentation and applications), Molecular luminescence spectroscopy (fluorescence, phosphorescence, chemi-luminescence), Mass spectroscopy.

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

Unit V Thermal Analysis Theory, methodology and applications of thermogravimetric analysis (TGA), Differential Thermal Analysis (DTA), and Differential scanning calorimetry (DSC). Principles, techniques and applications of thermometric titration methods.

Books Recommended

1. D.A. Skoog, Principles of Instrumental Analysis, 5th Edition (1998), Saunders College Publishing, Philadelphia, London.
2. G.W. Ewing, Instrumental Methods of Chemical Analysis, 5th Edition (1978), McGraw Hill Books Co., New York.
3. R.L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William, Modern Methods of Chemical Analysis, 2nd Edition (1976), John Wiley, New York.
4. J.H. Kennedy, Analytical Chemistry: Principles, Edition (1990), Saunders Holt, London. Edition (1990), Saunders Holt, London.

PGCHO9ICP - Inorganic practical

1. Separation and analysis of an inorganic mixture containing two common and two less common metal ions including the following:
   Common ions: Pb, Cu , Bi, Cd, Al, Ni, Co, Mn, Zn, Ba, Ca, Sr and Mg
   Less common ions: W, Se, Te, Mo, Ce, Th, Zr, Ti, V, U, and Li
2. Volumetric estimations using EDTA, Ammonium vanadate, ceric sulphate and potassium chlorate.
3. Colorimetric estimation of Cu,Cr,Fe,Ni,Ti and PO_4^{3-}
4. Preparation of any ten of the following complexes.
   i. Tetraamminecopper(II) sulphate
   ii. Potassium trioxalatochromate(III)
   iii. Potassium hexathiocyanatochromate(III)
   iv. Hexaureachromium(III) chloride
   v. Sodium trioxalatoferrate(III)
   vi. Hexaamminenickel(II) chloride.
   vii. Trithioureacopper(I) sulphate
   viii. Tris(acetylacetanato)copper(II)
   ix. Tris(ethylenediamine)nickel(II) chloride
   x. Cis(dichloro)-diammine cobalt(II) chloride
   xi. Nitrosylbis(diehtyldithiocarbamato)iron(I)
   xii. Penta thioureadicuprous nitrate
   xiii. trans-Potassium dioxalatodiaquaochromate(III)
   xiv. Hexathioureaplumbous nitrate(II)
   xv. Ruby powder by combustion method

Books recommended

1. Inorganic semi-micro analysis –V.V.Ramanujam, 3rd edition, The National publishing companay, 1997
2. Advanced Inorganic practical - Gurdeep Raj- Pragathi Prakasan –Meerut
3. Vogel's Text book of Quantitative analysis, Longman Group publishers, 5 th edition 1994.
4. Inorganic coordination compounds – G.B.Kauffmann – Heyden and son ltd
5. Synthesis of inorganic complexes – Burger

PGCH09OP1 Organic practical

1.Separation and analysis of an organic binary mixture and derivatisation of the components
2.Preparation of organic compounds (Any 8 from the following list)

- Benzoic acid from benzaldehyde
- Salicylic acid from methyl salicylate
- o-chlorobenzoic acid from anthranillic acid
- Resacetophenone from resorcinol
- para-bromoacetanilide from acetanilide
- para-nitroacetanilide from acetanilide
- Dibenzalacetone from acetone
- Benzhydrol from benzophenone
- Phenylazo-2-naphthol from aniline
- Glucose penta acetate from glucose
- Piperidone from ethyl acetoacetate
- Naphthylmethyl ether from β-naphthol

PGCH09PP1 - Physical chemistry practical

Electric experiments

Conductometry experiments

1. Titration of i. Strong acid Vs strong base
   ii. Weak acid Vs Strong base
   iii. Weak acid Vs weak base
2. Titration of a strong base Vs mixture of acids.
3. Precipitation titration i. $BaCl_2$ Vs $MgSO_4$
   ii. $AgNO_3$ Vs mixture of halides
4. Verification of Debye - Huckel – Onsager relation for a strong electrolyte
5. Dissociation constant of a weak electrolyte.
6. Solubility and solubility product of a sparingly soluble salt.

Potentiometry experiments

1. Dissociation constant of a weak acid titration method
2. Dissociation constant of a weak acid Henderson method
3. Redox titration $KMnO_4$ Vs Fe^{2+} / $KMnO_4$ Vs KI
4. Precipitation titration - $AgNO_3$ Vs mixture of halides
5. Standard reduction potential of Cu / Zn / Ag electrode
6. Formal redox potential of Fe^{2+} / Fe^{3+} or Ce^{3+} / Ce^{4+} system
7. Solubility product of a sparingly soluble salt by i. Single electrode method
   ii. Concentration cell method.

Non Electric experiments

1. Determination of partition coefficient of I_2 between water and CCl_4.
   Equilibrium constant for the formation of I^{3-} ion.
2. Construction of phase diagram for a pair of partially miscible liquids and the effect of added impurity.
3. Construction of phase diagram for a three partially miscible liquids.
4. Construction of phase diagram for a simple eutectic system
5. Construction of phase diagram for a system with compound formation
6. Determination M.wt of a non-volatile solute by Rast's method
7. Determination M.wt of a non-volatile solute by transition temperature method
8. Study of adsorption of oxalic acid on charcoal. (Verification of Freundlich's isotherm)
9. Determination of integral heat of solution by solubility method.
10. Determination of heat hydration of anhydrous $CuSO_4$.
11. Determination of rate, order of the reaction between $K_2S_2O_8$ and KI (clock reaction method)
12. Verification of Bronsted –Bjerrum equation with reaction between $K_2S_2O_8$ and KI.
13. Determination of order of the reaction for base hydrolysis of an ester- Condutomentric method
14. Kinetics of acid catalyzed iodination of acetone – spectrophotometeric method.
15. Determination of Arrhenius parameters for acid catalyzed hydrolysis of ester.

References

1. A.Finlay and J.A.Kitchener, "Practical Physical Chemisty", Longman
2. F.Daniels and J.H.Mathews, "Experimental Physical Chemistry", Longman
3. A.M.James, "Practical Physical Chemistry", J.A.Churchil
4. H.H.Willard, L.L.Merritt and J.A.Dean, "Instrumental Methods of Analysis", Affiliated East-West Press
5. D.P.Shoemaker and C.W.Garland, "Experimental Physical Chemistry", McGraw-Hill

Semester-III

PGCH0932 ORGANIC CHEMISTRY-III **Total 90 hours**

Unit I Separation Techniques

Chromatography – introduction and classification - principle and Theory of adsorption and partition chromatography – Paper - thin layer - column chromatographic methods - LC, HPLC and GC. Column matrices – Detectors (UV, IR, Diffractometers, DTCD, Ionisation, Electron capture detectors), - Affinity and chiral columns. **Solvent extraction** - Distribution law – efficiency of extractions- Successive extractions- continuous extraction – stripping- Craig method -Uses of oxine, dithizone, high molecular weight amines, dithiocarbamates and crown ethers in extraction - Normal and ultra-centrifugation.

Unit II UV-VIS, IR and Mass Spectrometry

Electronic spectra -Types of electronic transitions - Woodward-Fieser rules for enes- enones and aromatics - Effect of solvent polarity on UV absorption – **Vibrational spectra** - group frequencies –skeletal vibrations- combination and difference bands – interpretation of simple IR spectra -Hydrogen bonding and IR bands. Sampling techniques. **Mass spectrometry** – principle –Ionisation methods (including MALDI) - molecular ion peak – base peak –isotopic peaks – meta stable peak - Nitrogen rule – McLafferty rearrangement -Characteristic EIMS fragmentation modes of simple compounds including (alkanes, alkenes, acids, amides, aldehydes, ketones, alcohols, halo compounds.)

Unit III NMR Spectroscopy

NMR – principle – relaxation – types of relaxations -basic instrumentation – Chemical shift - τ and δ scales –factors affecting chemical shift - anisotropy effects - coupling constants – factors affecting J value - Spin-spin interactions –types of NMR spectra-1° order and complicated spectra (AB, ABX, AMX) - Simplification of complex spectra - high field NMR - shift reagents - chemical exchange - double resonance -Introduction of FT (pulse) NMR – pulse sequences- measurement of T1, T2 – NOE - DEPT 1 and DEPT2 - 2D NMR – COSY, ROSY, NOSY basic principles-MRI - **C^{13}NMR** - decoupled spectra- types of decoupling -chemical shifts - interpretation and structure identification- identification of structure of the molecules from the spectral data (combined problem).

Unit IV Reagents in Organic Synthesis

Applications of hydrogenation catalysts, hindered boranes, bulky metal hydrides, $NaCNBH_3$. DIBAL, Li trialkyl borohydrides, tri-n-butyl tin hydride, diimide, Kindlar catalysts and Rosenmund reduction. McFadeyan-Stevens reactions. Oxidation using SeO_2, lead tetraacetate, ozone, peracids,

DDQ and Cr(VI) reagents. Swern oxidation, Moffatt oxidation, allylic and benzylic oxidation Sommelet reaction. Elbs reactions. Oxidative coupling of phenols. Sharpless assymetric epoxidation Chemo and regioselectivity in reductions and oxidation. Use of XeF_2, SbF_5,VF_5,MoF_6,CF_3OF,SF_4, HF and F_2 as fluorinating agents

Unit V Methods in Organic Synthesis

Retrosynthetic analysis and disconnection approach. Synthetic strategy and synthons. Regioselectivity in enol and enamine alkylations Steroselective and stereospecific synthesis. Mitsonobu reaction. 1,3-dipolar cycloaddition in the construction of rings. Story synthesis. Olefin synthesis by extrusion reactions. Olefin metathesis. FMOC, BOC, Z, trityl, phthalimide, benzyl, tetrahydropyranyl, silyl, t-butyl, trichloroethyl, acetal and thioacetal as amino, hydroxy, thiol, caroxyl and carbonyl protecting groups in synthesis. Umpolung. Electrochemical reduction and oxidation reactions. Cathodic reduction of organic halogen, nitro and carbonyl compounds. Reductive coupling reactions. Conversions of C=O to $C=CH_2$; epoxide to alkene and alkene to *cis* and *trans* diols. Prevost and woodward procedures

References

1. D.A.Skoog, D.M.West and F.J.Holler, “Fundamentals of Analytical Chemistry”, Saunders College Publishing
2. R.A.Day and A.L.Underwood, “Quantitative Analysis”, Prentice Hall
3. D.H.Williams and I.Fleming, “Spectroscopic Methods in Organic Chemistry”, Wiley.
4. W.Kemp, “Organic Spectroscopy”, Longman
5. M.B.Smith, “Organic Synthesis”, McGraw Hill
6. H.O.House, “Modern Synthetic Reactions” Benjamin Cummins
7. R.K.Mackie, D.M.Smith, and R.A.Aitken, “Guide Book to Organic Synthesis Longman, 2Edn
8. W.Carruthers, “Some Modern Methods of Organic Synthesis”, Cambridge Univ. Press

PGCH09IA - INSTRUMENTATION ANALYSIS **Total 90 Hours**

Unit I Rotational, vibrational and Raman spectra

Microwave spectroscopy - Rotation of diatomic molecules. Rotational sepectrum: Intensity of spectral lines. Calculation of internuclear distance. Non-rigid rotors and centrifugal distortion. Rotational spectra of polyatomic molecules- linear and symmetric top molecules. Introduction to instrumentation**.**
Infrared spectroscopy: Vibrational spectra of harmonic and anharmonic diatomic molecules. Morse function. Fundamentals and overtones. Determination of force constants. Interaction of rotation and vibration. Different branches of spectrum. Asymmetry of vibrational-rotational spectrum. Vibrational spectra of polyatomic molecules. Vibrations of polyatomic molecules, normalmodes, classifications of vibrations: Stretching, bending, symmetric, asymmetric, parallel and perpendicular vibrations. Overtones, combinations and Fermi resonance. Finger print and group frequencies. Introduction to instrumentation and FT-IR.
Raman spectra: Scattering of light. Raman scattering. Polarisability and classical theory of Raman spectrum. Rotational and vibrational Raman sepctrum. Raman spectra of polyatomic molecules. Complimentary nature of Raman and IR spectra. Mutual exclusion principle. Introduction to instrumentation. Laser Raman spectrum. Electronic spectra: Term symbols of molecules. Electronic spectra of diatomic molecules. Vibrational coarse structure and rotational fine structure of electronic spectrum. Franck-Condon principle. Types of electronic transitions. Fortrat diagram. Predissociation. Calculation of heat of dissociation. Electronic spectra of polyatomic molecules: Electronic transtitions among molecular orbitals and absorption frequencies. Effect of conjugation of absorption frequencies. Introduction to instrumentation.

Unit II Electronic spectra and spectrometric methods

UV-Visible spectrophotometry: fundamental laws of photometry. Basic instrumentation. Simultaneous determination of two components. Flame emission and atomic absorption spectroscopy. Instrumentation for AAS. The flame spectra and flame characteristics. Atomiser used in spectroscopy. Hollow cathode lamp. Interference in AAS. Application of AAS. Mossbauer spectroscopy: principle and application. Photoelectron spectroscopy: Introduction to UV photoelectron and X-ray photoelectron spectroscopy. Electron deiffraction of gases. Incoherent scattering, Wierl's equation, correlation and radial distribution. Polarisation and dipole moment: Debye and Calusius-Mossotti equation. Determination of dipole moments. Structural information from dipole moments.

Unit III Spin Resonance spectroscopy

NMR spectrum. Nuclear spin. Interaction between nuclear spin and applied magnetic field. Proton nmr spectrum. Population of energy levels. Nuclear resonance. Chemical shift. Relaxation methods. Spin-spin coupling, Fine structure. Elementary idea of 2D and 3D nmr. Mention of nmr spectra of other nuclei. Introduction to instrumentation. ESR spectrum: Electron spin of molecules. Interaction with magnetic field. The g factor. Determination of g values. Fine structure and hyperfine structure. Elementary idea of ENDOR and ELDOR. Mossbauer spectroscopy: Principle, Doppler effect, recording of the spectrum, chemical shift, and quandrupole effect.

Unit IV Electroanalytical Methods

Potentiometric methods: Reference electrodes and indicator electrodes. The hydrogen, calomel, Ag-AgCl electrodes. The glass electrode – its structure, performance and limitations. Measurement of pH. Petentiometric titrations. Redox and precipitation titrations. Electrogravimety: Principle and method. Determination of Cu. Separation of metals. Conductometry: Principle and method. Conductance measurements. Conductometric titrations. Coulometry: Principle and method. Coulometric titrations.

Unit V Optical & Electron Microscopic techniques

Principle, instrumentations and applications of the following techniques AFM, SEM & TEM

References

1. C.N.Banwell, "Fundamentals of Molecular Spectroscopy", McGraw Hill
2. Manas Chanda, "Atomic Structure and Chemical Bonding including Molecular Spectroscopy", Tata McGraw Hill
3. G.Herzberg, "Molecular Spectra and Molecular Structure", D van Nostrand
4. D.A.Skoog, D.M.West and F.J.Holler, "Fundametals of Analytical Chemistry", Saunders College Publishing.
5. C.L.Wilson and D.W.Wilson, "Comprehensive Analytical Chemistry", Dan van Nostrand
6. J.G.Dick, "Analytical chemistry", McGraw Hill
7. W.W.Wendlandt, "Thermal Methods of Analysis", John Wiley & Sons

PGCH09MC - MATERIALS CHEMISTRY

Total 90 hours

Unit I Introduction to material chemistry

sMaterials and their classification, Role of Chemistry in Material design.

Unit II Synthesis and Characterization of Materials Preparative techniques: Ceramic methods; chemical strategies, chemical vapour deposition; preparation of nanomaterials, Langmuir- Blodgett Films. Fabrication of ordered nanostructures . Composition and purity of materials.

Unit III 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.

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

Unit V 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. A.R. West, Solid State Chemistry and its Applications, *(1984) John Wiley & Sons, Singapore.*

2. C.N R. Rao and J. Gopalkrishnan, New Directions in Solid State Chemistry, *(1997) Cambridge Univ. press.*

3. T. V. Ramakrishnan and C.N.R. Rao, Superconductivity Today, *(1992) Wiley Eastern Ltd., New Delhi.*

4. P. Ball, Designing the Molecular World: Chemistry at the Frontier, *(1994) Princeton Univ. Press.*

MC 401 ENVIRONMENTAL CHEMISTRY

Total 90 hours

Unit-I

Atmosphere

Atmospheric layers, Vertical temperature profile, heat/radiation budget of the earth atmosphere systems. Properties of troposphere, thermodynamic derivation of lapse rate. Temperature inversion. Calculation of Global mean temperature of the atmosphere. Pressure variation in atmosphere and scale height. Biogeochemical cycles of carbon, nitrogen, sulphure, phosphorus oxygen. Residence times.

Unit-II

Atmospheric Chemistry

Sources of trace atmospheric constituents : nitrogen oxides, sulphure dioxide and other sulphure compounds, carbon oxides, chlorofluorocarbons and other halogen compounds, methane and other hydrocarbons.

Tropospheric Photochemistry

Mechanism of Photochemical decomposition of NO2 and formation of ozone. Formation of oxygen atoms, hydroxyl, hydroperoxy and organic radicals and hydrogen peroxide. Reactions of hydroxyl radicals with methane and other organic compounds. Reaction of OH radicals with SO2 and NO2. Formation of Nitrate radical and its reactions. Photochemical smog meteorological conditions and chemistry of its formation.

Unit-III

Air Pollution

Air pollutants and their classifications. Aerosols-sources, size distribution and effect on visibility, climate and health.

Acid Rain

Definition, Acid rain precursors and their aqueous and gas phase atmospheric Oxidation reactions. Damaging effects on aquatic life, plants, buildings and health. Monitoring of SO2 and NOx. Acid rain control strategies.

Stratospheric Ozone Depletion

Mechanism of Ozone formation, Mechanism of catalytic Ozone depletion, Discovery of Antarctic Ozone hole and Role of chemistry and meteorology. Control Strategies.

Green House Effect

Terrestrial and solar radiation Spectra, Major green house gases and their sources and Global warming potentials. Climate change and consequences.

Urban Air Pollution

Exhaust emissions, damaging effects of carbon monoxide. Monitoring of CO. Control strategies.

Unit-IV

Aquatic Chemistry and Water Pollution

Redox chemistry in natural waters. Dissolved oxygen, biological oxygen demand, chemical oxygen demand, determination of DO, BOD and COD. Aerobic and anaerobic reactions of organic sulphure and nitrogen compounds in water acid-base chemistry of fresh water and sea water. Aluminum, nitrate and fluoride in water. Petrification. Sources of water pollution. Treatment of waste and sewage. Purification of drinking water, techniques of purification and disinfection.

Unit-V

Environmental Toxicology

Toxic heavy metals : Mercury, lead, arsenic and cadmium. Causes of toxicity. Bioaccumulation, sources of heavy metals. Chemical speciation of Hg, Pb, As, and Cd. Biochemical and damaging effects.

Toxic Organic Compound : Pesticides, classification, properties and uses of organochlorine and ionospheres pesticides detection and damaging effects.

Polychlorinated biphenyls : Properties, use and environmental continuation and effects.

Polynuclear Aromatic Hydrocarbons : Source, structures and as pollutants.

Soil and Environmental Disasters

Soil composition, micro and macronutrients, soil pollution by fertilizers, plastic an metals. Methods of re-mediation of soil. Bhopal gas tragedy, Chernobyl, three mile island, Minimtata Disease, Sevoso (Italy), London smog.

References

Environmental Chemistry, Colin Baird, W.H. Freeman Co. New York, 1998.
Chemistry of Atmospheres, R.P. Wayne, Oxford.
Environment Chemistry, A.K. De, Wiley Eastern, 2004.
Environmental Chemistry, S.E. Manahan, Lewis Publishers.
Introduction to atmospheric Chemistry, P.V. Hobbs, Cambridge.

PGCH09PO - POLYMER CHEMISTRY **Total 90 hours**

Unit-I

Importance of polymers. Basic concepts : Monomers, repeat units, degree of polymerization Linear, branched and network polymers. Classification of polymers. Polymerization : condensation, addition/radical chain-ionic and co-ordination and copolymerization. Polymerization conditions and polymer reactins. Polymerization in homogeneous and heterogeneous systems.

Unit-II

Polymer Characterization

Polydispersion-average molecular weight concept. Number, weight and viscosity average molecular weights. Polydispersity an molecular weight distribution. The practical significance of molecular weight. Measurement of molecular-weights. End-group, viscosity, light scattering, osmotic and ultracentrifugation methods. Analysis and testing of polymers-chemical analysis of polymers, spectroscopic methods, X-ray diffraction study. Microscopy. Thermal analysis and physical testing-tensile strength. Fatigue, impact. Tear resistance, Hardness and abrasion resistance.

Unit-III

Inorganic Polymers

A general survey and scope of Inorganic Polymers special characteristics, classification, homo and hetero atomic polymers.

Unit-IV

Structure, Properties and Applications of Polymers based on boron-borazines, boranes and carboranes. Polymers based on Silicon, silicone's polymetalloxanes and polymetallosiloxanes, silazanes.

Unit-V

Structure, Properties and Application of Polymers based on Phosphorous-Phosphazenes, Polyphosphates
Polymers based on Sulphure-Tetrasulphur tetranitride and related compounds.
Structure, Properties and Applications of Metal clusters. Co-ordination and metal chelate polymers.

References:

Inorganic Chemistry, J.E. Huheey, Harper Row.
Developments in Inorganic polymer Chemistry, M.F. Lappert and G.J. Leigh.
Inorganic polymers- N.H> Ray.
Inorganic polymers, Graham and Stone.
Inorganic Rings and Cages : D.A. Armitage.
Textbook of Polymers Science, F.W. Billmeyer Jr. Wiley.
Contemporary Polymer Chemistry, H.R. Al cock and F.W. Lambe, Prentice Hall.

PGCH09IL -INSTRUMENTATION LAB

PGCH09CP Programming in C and C^{++} **Total 90 hours**

Unit I Introduction to C: Character set - data types-variables –constants-key words-operators-expressions-hierarchy of evaluation. Control statements- if – if-else –nested if-else – while – do-while –for loop –nested loops –go to – break - continue –switch case statements

Unit II Functions and arrays: Types of functions-call by value – call by reference –call by address library and user defined functions-recursion –local and global variables –arrays –definition –initialization of an array –types of arrays – passing arrays to a function –structures-unions-pointers – pointer arithmetic.

Unit III C^{++} Fundamentals: Over view of C^{++} - classes and objects- console i/o operations – constructors and destructors –comparison between C and C$^{++.}$ Structures and unions in C++. Inline function – types of constructor-static members –structures, unions and class relationships-function overloading (polymorphism)

Unit IV Inheritance: Types of inheritance simple-multi level –multiple - hybrid-access specifiers for inheritance – late binding –pointers. Command line arguments – variable number of arguments (ellipsis)-standard library functions (ctype.h , string.h , math.h stdlib.h graphics.h)- Operator over loading

Unit V streams and files: stream and file classes- reading and writing charaters, strings, and structure variables with files -preprocessor-conditional computation directives-dynamic memory allocation. - templates – exception handling-name spaces.

References

1. C-complete reference – Hebert Schildt
2. Theory and problems of programming with C – Gotterfried.B
3. Encyclopedia of C – Robert A.Radcliffe
4. C^{++} : The complete reference - Hebert Schildt

PGCH09ICQ - INDUSTRIAL CHEMICAL ANALYSIS AND QUALITY CONTROL Total 90 hours

Unit I Analytical Chemo metrics: General introduction and its application in optimisation, Modelling and parameter estimation, Sampling, calibration, Factor analysis, Resolution, Signal processing, Structure-property relationship, Pattern recognition, Propagation of measurement uncertainties (inaccuracy and imprecision), Analytical validation techniques, Non-linear regression analysis,.

Unit II Analysis of Special Industrial Material (General Strategy for Analysis) : Analysis of dairy products, oils, soaps and synthetic detergents, food additives, petrochemicals (including liquid and gaseous fuels) pesticides, drugs and pharmaceuticals, fertilizers and paints.

Unit III Clinical Analysis : Sampling and selective analysis of biological fluids (using routine and automatic instruments): glucose, bilirubins, total cholesterol, haemoglobin, creatinine, total proteins, albumin, urea-nitrogen, carticosteroids and barbiturates. Immunological methods of analysis: ELISA, RIA and Immunodiffusion.

Unit IV Chemical Sensors : Principles, types of chemical sensors based on the modes of transductions, Types of chemical sensor based on the chemically sensitive materials (solid electrolyte, gas, semiconductor), Humidity sensors, Biosensors, Electrochemical sensors (Potentiometric sensors, Ion-selective electrodes, Membrane electrodes, Amperometric sensors, Clark and Enzyme electrodes).

Unit V Industrial safety Good manufacturing practice (GMP), Good lab practice (GLP), lab and industrial safety General types of occupational hazards and accidents in industries-methods to avoid accidents – specific examples-contamination in medicines – mutation problems in synthetic and biochemical plants-safety procedures-quality certification – environmental impacts of a plant -risk assessment – mitigation – preparedness-rehearsals.

References

1. S.J. Haswell , *Practical Guide to Chemometrics*, (1992) Marcel Deckker, Inc., New York.
(51)
2. D.C. Garratt, *The Quantitative Analysis of Drugs*, 2nd Edition (1992), Chapman and Hall Ltd., London.
3. F. J. Welcher, *Standard Methods of Chemical Analysis*, Vol. III A, 6th Edition (1966), Vol. III B, 5th Edition (1975), Van Nostrand Reinhold, London.
4. D.A. Skoog, *Principles of Instrumental Analysis*, 3rd Edition (1985), Saunders College Publishing, Philadelphia, London.
5. W. Horwitz (Editor), *Official Methods of Analysis*, 11th Edition (1970), Association of Official Analytical Chemists, Washington DC.