DEPARTMENT OF CHEMISTRY

TRIPURA UNIVERSITY

SURYAMANINAGAR – 799022

M. Sc. CHEMISTRY SYLLABUS

CHOICE-BASED CREDIT SYSTEM
(Revised 2017)

DEPARTMENT OF CHEMISTRY
TRIPURA UNIVERSITY
SURYAMANINAGAR 799 022
CHOICE BASED CREDIT SYSTEM (REVISED 2017)*

Course Curriculum – M. Sc. in Chemistry, Tripura University

Course Code	Name of the Courses	Credits
Semester –I (12 Credits core)		
CHEM 701C	Inorganic Chemistry-I	02
CHEM 702C	Organic Chemistry-I	02
CHEM 703C	Physical Chemistry-I	04
CHEM 704C	Chemistry Practical-I	04
Elective (Compulsory)		
CHEM 704E	Statistics	04
CHEM 705E	Computer	04
Semester – II (12 Credits core)		
CHEM 801C	Inorganic Chemistry-II	02
CHEM 802C	Organic Chemistry-II	04
CHEM 803C	Physical Chemistry-II	02
CHEM 804C	Chemistry Practical-II	04
Elective		
CHEM 805E	Spectroscopic Techniques in inorganic Chemistry	02
CHEM 806E	X-ray Crystallography and Solid state chemistry	02
CHEM 807E	Chemistry of Bio Molecules-I	02
CHEM 808E	Medicinal Chemistry	02
CHEM 809E	Advanced Group Theory	02
CHEM 810E	Surface Chemistry	02
Semester – III (12 credits core)		
CHEM 901C	Inorganic Chemistry-III	04
CHEM 902C	Organic Chemistry-III	02
CHEM 903C	Physical Chemistry-III	02
CHEM 904C	Chemistry Project-I	04
Elective		
CHEM 905E	Analytical and separation techniques in chemistry	02
CHEM 906E	Enzyme Chemistry	02
CHEM 907E	Bio-inorganic chemistry	02
CHEM 908E	Chemistry of Bio Molecules-II	02
CHEM 909E	Polymer Chemistry	02
CHEM 910E	Quantum Mechanics – II	02
Semester – IV (12 Credits core)		
CHEM 1001C	Inorganic Chemistry-IV	04
CHEM 1002C	Organic Chemistry-IV	02
CHEM 1003C	Physical Chemistry-IV	02
CHEM 1004C	Chemistry Project-II	04
Elective		
CHEM 1005E	Supra-molecular and Nano Chemistry	02
CHEM 1006E	Environmental and Green Chemistry	02
CHEM 1007E	Chemistry of Natural Products	02
CHEM 1008E	Photochemistry	02
CHEM 1009E	Computer Programming	02
CHEM 1010E	Statistical Mechanics	02

***Total minimum 72 credits should be obtained; core courses and two electives in first semester are compulsory**

First Semester courses from the Department of Chemistry

Course Code		Name of the Courses	Credits
CHEM	701C	Inorganic Chemistry-I	02
CHEM	702C	Organic Chemistry-I	02
CHEM	703C	Physical Chemistry-I	04
CHEM	704C	Chemistry Practical-I	04

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INORGANIC CHEMISTRY - I
PAPER – CHEM 701C

Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credit: 02

Unit-I Symmetry and Group Theory:

(a) Symmetry elements and operations, equivalent symmetry elements and equivalent atoms, point groups with examples, Group of very high symmetry, systematic procedures for symmetry classification of molecules and illustrative examples, molecular symmetry for compounds having coordination number 2 to 9, molecular dissymmetry and optical activity.

(b) Elementary idea of representation of theory, brief review of matrix, representation of groups, reducible and irreducible representation of point groups, definition of classes and character, the "Great Orthogonality Theorem", Orthogonality theorem for character tables, concept of character projection operator. Utilization of symmetry and group theory in constructing MO diagrams for polyatomic molecules (AB_n), the normal mode of vibration, symmetry of normal vibration, selection rules for IR and Raman Transitions.

Unit-II Stereochemistry and Bonding:

(a) VSEPR Theory; VBT (diatomic molecule); Polyatomic molecules; hyper-valence; localized bond, hybridization and energetics of hybridization; dπ-pπ bond; Bent's rule; Walsh Diagrams; MOT (simple LCAO); σ, π, δ M.O.; bonding and antibonding M.O. orbitals; criteria for stable molecular orbitals; orbital symmetry and overlap; homo-nuclear diatomic molecules; hetero-nuclear diatomic molecule; polyatomic molecules; molecular shapes in terms of molecular orbitals.

(b) Structure and bond properties; bond length, bond strength, electronegativity, group electronegativity, bond enthalpy, bond polarity, weak interactions:- hydrogen bonding, metallic bonding – band Theory, bonding in alloys, intermetallic compounds.

Text Books and suggested readings:

1. J. E. Huheey, E. A. Keiter, R. L Keiter and O. K. Medhi. Principles of Structure and Reactivity. First impression, Pearson Education 2006.
2. F. A. Cotton. Chemical Applications of Group Theory (3rd Edn) John-Wiley and Sons.
3. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry (5th edition) John Wiley
4. R. L. Dutta and A. Syamal, Elements of Magnetochemistry.
5. W. L. Jolly, Modern Inorganic Chemistry.
6. Gary L. Miessler and Donald A. Tarr, Inorganic Chemistry (4th Edition)
7. David M. Bishop Group Theory and Chemistry (Dover Books on Chemistry)
8. P. Atkins, T. Overton, J. Rourke, M. Weller & F. Armstrong, Shriver and Atkins Inorganic Chemistry, Oxford University Press (2006).
9. N. N. Greenwood & A. Earnshaw. Chemistry of the Elements, Pergamon Press (1984).
10. S. F. A. Kettle, Physical Inorganic Chemistry, Spectrum (1996).

ORGANIC CHEMISTRY -I

PAPER: CHEM 702C

Total Marks: 50 (Theory 35+ Internal Assessment 15)

Credit: 02

Unit I: Organic reaction mechanism

HSAB principle and its application in organic chemistry; Kinetic and non-kinetic methods for determination of reaction mechanisms; Linear free energy relationship; the Hammett equation-substitution and reaction constants; addition reactions of allenes and carbonyl compounds, stereochemistry of substitution, addition and elimination reactions; Substitution vs elimination reactions; neighboring group participation and anchimeric assistance.

Aromaticity; mechanism of formation of different aromatic ions and their stability

Unit II: Orbital symmetry reaction

Introduction to pericyclic reactions, orbital symmetry, electrocyclic, cycloaddition, sigmatropic and group transfer reactions; Woodward-Hoffmann rule and orbital motions in different pericyclic reactions; Rationalization based on FMO approach, correlation diagrams, Dewer-Zimmermann approach, Mobius and Huckel systems. Chelatropic reactions, Cope, aza-Cope, oxy-Cope, Claisen, Somelett-Hauser rearrangements.

Unit III: Reactive intermediates –I:

Introduction-structure, reactivity and stability of carbocations, carbanions, carbenes and nitrenes; Reactions involving these intermediates: pinacol-pinacolone rearrangement, Demjenov rearrangement, dienone-phenol rearrangement, Wolf rearrangement, cyclopropanation, Simon-Smith reaction, rearrangement of acylnitrenes etc.

Recommended text and reference books:

1. F. A. Carey and R. J. Sundberg. Advanced Organic Chemistry. 5thEdn. Plenum. Part – I, Part – II.
2. J. March, Organic Chemistry, Structure, Reactions and Mechanisms, 4thedn, John Willey
3. R.T. Morrison and R.N. Boyd, Organic chemistry, 6thedn, Prentice hall of India, New Delhi, 2003.
4. Michael B. Smith & Jerry March, Advanced Organic Chemistry Reactions, Mechanisms, and Structure. (2013) Wiley-Interscience.
5. T. Laue and A. Plagens, Named OrganicReactions,2nd edition (2005), John Wiley & Sons Ltd**.**
6. Reinhard Bruckner Advanced Organic Chemistry, Reaction Mechanisms (2002). Elsevier
7. R O C Norman and J M Coxon, Principles of organic synthesis, 3rd Edition, CRC Press.
8. A Guidebook to Mechanism in Organic Chemistry, P. A. Sykes, Longman Scientific, 1986.
9. B. Dinda, Essential of Pericyclic and organic photochemistry, Springer (2016).
10. J. Sing & J Singh, Photochemistry and pericyclic reactions, New Age International (Pvt. Ltd). 3rd Edition (2010).
11. Paula Y. Bruice, Organic Chemistry, Pearson, Seventh Edition (2016).
12. T. W. Graham Solomons, Craig B. Fryhle, Scott A. Snyder, Organic Chemistry, John Wiley & Sons Inc. 5th Edition.
13. Herbert O. House, Modern Synthetic Reactions, 2nd edition, The Benjamin/Cumings Publihing Company.

PHYSICAL CHEMISTRY - I
PAPER: CHEM 703C
Total Marks: 100 (Theory 70 + Internal Assessment 30)
Credit: 04

Group A: Marks- 50

UNIT –I

QUANTUM MECHANICS-I:

General Principles of Quantum Mechanics

Introduction; linear operators; Hermitian operators and related theorems; uncertainty principle; postulates; properties of wave functions; Schrodinger equation; separability of Schrodinger equation ; equation of motion.

Application to Simple Systems and Approximation Methods

Exactly solvable problems: Particle in a box, harmonic oscillator, rigid rotator, step potential, tunnelling effect and hydrogen atom. Antisymmetry principle and many-electron wave finctions.

Chemical Bonding

Born-Oppenheimer approximation (Introduction); valence bond (VB) theory and molecular orbital (MO) theory for diatomic molecules – hydrogen molecule ion, hydrogen molecule; excited states of H_2 – singlet and triplet; non-crossing rule and correlation diagram.

UNIT-II: SPECTROSCOPY-I

Rotational (microwave) spectra, rigid diatomic molecule, Energy expression; Rotational constant. Selection rules. Determination of bond length from observed rotational spectra. Spectral intensity-degeneracy of rotational energy levels and total relative population. The effect of isotopic substitution. Non-rigid rotator (energy expression only).Chemical analysis by microwave spectroscopy.

Vibrational (infra-red) spectra:Simple harmonic oscillator model. Corresponding selection rule. Anharmonic oscillator model-Morse function. Selection rules. Fundamental absorption and overtones. Hot bands. P-,Q-,R- branch in IR spectra. IR spectra of linear molecules. Parallel and perpendicular vibrations. Chemical analysis by IR techniques.

Raman spectroscopy: Rayleigh scattering and Raman scattering (classical and quantum mechanical consideration). Stokes and Anti-stokes lines. Selection rule. O- and S-branch in Raman spectra. Rotational Raman spectra of homonuclear diatomic molecules. Vibrational Raman Spectra .The rule of mutual exclusion. Structure determination from Raman and IR spectra.

Numerical problems.

Group B: Marks- 50

UNIT-III: Spectroscopy -II

NMR spectroscopy: Theory for NMR Population of energy levels. Larmor precession. Relaxation times: spin - lattice relaxation, spin-spin relaxation. Fourier transform spectroscopy in NMR . Chemical shift. Shielding and de-slielding mechanism. Fine structure, spin-spin splitting, coupling constant. Strongly coupled systems, shift reagent in NMR. Hyperfine structure. Nuclear overhauser effect (NOE), 1H and ^{13}C NMR. Two-Dimentional NMR. Chemical analysis by NMR techniques.

ESR spectroscopy : General background of ESR spectroscopy .Representation of ESR spectrum. 'g' - value, ESR spectra of simple organic free radicals; Hyperfine coupling, prediction of expected number of lines and their relative intensities, ESR spectra of transition metal complexes, metal-hyperfine coupling, anisotropic ESR spectra, zero field splitting, application of ESR spectroscopy examples.

UNIT-IV: Spectroscopy -III

***Photoelectron Spectroscopy (PES)*:** Frank- Condon principle, Basic principles of photoelectron and X-ray photoelectron spectroscopies and their applications for chemical analysis of surfaces; application of ESCA and Auger spectroscopy for the studies of solids.

NQR: Nuclear quadruple resonance, Energy levels of a nucleus in a non-uniform electric field. Quadruple coupling constant. NQR spectra of molecular compounds.

Mossbauer Spectroscopy: Principles of Mossbauer spectroscopy, Doppler shift, Application of Mossbauer spectra for chemical structure determination, Numerical problems.

Reference books:

1. G.W. Castellan, *Physical Chemistry*, (3 vol.), 1980. Wiley, New York.
2. D. A. MacQuarrie, *Quantum Chemistry*, (1983) Oxford University press,
3. A. K. Chandra, *Introductory Quantum Chemistry*, 4th Edition, Tata McGraw Hill, 1997.
4. I. Levine, *Quantum Chemistry*, (1994)Tata McGraw Hill, New Delhi.
5. L. Pauling and E.B.Wilson, *Introduction to Quantum Mechanics with Applications to Chemistry*, (1935), McGraw Hill, New York.
6. P.W. Atkins and R.S.Friedman, *Molecular Quantum Mechanics*, 3rd Ed.(1997) Oxford University Press.
7. Molecular Spectroscopy by G. Aruldhas
8. Molecular Spectroscopy by G. M. Barone
9. Molecular Spectroscopy by Banwell
10. Molecular Spectroscopy by Ira N Levine.

CHEMISTRY PRACTICAL-I
Paper: CHEM 704C
Credit: 04

Group A: Laboratory Course in Inorganic Chemistry

1. Semi micro qualitative analysis of Inorganic salt mixtures containing (06) six radicals including W, Mo, V, Ti, U, Th, Zr, Ce and at least one interfering radical ($F^-/PO_4^{3-}/BO_3^{3-}$).
2. Quantitative estimation involving volumetric (redox and complexometry), gravimetric and spectrophotometric methods of constituents in three component mixtures and alloys.
3. Preparation of the following inorganic compounds and characterization by IR, UV-Vis, Conductance & magnetic susceptibility measurements.
   Tris (acetyl acetonato)manganese (III)
   Tris (acetyl acetonato)iron (III)
   Linkage isomer of nitro & nitrido pentammine Cobalt (III) Chloride
   Tris (Ethylene diammine) Nickel (II) Chloride. dehydrate

Group B: **Laboratory Course in Physical Chemistry**

1. Determination of specific rotation of cane sugar and determination of concentration of supplied sample.(Quantitative-one day).
2. Potentiometric titration of Co(II) by $K_3[Fe(CN)_6]$ and determination of concentration of Co(II) in a solution. (Quantitative-one day).
3. Conductomectric titration of triple mixture containing KCl, NH_4Cl and HCl by $AgNO_3$ and by NaOH solution. (Quantitative-one day).
4. Verification of Beer's law and determination of concentration of unknown solution spectrophotmetrically(Quantitative-one day).
5. Determination of strengths of halides in a mixure , potentiometrically.
6. Determination of pH of buffer solutions and hence to calculate the E0 of quinhydrone electrode
7. Spectrophotometric determination of pKa of an indicator in micellar and microemulsion media.
8. Determination of specific rotation of sucrose and rate constant of its hydrolysis using a polarimeter.

Semester – II (12 Credits core)

CHEM	801C	Inorganic Chemistry-II	02
CHEM	802C	Organic Chemistry-II	04
CHEM	803C	Physical Chemistry-II	02
CHEM	804C	Chemistry Practical-II	04

Elective

CHEM	805E	Spectroscopic Techniques in inorganic Chemistry	02
CHEM	806E	X-ray Crystallography and Solid state chemistry	02
CHEM	807E	Chemistry of Bio Molecules-I	02
CHEM	808E	Medicinal Chemistry	02
CHEM	809E	Advanced Group Theory	02
CHEM	810E	Surface Chemistry	02

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INORGANIC CHEMISTRY - II
PAPER – CHEM 801C
Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credit: 02

Unit-I Coordination Chemistry

Brief review of theories of coordination compounds (VBT, CFT), Ligand Field Theory (LFT), Experimental evidences for metal-ligand orbital overlap, Calculation of ligand field parameters for complexes, MO Theory (LCAO) for complexes, application of MOT to octahedral, tetrahedral and square planar complexes, π-bonding in octahedral complexes and its effect on energy of molecular orbitals.

Unit-II Magneto-chemistry

Different types of magnetic behaviour of materials and their origin, magnetic susceptibility and magnetic moment, measurement of magnetic susceptibility (Gouy and Faraday methods), quenching of orbital moments, Interpretation of magnetic moments of complexes on the basis of various theories of complexes.

Magnetic behavior of multi-electron system, orbital coupling, spin-coupling, spin-orbit coupling (Russel Saunder's coupling), spin-orbit coupling constant, spin-orbit interaction energy, j-j coupling, micro-states and term symbols, Hund's rule for ground state term symbol, Lande interval rule, Derivation of Curie equation for magnetic moment, Curie and Curie-Weiss law, Thermal energy and magnetic moment, anti-ferromagnetism and its exchanged pathways.

Unit – III Bioinorganic Chemistry -1

Essential and trace element in biological system. Structure and function of biological membranes, mechanism of ion transport across membranes; Crown either complexes of Na and K, Ionophores, Valinomycin, Sodium and Potassium pump; Catalysis of phosphate transfer by Mg^{2+} ion; Metalloporphyrins: Structure and function.

Suggested reading:

1. Inorganic Chemistry-Principles of Structure and Reactivity, 5th Edn. J. Huhee, E.A. Keiter, R.L.Keiter & O.K. Medhi Pearson Education, New Delhi.
2. Shriver & Atkins - Inorganic Chemistry, Atkins, Overton, Rourke, Weller, Armstrong, South Asia Edn. 5th Edn. Oxford University Press, 2010.
3. Bioinorganic Chemistry, Asim K. Das, Books & Allied Ltd, 2013.
4. Bioinorganic Chemistry (Bertini, Ivano; Gray, Harry B.; Lippard, Stephen J.; Valentine, Joan Selverstone), University Science Books, CA, 1994.

ORGANIC CHEMISTRY - II
PAPER – CHEM 802C

Total Marks: 100 (Theory 70 + Internal Assessment 30)
Credit: 02

Group A

Unit I: Advanced Stereochemistry

Symmetry elements and point groups, axial and planar chirality, correlation of axial dissymmetry and Centro dissymmetry, atropisomerism, stereochemistry of allenes, biphenyls and spiro compounds. Topicity, acyclic systems up to 4 chiral centers, Compounds with asymmetric carbons in branched chains, asymmetric synthesis, Winstein- Holness equation and the Curtin- Hammett principle, conformational analysis of cyclic compounds such as substituted cyclohexanes, fused ring systems (decalins, PHA, PHP), allylic strains, alkylketone effects, haloketone rule.

Unit –II: Reactive intermediates - II

Arynes: Generation, structure and stability; Benzyne mechanism for aromatic nucleophilic substitution; Rearrangement and cyclo-addition reactions of arynes, synthetic application.

Enamines: Generation, structure and stability of enamines; synthetic applications.

Free radicals: Generation, structure and stability of radicals, radical- initiator, scavenger substitution and addition reactions involving radicals,tributyl tin hydride mediated radical reactions, exo- and endo cyclisation.

Group B

Unit I: Strategies and reagents in organic synthesis

Designing of organic synthesis - Retrosynthetic and Disconnection approach; Reversal of dipoles (umpolung of reactivity) and it's applications; Synthons and retrons, linear and convergent synthesis, protection and deprotection strategies, protecting agents for common functional groups; Trans metallation approach and metal catalyzed cross coupling reactions.

Uses of the following reagents/reactions in organic synthesis: PCC, PDC and Collin's reagent; IBX, Dess-Martin periodinane, ceric ammonium nitrate, Thallium(III) nitrate, chloranil, DDQ, m-CPBA, K-selecteride and L-selecteride, sodium cyanoborohydride, super hydrides, 9-BBN, Mukaiyama reagent, Gilman's reagent, LDA, dicyclohexylcarbodimide, tri-n-butyltin hydride, NCS, NBS, NIS, Corey-Nicolaou reagent, baker's yeast, CBS reagents, diimide, crown ether, phase transfer catalyst.

Unit III: Selective named reactions (1 credit)

Arndt Eistert synthesis, Swern oxidation, Moffat oxidation, Prevost and Woodward hydroxylation; Henry reaction, Wittig reaction and Horner-Wordwoth-Emmons reaction (stabilized and non-stabilized ylide); Nazarov cyclization, Pictet-Sprengler reaction, Biginelli reaction, Passerini reaction, Ugi reaction, Peterson's synthesis, McMurry olefination, Julia olefination, Tebbe Olefination. Shapiro reaction, Chichibabin reaction, Baeyer-Villiger oxidation, Baylis-Hillman Reaction, Staudinger Reaction, Stobbe Condensation.

Recommended text and reference books:

1. W. Carruthers, *Some Modern Methods of Organic Synthesis*, Cambridge University Press (2004).
2. L. Stryer, Biochemistry, 5th Edition (2002), Freeman & Co, New York.
3. H. O. House, Modern Synthetic Reactions, 3rd Edition (1992), Benjamin Publishing Co.
4. S. Warren, Organic Synthesis, Disconnection Approach, 1982, Wiley Interscience, NY
5. Francis A. Carey and Richard J. Sundberg, Advanced Organic Chemistry Part A and Part B.
6. T. Laue and A. Plagens, Named Organic Reactions,2nd edition (2005),John Wiley & Sons Ltd

7. *Reinhard Bruckner* Advanced Organic Chemistry, Reaction Mechanisms (2002). Elsevier
8. R O C Norman and J M Coxon, Principles of organic synthesis, 3rd Edition, CRC Press
9. J. March, Organic Chemistry, Structure, Reactions and Mechanisms, 4thedn, J. Willey
10. D. Nasipuri, Stereochemistry, Conformation and mechanism, 2ndEdn. John Wiley
11. R.T. Morrison and R.N. Boyd, Organic chemistry, 6thedn, Prentice hall of India, New
12. E. L. Eliel, Stereochemistry of Carbon Compounds, Tata McGraw Hill, 2007.
13. S. Sengupta Basic Stereochemistry of Organic Moleclules, Book Syndicate Pvt. Ltd. 2nd Edition.
14. P.S. Kalsi, Stereochemistry, Conformation and Mechanism, 8th Edition. New Age Int., 2015.

PHYSICAL CHEMISTRY - II
PAPER – CHEM 803C
Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credit: 02

UNIT-I: CHEMICAL THERMODYNAMICS

Nernst heat theorem and the third law of thermodynamics, Calculation of entropy changes in chemical reactions, Mathematical and thermodynamic probability. Entropy and probability. The free energy of a mixture. Dependence of thermodynamic functions on composition. Partial molar quantities.

Thermodynamic properties of gases with special reference to real gases in the pure state and in mixtures. Concept of fugacity.

Analytical form of the chemical potential in ideal solutions. Chemical potential of the solute in a binary solution Application of Gibbs-Duhem equation.

The concept of activity:the rational concept and the practical concept. Colligative properties and activity of solute. Activities and reaction equilibria, experimental determination of activity coefficients of non-electrolytes, Numerical problems.

Unit -II: Kinetic theory and transport properties of gases

Derivation of Maxwell's distribution of molecular speed**;** The general equation for transport, Thermal conductivity of gases, Molecular collisions and mean free path, Viscosity of gases, Diffusion , Introduction to the concept of non-steady state, Numerical problems.

Unit-III: Chemical kinetics-1

Opposing and consecutive reactions, complex reactions, Atomic and free radical chain reactions. Kinetic salt effect; Effect of solvent on rate constant (Single sphere and double sphere model): Non-Arrhenius equations and its significance. Theory of absolute reaction, rate (statistical) and comparison with that of collision theory; Kinetics of enzyme reaction (effect of pH) Michaels- Menton Law, derivation; Numerical problems

Reference books:

1. G.W. Castellan, *Physical Chemistry*, (3 vol.), 1980. Wiley, New York.
2. D. A. MacQuarrie, *Quantum Chemistry*, (1983) Oxford University press,
3. A. K. Chandra, *Introductory Quantum Chemistry*, 4th Edition, Tata McGraw Hill, 1997.
4. I. Levine, *Quantum Chemistry*, (1994)Tata McGraw Hill, New Delhi.
5. L. Pauling and E.B.Wilson, *Introduction to Quantum Mechanics with Applications to Chemistry*, (1935), McGraw Hill, New York.
6. P.W. Atkins and R.S.Friedman, *Molecular Quantum Mechanics*, 3rd Ed.(1997) Oxford University Press.
7. K.J.Laidler, Chemical Kinetics, 3rd Ed.(1967), Harper and Row Publishers, New York.
8. H.Eyring, S.H. Lin and S.M.Lin, *Chemical Kinetics*, (1999)Jhon Willey, New York.
9. K. Zeemanski, *Thermodynamics*

CHEMISTRY PRACTICAL-II

PAPER: CHEM 804C

Credit: 04

Group A: Laboratory Course in Organic Chemistry

1. Separation, purification and identification of compounds of binary solid mixtures by systematic analysis
2. Identification of organic liquid compounds by systematic analysis
3. Organic preparation
4. Organic estimation - Estimation of some organic compounds

Group B: Laboratory Course in Physical Chemistry

1. Determination of rate constant and order of the reaction between $KBrO_3$ and KI in acid medium.(Qualitative- one day)
2. Kinetic study of decomposition of $K_2S_2O_8$ by KI and effect of added salt. (Qualitative- two day)
3. Determination of formula of cupro-ammonium ion. (Qualitative- one day)
4. Determination of distribution coefficient of C_6H_5COOH between H_2O and an organic solvent (verification of dimerization of benzoic acid in organic solvent). Qualitative- one day)
5. Determination of standard electrode potential of quinhydrone electrode. (Qualitative-one day).
6. Determination of composition and stability constant of Ferric-salicylic acid complex by Job's method. (Qualitative-two day).
7. Determination of critical micellar concentration(CMC) of sodium lauryl sulphate from the measurement of conductivities at different concentrations.

Reference books:

1. Practical Organic Chemistry, A. I. Vogel, ELBS, 2002.
2. Laboratory Manual in Organic Chemistry, R. K. Bansal, Wiley Eastern, 1980.
3. Comprehensive Practical Organic Chemistry : Qualitative Analysis, V. K. Ahluwalia and S. Dhingra, Universities Press (India) Ltd, 2000.
4. N. K. Visnoi, Advanced organic Chemistry practical
5. D. P. Shoemaker, C. W. Garland and J. W. Niber, *Experiments in Physical Chemistry*,(1996) McGraw Hill Interscience.
6. Findlay's Practical Physical Chemistry, 9th Ed. Revised by B.P. Levitt, Longman.1973.
7. R. K. Bansal. *Laboratory Manual of Organic Chemistry* (3rd edn.), Wiley-Eastern (1994).
8. R. G. Brewster & W.E. Mcwedn. *Unitized Experimental Organic Chemistry* (4th edn.), East-West Press (1977).

PAPER – CHEM 805E
(Spectroscopic methods in inorganic Chemistry)
Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credit: 02

Unit I:

Nuclear Magnetic Resonance Spectroscopy:

Basic principle, Relaxation time-spin lattice and spin–spin relaxation, Chemical shift, factors that affect chemical shift. Use of chemical shifts and spin-spin couplings for structural determination. Application of ^{1}H, ^{13}C, ^{19}F and ^{31}P in the structural assignment of selected inorganic compounds.

Electron Spin Resonance Spectroscopy:

Basic principle, the g-value and the factors affecting thereof; Hyperfine splitting (isotropic systems); interactions affecting electron energies in paramagnetic complexes (Zero – field splitting and Kramers degeneracy); Anisotropic effects (the g-value and the hyperfine couplings). Application of ESR spectra of simple free radicals, transition metal complexes (d^1 and d^9 ions in cubic and tetrahedral fields),anisotropic nature of g-values, hyperfine coupling constant, ESR spectra in structural assessment of inorganic compounds.

Unit II :

Infrared and Raman Spectroscopy:

Basic principle of IR and Raman spectroscopy; application of vibrational spectroscopy in investigating - Symmetry and shapes of simple AB_2, AB_3 and AB_4 molecules.

Structural elucidation (by IR & Raman spectra) of co-ordination compounds containing the common ligands such as: NH_3, H_2O, OH^-, $NO3^-$, $SO42^-$, ClO_4^-, CN^-, SCN^-, N_3^-, H^-, PR_3, OPR_3, halides, dioxygen, $-COO^-$, aminao acids.

Mass Spectroscopy:

Basic principle of mass spectrometry, concept of metastable ions and transitions, recognition of the molecular ion peak, Stevensan's rule.

Application to metal compounds containing ligand such as carbonyl/ nitrosyl/ alkyl/ cyclopentadienyl and acetyl acetonate. Interpretation of mass spectra for structural characterization. Effect of isotopes on the appearance of mass spectrum.

Mossbauer spectroscopy:

Principles, isomer shift, quadruple effect of magnetic field, application to iron and tin compounds.

Recommended Books:

1. R.S. Drago, Physical Methods for Chemists (1992), Saunders College Publishing, Philadelphia.
2. K. Nakamoto, Infrared Spectra of Inorganic and coordination compounds, 2nd Edn. 1970, Wiley-Interscience, London.
3. Inorganic Spectroscopic Methods. Alan. K. Brisdan, Oxford Science Publication (Zeneca) 1997).

PAPER: CHEM 806E

X-ray Crystallography and solid state Chemistry

Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

Unit I

Crystals Lattices and symmetry: Definition of a crystal, Lattice points, Unit Cells, Unit Cell calculations; Definition of symmetry, Symmetry operations and elements of symmetry, Point groups, Classification of unit cells, Crystal systems, Herman-Mauguin notation, Bravais Lattices, Distinction between trigonal and hexagonal systems, Crystal planes and indices Law of rational indices. ***Space groups and equivalent positions:*** Screw axis, Glide planes, Space groups, Relationship between space groups, point groups, and physical properties, Equivalent positions, Special positions, Space group tables in International Tables for X-ray crystallography.

Unit II

X-ray diffraction*:* Periodicity and structural information, The diffraction grating, Diffraction of X-ray by crystals, The Laue equations, Bragg's Law, Generalization of Miller indices, Electron density function, Fourier series, Fourier expansion of electron density, Intensities of diffraction spots, The phase problem, Calculation of structure factors, Effect of thermal vibrations, Structure factors of centro-symmetric crystals, Friedel's law, Laue groups, Structure factors of sodium chloride

Determination of atomic positions*:* Solutions of structure factor equations, The Patterson function Heavy-atom methods, Isomorphous replacement, Superposition methods, Inequalities, Sayre-Cochran-Zachariasen relationship, Hauptman-Karle methods, Summary of phase-determining methods, Refinement, Description of procedure for X-ray structure analysis (NaCl and CsCl)

Unit III: Solid state Chemistry: Solid State Reactions: Types; sintering; nucleation; Factors influencing the reactivity of solids;Precursors to solid state reactions; Tammann and Hedvall mechanism; Wagner's Diffusion theory of reaction; Material transport in solid state reaction—counter diffusion, Kirkendall effect; Huttig's mechanism; Kinetic model: Reaction in powder compact, parabolic rate law, Jander'srate equation. Crystal Defects: Types of defects, thermodynamics of Schottky and Frenkel defect formation, Kroger-Vink notation for crystal defects Atomic theory of diffusion—self diffusion mechanism.

Recommended Books:

1. Introduction to Crystallography, Donald E. Sands, Dover Publications, INC. New York.
2. Crystal Structure Analysis for Chemists and Biologist, Jenny P. Glusker, Mitchell Lewis, Miriam Rossi, Wiley VCH, 1994.
3. Crystal Structure Determination, William Clegg, Oxford University Press, 1998.
4. Structure Determination by X-ray Crystallography, Mark Ladd and Rex Palmer (September 30, 2003).
5. Crystal Structure Determination, Werner Massa (March 31, 2004).
6. Crystal Structure Analysis, Jenny Glusker and Kenneth Trueblood (August 1992).
7. A. R. West. *Solid State Chemistry and its Applications*, John Wiley (1998).
8. N. B. Hannay. *Solid State Chemistry*, Prentice-Hall (1979).
9. D. K. Chakraborty. *Solid State*, New Age International, New Deldi (1996)

PAPER - CHEM 807E

Chemistry of Biomolecules-I

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

Unit I:

Chemistry of amino acids and peptides: Introduction to amino acids, essential amino acids; nomenclature of α-amino acids;structures, properties and synthesis of natural and non-natural α-amino acids; application of amino acids as building block and chiral ligand in organic synthesis; peptides and peptide synthesis, different strategies in peptide synthesis, solid phase methods; sequencing of polypeptides; enzymatic cleavage of peptide bond; preliminary concept of protein and their structures; protein denaturation; biosynthesis of amino acids.

Unit II:

Chemistry of carbohydrates: Classification; structure, nomenclature, stereochemistry, conformation, reactions of monosacharides (isomerization, glycoside formation, hydrazones and osazones, alditols by reduction, oxidation and oxidative cleavage); protective groups for monosaccharides; synthesis of monosaccharide and disaccharides (sucrose, maltose, lactose); carbohydrate metabolism; role of sugars in biological recognition. Structure and function of sugar derivatives (deoxy, amino, branched chain sugars); Polysaccharides of biological importance, dextran, sialic acid

Recommended text and reference books:

1. J. Clayden, N. Greeves, S. Warren, and P. Wothers, Organic Chemistry, (2001) Oxford Univ. Press, Oxford.
2. G. C. Barrett and D. T. Elmore, Amino acids and peptides (2004), Cambridge University press.
3. F. D. Gustone, Fatty acid and Lipid Chemistry (1996), Wiley
4. S. P. Bhtani, Chemistry of Biomolecules (2010), CRC Press
5. Norbert Sewald and Hans-Dieter Jakubke,Peptides: Chemistry and Biology.. Wiley-VCH
6. Ward, Selectivity in organic synthesis (1999), Wiley-VCH, 1999.
7. T. W. Greene, Protecting groups in Organic synthesis (2000), Wiley-VCH, 2000.
8. Chemistry of Biomolecules : An Introduction, R. J. Simmonds, Royal Society of Chemistry, 1992.

PAPER - CHEM 808E

Medicinal Chemistry

Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

Unit I:

Drugs and drug design: Concepts of drugs, classification, analogues and pro-drugs, theories of action, assay and metabolism of drugs;

Drug design, theory of drug design, structure activity relationship (SAR), Quantitative structure activity relationship (QSAR); introduction to combinatorial synthesis in drug discovery; Development of new drugs, procedures followed in drug design and development.

Unit II:

Synthesis and uses of the following drugs of different pharmacological activities:

a) Antimalerials: Quinine, chloquine, Trimethoprim

b) Analgesic & Antipyretics: Paracetamol, Meperidine, methadone, Aminopyrine.

c)Anti-inflammatory: Aspirin, Ibuprofen, Oxyphenylbutazone, Diclophenac, Indomethacin, coxib, celecoxib.

d) Antitubercular and antileprotic:Ethambutol, Isoniazide&Dapsone

e) Anaesthetics: Lidocaine, Thiopental.

f) Antihistamines: Phenobarbital, Diphenylhydramine.

g) Tranquilizers: Diazepam, Trimeprazine

h) Cardiovascular: Synthesis of dilliazem, quinidine, methyldopa, atenolol, oxyprenol

i) Anti-neoplastic drugs: Cancer chemotherapy, Synthesis of mechloraethamine, cyclophosphamide, Mephalan, uracils, mustards.

Unit II: Antibiotics: Preparation of semi synthetic penicillin, conversion of penicillin into cephalosporin, synthesis of chloramphenicol (diastereoselective and enantioselective) general account of tetracycline & macrocyclic antibiotics (no synthesis)

Recommended text and reference books:

1 A. Kar, Medicinal Chemistry, New Age publications
2 Thomas Nogrady, Donald F. Weave, Medicinal Chemistry-A Molecular and Biochemical Approach, Oxford University Press.
3 Burger. Medicinal Chemistry and Drug Discovery, Vol-1, Ed. M. E. Wolff, John Wiley (1994).
4 Goodman & Gilman. Pharmacological Basis of Therapeutics, McGraw-HilI (2005).
5 S. S. Pandeya& J. R. Dimmock.Introduction to Drug Design, New Age International.(2000).
6 D. Lednicer. Strategies for Organic Drug Synthesis and Design, John Wiley (1998).
7 Graham & Patrick. Introduction to Medicinal Chemistry (3rd edn.), OUP (2005).

PAPER - CHEM 809E

Advanced group theory

Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

GROUP THEORY – I:

The concept of groups; group multiplication tables and the rearrangement theorem; subgroups, classes and the related theorems; commutative groups (Abelian), cyclic group; isomorphism and homomorphism. Examples.

Molecular point groups (in Brief) , similarity transformation and the invariance of characters of matrices under such transformation, matrix representation of point groups; reducible, irreducible and equivalent and inequivalent representations; the great orthogonality theorem (no derivation) and its corollaries, character tables, construction of character tables in complex cases such as $D_{6h,}$ T_d etc; the group of Schrodinger equation; basis function for irreducible representation "projection" operator; direct product representation .

GROUP THEORY - II (Physical Applications):

Symmetry factoring of secular equations; LCAO -MO ,II bonding and Huckel's theory ;some examples: ethylene ,bengene ,Naphthalein. symmetry based "selection rules" for cyclization reaction (Woodward Hoffmannrule) Hybrid orbital and Molecular orbitals for AB_n -type molecules. Crystal field theory (CFT) Splitting of energy levels, and terms in a chemical environment. Determining the symmetry types of the normal modes;selection rule for fundamental (infra-red and Raman) vibrational transitions. Mutual Exclusion rule.

Reference books:

1. Chemical Application of Group Theory – F.A. Cotton,3rd edition, A Wiley Interscience publication
2. Group Theory and Quantum Mechanics, M.Tinkham, Tata McGraw Hill, publishing Ltd.
3. Group Theory and Chemistry, David M. Bishop, Clarendon Press Oxford.
4. Group Theory and its application to Physical Problem, M. Hamermeah, Dover publication.

PAPER - CHEM 810E

Surface Chemistry

Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

ADSORPTION ISOTHERM:

Thermodynamics of adsorption isotherm, Different adsorption isotherms, Adsorption at solid-liquid, liquid-gas, liquid-liquid interfaces, Effect of added electrolyte on the surface excess of ionic surfactants.

MIXED SURFACTANTS:

Different types of mixed micelle, cmc of mixed micelle, Clint's equation for cmc, counter ion binding in mixed surfactants.

SOLUBILISATION AND EMULSIFICATION:

Solubilization and Emulsification by Surfactants: Factors determining extent of solubilization, formation of emulsions, factors determining emulsion stability, microemulsions, conductance behaviour of microemulsions and applications.

Reference books:

1. N.K.Adams, *Physics and Chemistry of Surface,*
2. A.W.Adamson, *Physical Chemistry of surface,*
3. M.J.Rosen, *Surfactants and Interfacial Phenomena,* (1978) John Willey, New York.
4. Y.Moroi, *Micelles: Theatrical and Application Aspects,* (1992) Plenum Press, New York

SEMESTER – III

Semester - III

CHEM	901C	Inorganic Chemistry-III	04
CHEM	902C	Organic Chemistry-III	02
CHEM	903C	Physical Chemistry-III	02
CHEM	904C	Chemistry Project-I	04
		Elective	
CHEM 905E		Analytical and separation Techniques in Chemistry	02
CHEM 906E		Enzyme Chemistry	02
CHEM 907E		Bioinorganic Chemistry	02
CHEM 908E		Chemistry of Biomolecules - II	02
CHEM 909E		Polymer Chemistry	02
CHEM 910E		Quantum Chemistry - II	02

PAPER - CHEM 901C

Inorganic Chemistry - III

Total Marks: 100 (Theory 70 + Internal Assessment 30)

Credits: 04

Unit I: Kinetics and Mechanism of Inorganic Reactions

(a) Energy profile of a reaction, Labile and inert complexes, dissociative, associative and interchange mechanisms of ligand substitution reactions, ligand substitution reactions in square planar and octahedral complexes, the trans effect, mechanism of isomerization, acid & base hydrolysis and racemization of tris-chelate complexes, Ray-Dutta and Bailar twist mechanisms.

(b) Mechanism of electron transfer (redox) reactions: various types of electrons transfer reaction (inner and outer sphere reactions, complementary and non-complementary reactions), Marcus-Husch theory and its applications, stereochemical non-rigidity and fluxional molecules.

(c) Study of complexes in solution: Stability of a complex in solution, thermodynamic and kinetic stability of complexes, factors affecting thermodynamic and kinetic stability of complexes, stability constant, determination of composition and stability constants of complexes by modern methods, conditional stability constants and their importance. Study of polynuclear and mixed ligand complexes.

Unit II: Transition and Inner transition metal chemistry

(a) Chemistry of Platinum metals: Important compounds of Platinum metals, comparative study of Lanthanides and Actinides with reference to oxidation states, complex formation, magnetic properties, colour and spectral properties, Lanthanide shift reagents.

(b) Transition metal π-acid complexes: π-acid ligands (CO, NO, tertiary phosphine, arsine etc.), structure, bonding, synthesis and reactivity of complexes of CO, NO, tertiary phosphine, metal carbonyl hydrides.

Unit III: Electronic Spectra of Transition metal complexes:

Spectroscopic states: micro states, terms of d^n configurations, Selection rules, Orgel diagram, Correlation diagram, Tanabe-Sugano diagram, calculation of ligand field parameters (dq, B and β values), Band intensities and band width, Spectra of high spin octahedral and tetrahedral complexes for d^1-d^9 systems, charge transfer spectra, Application of electronic spectra for structural characterization of coordination compounds.

Unit IV

Cluster Compounds: Classification of Clusters – Low Nuclearity Clusters: M_3 and M_4 clusters, structural patterns in $M_3(CO)_{12}$ (M=Fe, Ru, Os) and $M_4(CO)_{12}$ (M=Co, Rh, Ir) Clusters. Polyhedral skeletal electron pair theory and Total Electron Count theory – Wades rules – Capping rule, Mingo's Rules (selected examples). Carbide Clusters.

Metal Halide clusters: Dinuclear, Trinuclear, Tetranuclear Metal-Metal systems – Edge sharing, Face sharing Bioctahedra, Tetragonal prismatic and Trigonal antiprismatic structures, Quadruple bond, Structure and bonding in Octahedral halides of $[Re_2Cl_8]^{2-}$, $[Mo_6(Cl)_8]^{4+}$.

Boranes, carboranes, metalloboranes, metallocarboranes.

Reference book

1. Advanced Inorganic Chemistry. F.A.Cotton, G. Wilkinson, C.A.Murillo and M. Bochmann, 5th Edition, Wiley Interscience, N.Y
2. Inorganic Chemistry, J.E.Huheey, K.A.Keiter and R.L.Keiter 4th Edition Harper Cottens College Publications (1993).
3. The Chemistry of Metal Cluster Complexes. D.F.Shriver, H.D.Kaerz and R.D.Adams (Eds), VCH, NY (1990).
4. Inorganic Chemistry, Keith F.Purcell and John C.Kotz, Holt-Saunders International Editions, London (1977).
5. J. Huhee, E.A. Keiter, R.L. Keiter & O.K. Medhi-Inorganic Chemistry-Principles of Structure and Reactivity, 5th Edn..Pearson Education, 2007.
6. G.L. Miessler & D.A. Tarr-Inorganic Chemistry, 3rd Edn, Pearson Education, 2007.
7. Allan K. Brisdon-Inorganic Spectroscopic methods, Oxford.
8. Introduction to Ligand field Theory- B.N.Figgis

PAPER - CHEM 902C

Organic Chemistry - III

Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

Unit I: Nuclear magnetic resonance spectroscopy for organic compounds

NMR sample handling and solvent for NMR study, chemical shift, internal standards, factors affecting the chemical shift, NMR shift reagents, coupling constant, spin-spin coupling – vicinal and geminal coupling, long range coupling – two bond coupling (2J) three bond coupling (3J), Karplus relationship, multiplicity of splitting and relative intensity of lines, spin decoupling, coupling constants. First order spectra- A_3X, AX and AMX systems. Second order spectra- AB and A_2B_2 systems; Nuclear overhauser effect (NOE), chemically induced dynamic nuclear polarization (CIDNP), introduction of ^{13}C NMR spectroscopy: Principle, instrumentation; multiplicity, proton –decoupling, off-resonance decoupling, noise-decoupling, ^{13}C chemical shifts values, DEPT and INEPT terminology; Two dimensional NMR spectroscopy: magnetic resonance imaging (MRI).Application of NMR in the structure elucidation of organic compounds.

Unit II: Mass spectroscopy for organic compounds

Introduction – basic theory, instrumentation and sample handling. Methods of generation of mass ions – electron impact (EI), chemical ionization (CI), electron spray ionization (ESI) and fast atom bombardment (FAB) techniques, TOF-MALDI and SELDI; Tandem mass spectroscopy, general mass fragmentation pattern of organic compounds, base peak, molecular ion, relative intensity, mass ions fragmentation, metastable ions, even electron rule, nitrogen rule, HDI, application of mass spectroscopy.

Unit III: Main group Organometallic Chemistry:

Introduction: Definition, a brief history of organometallic chemistry, importance of organometallic compounds as reagents, additive and catalyst. Organometallic chemistry of lithium, magnesium, zinc, copper, aluminium, cadmium and mercury: synthesis, structures and reactivity. Metal alkyls, aryls and hydrides: Stability, preparation and reactivity.

Applications of main group organometallics in organic synthesis:

Recommended Books:-

1. Spectroscopic identification of organic compounds (8th edition). R.M. Silverstein and F.X. Webster, John Wiley & Sons, Inc (2014).
2. Spectroscopic methods in organic chemistry (sixth edition). D. H. Williams and I Fleming, Tata McGraw Hill (2005).
3. Organic spectroscopy (3rd edition). William Kemp, MacMillan (1991).
4. Applications of Absorption Spectroscopy of Organic Compounds. J.R. Dyer. Prentice Hall (Digitized 2008)
5. Introduction to Spectroscopy (5thEdn), Donald L. Pavia, Gary M. Lampman, George S. Kriz, James A. Vyvyan (2009)
6. Inorganic Chemistry G.L. Miessler& D.A. Tarr-, 3rdEdn, Pearson Education, 2007.
7. Basic Organometallic Chemistry - Concepts, Syntheses and Applications by B. D. Gupta, A. J. Elias, Universities Press (2010).
8. Organometallic Chemistry: A Unified Approach by R. C. Mehrotra, Anirudh Singh, 2nd Edition, New Age International, Publication Year: 1991, reprint (2014).
9. Organolithium reagents, Jonathan Clayden,

PAPER - CHEM 903C

Physical Chemistry - III

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

UNIT – I: Statistical thermodynamics

Independent subsystems and distinguishability. Boltzmann distribution (nondegenerate and degenerate cases). Review of partition function: Thermal De Broglie wavelength. Partition functions for electronic, nuclear, rotational and vibrational degrees of freedom. Thermodynamic quantities in terms of partition functions. Entropy of ideal gas. Gibbs paradox. Equilibrium constants (ideal gas reaction) in terms of partition function.

The mathematical proof of the equipartition of energy principle. Specific heats of solids, fluctuations.

UNIT-I I: IRREVERSIBLE THERMODYNAMICS

Entropy of irreversible processes – Clausius inequality; entropy production and entropy flow, Rate of entropy production – generalized forces and fluxes (heat flow, chemical reactions, electrochemical reactions); Entropy production in open system; Phenomenological equations, Onsager reciprocity relation; Electrokinetic phenomena; Stationary non-equilibrium states -states of minimum entropy production, Curie Prigogine principle.

UNIT II: NON EQUILIBRIUM THERMODYNAMICS

Non-equilibrium statistical mechanics: Random Processes; Time-correlation functions; Brownian motion; Langevin equation for random motion; Random walk in one dimension; Time dependence of fluctuation; Fluctuation-dissipation theorem; Fokker-Planck equation.

Reference books:

1. C. Kalidas and M.V.Sanganarayana, Non Equilibrium Thermodynamics – Principles and application, Macmillan India (2002).
2. I. Prigogine, Introduction to Thermodynamics of Irreversible Processes, Interscience (1960).
3. D. A.McQuarrie, *Statistical Mechanics,* (2003), Viva Books Pvt. Ltd. New Delhi.
4. M. C.Gupta, *The statistical Thermodynamics*,(1990), New Age International (P) Ltd. New Delhi.
5. M. Dole, Introduction to Statistical Thermodynamics

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PAPER - CHEM 904C

Chemistry Project- I

Total Marks: 100 (Theory 70 + Internal Assessment 30)

Credits: 04

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PAPER - CHEM 905E

Analytical and separation Techniques in Chemistry
Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

Unit I: Electrochemical techniques

Electrode processes and thermodynamics of cells: Introduction, Electrochemical Cells and reactions, Faradaic and nonfaradaic processes, nonfaradaic processes and the nature of the electrode solution interface, faradaic processes and factors affecting rates of electrode reactions, Basic electrochemical thermodynamics, formal potentials, reference electrodes, Liquid junction potentials. Currents in Polarography: Charging or condenser current, Migration current, Diffusion current, Ilkovic equation, influence of supporting electrolyte, limiting current measurements. Potential sweep methods: Introduction, reversible systems peak current and potential, totally irreversible systems peak current and potential, quasi reversible system, cyclic voltammetry.

Unit II: Atomic Emission-Absorption Spectroscopy and thermo analytical techniques

Flame Atomic Absorption Spectroscopy: Principles of atomic absorption spectroscopy, Radiation sources, Flame and electrothermal atomization, Limitations in atomic absorption, Interferences, Comparison of absorption spectrometry techniques-flame and graphite furnace, Quantitative Analysis, inductively coupled plasma-mass spectroscopy (ICP-MS).

Flame Atomic Emission Spectroscopy: Atomic emission, Principles of flame emission photometry, Limitations of flame emission photometry, Interference, Qualitative Analysis, Quantitative Analysis, Comparison of flame atomic emission and absorption spectroscopy. Excitation sources in atomic emission spectroscopy, ICP-AES spectroscopy.

Thermo-analytical Techniques: Thermo gravimetric analysis (TGA), differential thermo gravimetric analysis (DTA), differential scanning calorimetry (DSC), Thermometric titration (principle, technique and application)

Unit III: Chromatographic techniques:

Basic concept of chromatographic separation – adsorption and partition chromatography, theory and handling of different chromatographic techniques – column, thin-layer, and paper chromatography. Gas chromatography: Basic principle, basic equipment; types of column and their selection; detectors (FID, TCD, ECD, NPD); sample separation and applications. High performance liquid chromatography (HPLC): Instrumentation - basic equipment; pumping and injection system, column and its packing, normal and reverse phases; detectors, sample separation and application. Gel permeable (filtration) chromatography, Size exclusion chromatography, gel electrophoresis

Recommended books:

1. Electrochemical Methods: Fundamentals and Applications by Allen J. Bard & Larry R. Faulkner, 2nd edition, Wiley India, Copyright 2004, reprint (2006).
2. Principles of Polarography by R. C. Kapoor & B. S. Aggarwal, Wiley Eastern Limited, (1991).
3. A Text-book of Quantitative Inorganic Analysis including Elementary Instrumental Analysis, by A.I. Vogel, 3rd Edition, The English language book Society and Longmans, Green & Co Limited, (1956).
4. Atomic Absorption Spectrometry by B. Welz, M. Sperling, 3rd Edition, Wiley-VCH (1999).
5. Vogel's Text Book of Quantitative Chemical Analysis (6th Edition), Prentice Hall (2000).
6. Principles and Practice of Modern Chromatographic Methods, (1st Edition), Robards, Jackson & Haddad, Academic press (1994).
7. Chromatographic Methods (5th Edn), A. Braithwaite, J.F. Smith, Kluwar Academic Publisher.

PAPER - CHEM 906E

Enzyme Chemistry
Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

Unit I: Enzymes and Mechanism of Enzyme Action: General aspects of enzymes; nomenclature, classification and specificity, isolation, purification and function of enzymes. enzyme specificity activesites, Mechanism of enzyme action: mechanism at active sites,Transition state theory, orientation and steric effect, acid base catalysis, strain or distortion.covalent catalysis, acid base catalysis, proximity and orientation effects, zymogen, multi enzyme complexes, enzyme technology.

Kinetics of enzyme action – Michaeli's-Menten equation, Different plots for determination of K_m and V_{max} and their physiological significance; Enzyme regulation & drug design, Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors affinity labeling and enzyme modification by site directed mutagenesis.

Unit –II: Co-enzyme Chemistry: Definition, classification, sources, biological functions of coenzymes; cofactors as derived from vitamins; coenzymes, prosthetic groups, and apoenzymes. Structure and biological functions of coenzyme A, thiamine Pyrophosphate, Pyridoxal phosphate, lipoic acid, tetrahydrofolic acid, flavin coenzyme and heme coenzyme. Structure and functions of thiamine, riboflavine, pyridoxine, biotin, Vitamin B -complex, tocopherol and ascorbic acid and Vitamin -D, NAD^+, $NADP^+$, FMN, FAD and vitamin B_{12}.

Application and enzyme catalytic organic reactions – Oxidation, reduction, isomerization, epimerization, hydrolysis, phosphorylation, acylation, methylation, decarboxylation, dehydration. Enzymatic hydrolysis of peptides (carboxy peptidase, trypsin, chrymotrypsin and Lys C);

Recommended Books:

1. Lehninger Principles of Biochemistry, David L. Nelson and Michael M. Cox. 7th Edition. W H Freeman & Co (Sd). 2017.
2. Bioorganic and Bioinorganic and Supramilecular Chemistry. P.S. Kalsi, New Age International (Pvt. Ltd.) 2nd edition 2010.
3. Biochemistry, C.B. Power and G.R. Chatwal. Himalayan Publishing House. 4th edition 1999.
4. Instant notes on Medicinal Chemistry. G Patrick. Viva Books Pvt. Ltd. 1st edition 2002.

PAPER - CHEM 907E

Bioinorganic Chemistry
Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

Unit I

Calcium in Biology: Biochemical role of calcium, Storage and transport of calcium, Role of Ca^{2+} in muscle contraction, Blood clotting mechanism, Biological calcification.

Unit II

Metallo-proteins and Metallo-enzymes of Fe : Ferritin, Transferrin, bio–mineralization and Siderophores, Peroxidase, Catalase, Hemerythrin, Cytochromes, Cytochrome P-450, Iron sulphur proteins, Rubredoxins, Ferredoxins.

Unit III

Metallo-enzymes and proteins of copper and zinc : Blue-copper proteins, Ceruloplasmin, Hemocyanin, Cytochrome -c oxidase, Superoxide dismutase, Carbonic anhydrase, Alcohol dehydrogenase, Carboxy peptidase, Metallothionein, inter changeability of Zn and Co in enzymes.

Unit IV

Biochemical role of Co, Mo and Mn, : Biological nitrogen fixation, Vitamin B12, B12 coenzyme, Cobalamines, Xanthine oxidase, Sulphite oxidase, Nitrite reductase, Arginase, Mn-SOD, Chlorophyll, Photosystem I and II, cleavage of water.

Unit V

Metals in medicines: Toxicity of Hg, Cd, Pb, Cr, Be, Se, and As. Biological defence mechanism, Chelation therapy, Metals used for diagnosis and Chemotherapy, Pt- complexes as anticancer drugs, complexes of Au, Cu, Zn, As, Hg, as drugs.

Suggested Reading:

1. Bioinorganic Chemistry, Asim K. Das. Books & Allied Ltd, 2013
2. Bioinorganic Chemistry (Bertini, Ivano G, Harry B ,Lippard, S. J, Valentine, J.S.), University Science Books, CA, 1994.
3. J.A. Cowan, Inorganic Biochemistry: An Introduction, 2nd Edition, Wiley-VCH , 1997
4. R. P. Hanzlik, Inorganic Aspects of Biological and Organic Chemistry,, Academic Press, New York, 1976

PAPER - CHEM 908E

Chemistry of Biomolecules-II
Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

Unit I: Classification of lipids, biological importance of fatty acids and lipids, even chain and odd chain fatty acids, essential fatty acids: ω-3and ω-6 fatty acids; Oxidation of fatty acids (alpha, beta, and omega): saturated and unsaturated;odd carbon atom and even carbon atom fatty acids; saturated and unsaturated fats, ketone bodies, fatty acid metabolism, biological membranes, lipid peroxidation, properties and function of lipid bilayers and liposomes; self association of lipids-micelles, reverse micelles and membranes, transport of cations through membranes.

Unit II: Structure and functions of prostaglandins, and thromboxanes; Ecosanoids and prostaglandins, Source, synthesis and biological activities of prostaglandins and thromboxanes (PGE_1,PGE_2, PGE_3,PGF_1, PGF_2,PGF_3,PGG_2,PGI_2, PGH_2, TXA and TXB), biosynthesis of prostaglandins, inhibition of prostaglandin synthesis.

Unit –III: Synthesis, stability, reactivity and rearrangement of macrocyclic compounds, synthesis of mucone, civetone, exaltone and their bioactivity.

Books recommended:

1. Chemistry of Biomolecules: An Introduction, R. J. Simmonds, Royal Society of Chemistry, 1992.
2. Lehninger Principles of Biochemistry, David L. Nelson and Michael M. Cox. 7th Edition. W H Freeman & Co (Sd). 2017.
3. 2. Bioorganic and Bioinorganic and Supramilecular Chemistry. P.S. Kalsi, New Age International (Pvt. Ltd.) 2nd edition 2010.
4. 3. Biochemistry, C.B. Power and G.R. Chatwal. Himalayan Publishing House. 4th edition 1999.
5. J. Clayden, N. Greeves, S. Warren, and P. Wothers, Organic Chemistry, (2001) Oxford Univ. Press, Oxford. .
6. F. D. Gustone, Fatty acid and Lipid Chemistry (1996), Wiley
7. S. P. Bhtani, Chemistry of Biomolecules (2010), CRC Press
8. Norbert Sewald and Hans-Dieter Jakubke,Peptides: Chemistry and Biology.. Wiley-VCH
9. *Maitland, Jr Jones, Organic Chemistry (1998).*
10. *J. Hopkins, C.W McLaughlin, S. Johnson, M.Q Warner, D. LaHart, J.D Wright .Human Biology and Health.Michelle (1993). Prentice Hall.*
11. *J.E Vance, D.E Vance, Biochemistry of Lipids, Lipoproteins and Membranes. Amsterdam: Elsevier (2002).*

PAPER – CHEM 909E

POLYMER CHEMISTRY
Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

UNIT-I:

Polymer and Characterisation:-Banz concepts of polymer science, Molecular forces and chemical bonding in polymers. Polymer solution and fractionation. Gel permeation Chromatography and molecular weight determination by viscometry, osmometry, light scattering and ultra centrifugation, molecular weight distribution curve.

UNIT-II:

Polymerization:- mechanism and kinetics of step growth and chain growth polymerization- radical, ionic and ring opening polymerization, copolymerization, polymerization techniques and polymer reaction, polymer structure and physical properties: configuration of polymer chain crystal structure of polymers: speciality polymers: Block copolymer, polymer colloids and biomedical polymers.

Unit III: Organic and inorganic polymer

Organic polymer: Manufacturing process, general properties, compounding and applications of SBR, Polyisoprene, Polybutadiene, Butyl rubber, Ethylene –propylene rubber, Neoprene rubber, Speciality rubbers: Silicon rubbers, Nitrile rubbers, Polyacrylic rubbers –Polyurethane rubbers – foam rubber

Inorganic polymers:

Classification of inorganic polymer, inorganic polymerisation reactions (addition, condensation and coordination polymerisation). Polysiloxanes, polysilanes, poly phosphazenes, polymeric sulfur. Syntheisis, structure, properties and application of coordination polymers & organometallic polymers.

Reference books:

1. C. Tanford, Physical Chemistry of Macromolecules, Wiley, Newyork, 1961
2. V.R. Gowariker, Polymer Science, New Age International New Delhi, 1986
3. Y. Morai, Micelles: Theoretical and Applied Aspects, Plenum (1992).
4. G. Odien, Principles of Polymerization, 3rd edition (1991) John Wiley & Sons, Singapore.
5. P. Bahadur and N.V. Sastry, Principles of Polymer Science, (2002) Narosa, New Delhi.
6. F.W. Billmayer, Jr., Text Book of Polymer Science, 3rd Edition (1984), Wiley-Interscience, New York.

PAPER – CHEM 910E
QUANTUM CHEMISTRY-II
Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

Group A: QUANTUM MECHANICS

UNIT-I

Interpretation of wave function (probability density). Box normalization. Superposition principle and expansion theorem. Derivation of the expression of L_z in polar coordinate system.P_x, L_z and $\hat{H}$ operators are Hermitian: Proof. Unitary and projection operators. Some important theorems. Schmidt orthogonalization. Dynamical variables and operators, dynamical states. Expectation value and average value. Linear vector spaces in quantum mechanics. Completeness theorem. Equations of motion of classical mechanics (in brief). Poisson bracket and Dirac's version of Correspondence principle. Ehrenfest theorem. Constants of motion.

The Heisenberg Uncertainty relations (position and momentum, angle and angular momentum , time and energy relations) : proof. Commutability and compatibility. Complete set of commuting operators. Fourier transform. Wave packet. Momentum space wave function.

Angular momentum operators (single particle system). Step up and step down operators. Spin angular momentum operators. Angular momentum operators (many electron system) and their commutation with spin free Hamiltonian operator. coupling of angular momenta, L-S coupling and j-j coupling. Term symbols and spectroscopic states. Pauli spin matrices and anti-commutation relations.

UNIT-II

Time independent non-degenerate perturbation theory (RSPT). Application: ground state of He atom. Degenerate RSPT. Applications: Stark effect, normal and anomalous Zeeman effect.

Rayleigh- Ritz variation principle. Linear variation method. Applications: ground state energy of He atom, harmonic oscillator.

Time dependent RSPT (First order). Fermi-Golden rule. Born-Oppenheimer approximation(in detail). Antisymmetrized wave Function. Slater determinant and Pauli exclusion principle.

Reference books:

1. L.I. Schiff, *Quantum Mechanics*, Third Edition, McGRAW-HILL BOOK COMPANY, 1985.
2. P.W. Atkins and R.S.Friedman, *Molecular Quantum Mechanics*, 3rd Ed.(1997) Oxford University Press.
3. B.H. Bransden & C.J. Joachain, *Physics of Atoms and Molecules*, Longmann Scientific and Technical, 1994.
4. B.H. Bransden & C.J. Joachain, *Quantum Mechanics*, Second edition, low price edition, PEARSON Education, First Indian Reprint, 2004.
5. J. L. Powell and B. Crasemann, *Quantum Mechanics*, Addison-Wesely Publishing Company.
6. Eugene Merzbacher, *Quantum Mechanics*,Wiley International Edition, 1970.

SEMESTER –IV

Semester – IV

Core (12 credits)

CHEM	1001C	Inorganic Chemistry-IV	04
CHEM	1002C	Organic Chemistry-IV	02
CHEM	1003C	Physical Chemistry-IV	02
CHEM	1004C	Chemistry Project-II	04

Elective

CHEM	1005E	Supra-molecular and Nano Chemistry	02
CHEM	1006E	Environmental and Green Chemistry	02
CHEM	1007E	Chemistry of Natural Products	02
CHEM	1008E	Photochemistry	02
CHEM	1009E	Computer Programming	02
CHEM	1010E	Statistical Mechanics	02

PAPER: CHEM 1001C

Inorganic Chemistry-IV
Total Marks: 100 (Theory 70 + Internal Assessment 30)
Credits: 04

Group A

Transition Metal–Carbon Bond

(a) Transition Metal–Carbon σ-Bond: Brief review of metal alkyl compounds; transition metalcarbene and transition metal-carbyne compounds; transition metal vinylidene and transition metal allenylidene compounds.

σ – bonded ligands : Metal alkyls, aryls and hydrides. Stability, preparation and reactivity.

Metal- carbonyls / Metal- phosphines / metal- nitrosyls / metal isocyanide: structures, reactivity and bonding.

Metal- carbenes, metal-carbynes, Fischer carbenes, Schrock carbenes , N-heterocyclic carbenes, olefin metathesis.

(b) Transition Metal-Carbon π-Bond: Cyclopropenyl cation as a ligand; C4R4 as a ligand (R = H, Me, Ph); Synthesis and reactions of cyclopentadienyl metal carbonyls, cyclopentadienyl metal hydrides, cyclopentadienyl metal halides, arene metal carbonyls, η6-arene-chromium tricarbonyl in organic synthesis.

π - bonded ligands: Metal-olefins, metal alkynes, metal-dienes, Metal-Cp Metal-Cp* complexes. Synthesis, structure, bonding and reactivity.

Group B

1. Catalysis Using Organometallic Compounds: Terminology in catalysis (Turnover, Turnover number, Turnover frequency or turnover rate, mole fraction, eantioselectivity, stereoselectivity, chemoselectivity, regioselectivity); Comparison of Homogenous and Heterogeneous Catalysis; Catalytic Hydrogenation of alkenes and related reactions: Hydrogenation catalysts, Catalytic cycle

of Wilkinson's catalyst, Catalytic asymmetric synthesis, the mechanism of asymmetric hydrogenation using a chiral catalyst.

2. Olefin Metathesis: Well-known olefin metathesis catalysts and their properties, synthesis of Grubbs' and Schrock catalysts, Mechanism of olefin metathesis, ring opening metathesis, cross metathesis, ring closing metathesis, ring opening polymerization metathesis, acyclic diene metathesis polymerization, enyne metathesis, comparison of catalysts, application of catalytic olefin metathesis.
3. Palladium catalyzed C–C coupling reactions: The Heek reaction, Suzuki-Miyaura coupling, Sonogashira coupling, Stille coupling, Kumada coupling, Negishi coupling.
4. Olefin polymerization and oligomerisation reactions: The Ziegler-Natta catalyst, site control and chain end control mechanisms, metallocene based catalysts, post metallocenes catalyst.

PAPER: CHEM 1002C

Organic Chemistry-IV
Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

Unit I: Heterocyclic chemistry

Hantzsch-Widman nomenclature for monocyclic, fused and bridged heterocycles; Basicity and aromaticity of heterocycles; Synthesis, properties and reactions (ring openings & heteroatom extrusion) of 3- membered heterocycles (aziridines, oxiranes and thiiranes), 4- membered heterocycles (azetidine, oxetanes and thietanes); Synthesis and reactivity of azoles (imidazole, pyrazole, oxazole, isoxazole, thiazole, isothiazole& their benzo derivatives) and azines (6-membered heterocycles with two hetero atoms -pyridazines, pyrimidines and pyrazines), caffeine; theobromine and theophylline.

Unit III: **Nucleic acid chemistry**

Nucleic acids, nucleic acid bases, Purine and pyrimidine bases of nucleic acids, nucleosides and nucleotides, their structures and nomenclature, structures and functions of NADH, NADP and ATP, Structures of RNA and DNA; replication of DNA; base-pairing, double helical structure of DNA.

Recommended Books:

1. Heterocyclic Chemistry Vol. 1-3, R.R. Gupta, M. Kumar and V.Gupta, Springer Verlag.
2. The Chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme.
3. Heterocyclic chemistry J. A. Joule, K. Mills and G.F. Smith, Chapman and Hall.
4. Heterocyclic Chemistry, T.L. Gilchrist, Pearson Education.
5. Contemporary Heterocyclic Chemistry, G.R. Newkome and W.W. Paudler, Wiley-Inter Science.
6. An Introductiion to the Heterocyclic Compounds, R.M. Acheson, John-wiely.
7. Comprehensive Heterocyclic Chemistry, A.R. Katrizky and C.W. Rees, eds. Pergamon Press.
8. Medicinal Natural Products, A Biosynthetic Approach 3rd Edition, Paul M Dewick, John Wiley & Sons Ltd.
9. Organic Chemistry Volume 2: Stereochemistry and the Chemistry of Natural Products, I. L. Finar, Fifth Edition, ELBS.
10. R.T. Morrison and R.N. boyd, Organic chemistry, 6^{th}edn, Prentice hall of India, New delhi, 2003.

PAPER: CHEM 1003C

Physical Chemistry-IV

Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

UNIT – I

A. ELECTROCHEMISTRY–I: Activity in electrolytic solutions. Freezing point depression and the mean ionic activity coefficient. The Debye-Huckel theory for dilute ionic solutions (derivation) and correction for concentrated solutions Equilibrium in ionic solutions. Ion association.

B. ELECTROCHEMISTRY–II: Electrodics - The basic electrodic equation: Butler-Volmer equation, over potential, polarisable and non-polarizable interfaces; Faradaic and non -faradaic Currents, Over-potentials, aspects of deviation from equilibrium. Electrical conductance of solutions; The Debye Huckel Onsagar equation for conductance (derivation); Conductance at high fields and high frequencies, Conductance in non-aqueous solvents. Fuel Cells: H_2-O_2 cell, Air-H cell; Electricity producing cells: Na-S, Sb-S.

Numerical problems.

UNIT-II

C. BIO-PHYSICAL CHEMISTRY: Hydrophobic effect and self organising systems, structure and functions of proteins and nucleic acids and their stability. Structure and functions of cell membranes; Ion transport through cell membranes and nerve conduction; Multiple equilibria; stacking and cooperative interactions in biological systems. Muscle contraction; Techniques for study of structure and functions of proteins and nucleic acids.

D. CHEMICAL KINETICS-II: Theory of reaction rates; Temperature effect on reaction rates; Rate constant for simple; Bi-molecular reactions; Collision theory; Activated complex theory. Reactions in solutions: Diffusion controlled and activation controlled reactions; Thermodynamic formulation of rate constant: effect of pressure & ionic strength; Reaction in surfaces: Langmuir adsorption isotherm; kinetics of surface catalyzed uni-molecular and bimolecular reactions; Applications in ammonia synthesis and oxidation of carbon-monoxide.

Reference books:

1. J.O'M, Bockris and A.K.N. Reddy, *Modern Electrochemistry*, Vol.1&2 (1998), Plenum Press, New York.
2. K. J. Laidler, Chemical Kinetics, 3rd Ed.(1967), Harper and Row Publishers, New York.
3. H. Eyring, S. H. Lin and S. M. Lin, *Chemical Kinetics* (1999), Jhon Willey, New York.
4. K. Zeemanski, *Thermodynamics*

PAPER: CHEM 1004C

Chemistry Project II

Total Marks: 100 (Projrct 70 + Internal Assessment 30)
Credits: 04

PAPER: CHEM 1005E

Supra-molecular and Nano Chemistry
Total Marks: 50 (Theory 35 + Internal Assessment 15)
Credits: 02

Unit-I: SUPRAMOLECULAR CHEMISTRY

Concepts and Languages of supramolecular chemistry - Molecules, super molecules and supramolecular Chemistry; factors leading to strong binding (non-covalent interactions); molecular receptors – design and principles; Types of interactions between host and guest molecules; Thermodynamics of host-guest complexation; Enthalpy and entropy contributions, complexation free energies; Molecular recognition – factors involved; Molecular receptors – for alkali metal ions, ammonium ions, anions and neutral molecules. Crown ethers, cryptands, spherands and ionophores; Creation of rotaxanes and catenanes; Supramolecular catalysis- Catalysis by Reactive Macrocyclic Cation Receptor Molecules. Catalysis by Reactive Anion Receptor Molecules; Catalysis with Cyclophane Type Receptors; Catalysis of Synthetic reactions; Supramolecular Chemistry in solution: Cyclodextrin, Micelles, Dendrimmers, Gelators. Various types of supramolecular devices.

Unit –II: NANO CHEMISTRY

Background to Nano-science Science and Technology - Implications for Physics, Chemistry, Biology and Engineering - Classifications of nanostructured materials - nano particles - quantum dots, Nanowires, nano-tubes – ultra – thinfilms – multilayered materials. Typical syntheses of nano particles, oxide nano tubes and fibres, metal nano particles; Length Scales involved and effect on properties: Mechanical, Electronic, Optical, Magnetic and Thermal properties.

Synthesis of nanoparticle: Bottom-up Synthesis -Top-down Approach: Precipitation, Mechanical Milling, Colloidal routes, Self-assembly, Vapour phase deposition, MOCVD, Sputtering, Evaporation, Molecular Beam Epitaxy, Atomic Layer Epitaxy, MOMBE.

Characterization of nano particles- X-ray diffraction technique, Scanning Electron Microscopy - environmental techniques, Transmission Electron Microscopy including high-resolution imaging, Surface Analysis techniques

Application of nano-structured material in organic synthesis, dendrimers, bucky balls and nano tubes (properties and applications), drug delivery systems; Nanotechnology for sustainability, Nanomedicine, Environmental, health, and safety issues

Suggested reading:

1. Lehn, J.M. Supramolecular Chemistry, VCH, Wienheim, 1995.
2. A.S. Edelstein and R.C. Cammearata, eds., Nanomaterials: Synthesis, Properties and Applications, (Institute of Physics Publishing, Bristol and Philadelphia, 1996)
3. N John Dinardo, Nanoscale charecterisation of surfaces & Interfaces, Second edition, Weinheim Cambridge, Wiley-VCH, 2000
4. G Timp (Editor), Nanotechnology, AIP press/Springer, 1999
5. Akhlesh Lakhtakia (Editor) The Hand Book of Nano Technology, "Nanometer Structure", Theory, Modeling and Simulations. Prentice-Hall of India (P) Ltd, New Delhi, 2007.

PAPER: CHEM 1006E

Environmental and Green Chemistry

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

Unit – I: Environmental Chemistry (Credit – 01)

Concept and scope of environmental chemistry, Environmental terminology and nomenclatures, Environmental segments, Ozone depletion, The green-house effect and Global warming, El-Nino phenomenon. 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, microbiologically mediated redox reactions and Nitrogen transformation by bacteria. Water pollutants: Water-quality parameters and standards: physical and chemical parameters (colour, odour, taste and turbidity, DO, BOD, COD etc.); industrial and waste-water treatment; Chemical hazards, chemical disaters, pollution of environment-man made, industrial, natural disasters, environmental biochemistry, toxicological chemistry; analysis of water and waste water, solid wastes and air pollution-Photochemical smog, Auto exhausts, Acid-rains, Air-quality standards. Toxic chemicals in the environments, Impact of toxic chemicals on enzymes, Biochemical effects of arsenic, cadmium, lead, mercury, carbon monoxide, nitrogen oxides, sulphur oxides, ozone, PAN, cyanide, pesticides, insecticides and carcinogens.

Unit – II: Green Chemistry (Credit – 01)

Definition, Concepts and basic principles of green chemistry, need of green chemistry, green chemistry as an alternative tool for reducing pollution, atom economy, less hazardous chemical syntheses, atom economy in rearrangements, addition and pericyclic reactions, less hazardous chemical syntheses, designing safer chemicals, safer solvents and auxiliaries, design for energy efficiency, Green synthesis, clean routes, supercritical solvents, ionic liquids, green catalyst, auto-exhaust catalyst and clean technology. Development of new methods for organic synthesis such as Green Synthesis: use of sonochemistry, use of ionic liquids, use of microwaves, bio-catalysis. Selection of solvent: i) Aqueous phase reactions ii) Reactions in ionic liquids iii) Solid supported synthesis iv) Solvent free reactions, Green catalysts: i) Phase transfer catalysts (PTC) and ii) Biocatalysts. Microwave and Ultrasound assisted green synthesis: Aldol condensation, Cannizzaro reaction, Diels-Alder reactions, Strecker synthesis, Willaimson synthesis and Dieckmann condensation.

Book Suggested:

1. *Handbook of Environmental chemistry*, Springer-Verlag, O. Hutzinger.
2. M. Bernhard, F.E. Brinckman & P.J. Sadler.*The Importance of Chemical Speciation in Environmental Processes*, Springer-Verlag,
3. L.J. Fristschen, & L.W. Gay, *Environmental Instrumentation*, Springer-Verlag,.
4. Real World Cases in *Green Chemistry*, ACS, M.C. Cann & M.E. Connelly.
5. P.T. Enastas and T.C. Williamson, Green Chemistry: Designing Chemistry for Environment, ACS,
6. *Green separation processes, methods and application*, Fonso, National Scientific Book Agency, Delhi-110053.
7. G.W. Vanloon, S.J. Duffer, *Environmental Chemistry* - A Global Perspective, (2000) Oxford University Press.
8. F.W. Fifield and W.P.J. Hairens, *Environmental Analytical Chemistry*, 2nd Edition (2000), Black Well Science Ltd.
9. Colin Baird, *Environmental Chemistry*, (1995) W.H. Freeman and Company, New York.
10. A.K. De, *Environmental Chemistry*, 4th Edition (2000), New Age International Private Ltd., New Delhi.
11. Peter O. Warner, *Analysis of Air Pollutants*, 1st Edition (1996), John Wiley, New York.
12. S.M. Khopkar, *Environmental Pollution Analysis*, 1st Edition (1993), Wiley Estern Ltd., New Delhi.
13. S.K. Banerji, *Environmental Chemistry*, 1st Edition (1993), Prentice-Hall of India,New Delhi

PAPER: CHEM 1007E

Chemistry of Natural products

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

UNIT – I

General: Sources and types of natural products, method of isolation and structure elucidation, importance of natural products, biosynthesis of some common type of natural products – terpeneoids, steroids, flavonoids and alkaloids.

Chemistry of terpenoids, **steroid and hormones:** Terpenoids – sesquiterpenoids, diterpenoids with special reference to the isolation, structure and stereochemistry: alpha-santonin, Caryophyllene and isocaryophyllene, abietic acid and Gibberellic acid.

Steroids and hormones – Cholesterol, oestrone, progesterone, testosterone.

UNIT- II Alkaloids and Phenolics - Chemistry of quinoline, isoquinoline, phenanthrene and indole group of alkaloids - papaverine, cimchonine quinine, morphine, thebaine, codeine, reserpine with special reference to isolation, structure and stereochemistry. Plant phenolics with special reference to the general structures, reactions and synthesis of anthocyanins, anthocyanidins, flavones flavonols, isoflavones, chalcones, coumarins, quinines and tannins.

Reference books:

1. Organic Chemistry, I.L. Finar, volume 2, ELBS, 5th edition (1975).
2. Organic Chemistry. Morrison Boyd and Bhattacharjee, 7th edition (2013), Pearson.

PAPER: CHEM 1008E

Photochemistry

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

UNIT- I : Physical processes of Photochemistry

Physical properties of excited molecules: Nature of changes on electronic excitation, Potential energy diagram, Absorption band shape and Franck-Condon Principle, Emission Spectra, Environmental effects on absorption and emission properties, Excited state dipole moment, Redox potential and acidity constants of aromatic acids. Polarised luminencence, non radiative intra-molecular electronic transition, internal conversion, intersystem crossing, crossing potential energy surface (Franck- Condon factor).

Photo-physical processes in excited state: Types of photophysical pathways, Radiation less transitions, Fluorescence emission, Triplet state and phosphorescence emission, Fluorescence quenching, Stern-Volmer equation, Concentration quenching and excimer formation, Quenching by foreign substrates, Exciplex formation. Mechanism of quenching, energy transfer process (Forster dipole coupling), electron transfer phenomenon (Marcus theorem, Rehm Weller theorem), eximer.

Unit II: Inorganic photochemistry and organic photochemistry

Introduction to inorganic photochemistry, Ligand field states,L-F excited states, charge transfer states , L-M-C-T states, M-L-C-T states, Thexi (and Dosenco states), photochemical reactions, substitutions, redox reactions of Cr(III), Ru(II) and RU(III) complexes. Application (synthesis and catalysis, chemical actinometry, photochromism, sensitization). Laser: Basic principles, population-inversion, qualitative description of ruby and He-Ne lasers.

Organic photochemical process: Quantum yields, photosensitization and its uses. Photochemistry of olefins and carbonyl compounds, Norrish – I and Norrish – II type reactions, photo oxygenation and photo fragmentation, Paterno-Buchii reaction, Barton reaction, Di-π-methane rearrangement, Photo-cycloaddition and Photochemistry of arenes. Photochemistry in vision process.

Reference books:

1. K. K. Rohtagi-Mukherjee, *Fundamental of Photochemistry*,(1986) New Age International New Delhi.
2. J. G. Calvert and J. N. Pitts, Jr., *Photochemistry* (1966) John Wiley & Sons, New York.
3. R. P. Wayne, *Principles and Application of Photochemistry* (1988), Oxford University Press, Oxford.
4. N. J. Turro, *Modern Molecular Photochemistry*, (1991) Univ. Science Books, Sansalito.
5. J. F. L Lakowicz, *Principles of Fluorescence Spectroscopy*, 2nd Edn. (1999) Planum Publishers, New York.

PAPER: CHEM 1009E

Fortran and C, C+, C++ Programming

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

UNIT-I

FORTAN programming F77:

FORTAN programming preliminaries; FORTAN constants and variables; Arithmetic Expressions. Input-output statements. Simple computer programmes. Control statements. The Do statements. Subscripted variables. Elementary Format Specifications. Logical Expression. Function and subroutines. Processing files in FORTRAN. Use of common statements. FORTAN 90, 95(Introduction).

UNIT-II

C, C+ , C++

PAPER: CHEM 1010E

Statistical Mechanics

Total Marks: 50 (Theory 35 + Internal Assessment 15)

Credits: 02

UNIT-I

Classical monatomic liquids-radial distribution function (RDF); Relating RDF with the thermodynamic properties; integral equations; Potential of mean force; the direct correlation function.

Statistical mechanical perturbation theory of liquids: theory and its application to derive van der Waals equation of state.

UNIT-II: Non-equilibrium statistical mechanics: Random Processes; Time-correlation functions;

Brownian motion; Langevin equation for random motion; Random walk in one dimension; Time dependence of fluctuation; Fluctuation-dissipation theorem; Fokker-Planck equation.

Reference books:

1. B. J. Mcclelland, *Statistical Thermodynamics*
2. M. Dole, *Introduction to Statistical Thermodynamics*
3. M. C. Gupta, *The statistical Thermodynamics* (1990), New Age International (P) Ltd. New Delhi
4. Anrew Maczek, S*tatistical Thermodynamics* (1978), Oxford University Press Inc. New York
5. D. A. McQuarrie, *Statistical Mechanics* (2003), Viva Books Pvt. Ltd. New Delhi.