MASTER OF SCIENCE (CHEMISTRY) – FIRST SEMESTER

First Semester			
S. No.	Name of Subject	Credits	Total Marks
1	Inorganic Chemistry – I	4	100
2	Organic Chemistry – I	4	100
3	Physical Chemistry – I	4	100
4	Green Chemistry	2	100
5	Analytical Chemistry - I	2	100
6	Lab-I	6	100
Total		22	

Subject: - Inorganic Chemistry - I

Course A: Stability constants of metal complexes and their applications

Stoichiometric and thermodynamic equilibrium constants, stepwise formation of complexes, formation functions, φ, n and $\propto C$ and relationship between different functions. Calculation of stability constants. Graphical Methods: using sets of data $\{\varphi,[A]\}$; $\{\propto C,[A]\}$ and $\{n,[A]\}$.

Curve fitting method, Elimination method, Numerical method, Potentiometric method. Method of corresponding solutions, Ion exchange method, Solvent extraction, Polarographic method, and Spectrophotometric methods which include Job's method of continuous variation, Logarithmic method. Bent and French mole ratio method. Turner and Anderson methods and Yatsimirskiis method.

Errors and Evaluation: Definition of the terms- mean and median, precision —standard deviation, relative standard deviation, accuracy-absolute error. Types of errors in experimental data determination (systematic), indeterminate (random) and gross. Sources of errors and their effect upon the analytical results. Methods for reporting analytical data. Statistical evaluation of data -indeterminate errors. The use of statistics.

Analytical applications of complex formation; gravimetric analysis, complexometric titrations (Conditional constants, titration curves, titration error, detection of end point using metal indicators and instrumental methods. Indicator errors, Indicator correction etc. Simultaneous titrations, stepwise titrations, back titrations). Use of masking and demasking agents in complexometric titrations.

Course B: Supramolecular and Photoinorganic Chemistry

Molecular recognition: Receptors, design and synthesis of co-receptors and multiple recognition, Hydrogen bonds, strong, weak and very weak H-bonds, Utilisation of H-bonds to create supramolecular structures, Use of H-bonds in crystal engineering and molecular recognition, Chelate and macrocyclic effects.

Cation binding hosts, binding of anions, binding of neutral molecules, binding of organic molecules.

Supramolecular reactivity and catalysis. Transport processes and carrier design. Supramolecular devices, supramolecular photochemistry.

Redox reactions of metal complexes in excited states, excited electron transfer, examples using [Ru(bpy)3]2+ complex and [Fe(bpy)3]2+ complex. Role of spin-orbit coupling, lifetimes of excited states in these complexes.

Metal complex sensitizers: Electron relay, semiconductor supported metal oxide systems, water-photolysis, nitrogen fixation and C02 reduction.

Recommended Texts:

1. Inczedy, J. Analytical applications of complex equilibria Halsted Press: New York, NY (1976)..
2. Martell, A. E. & Calvin, M. Chemistry of the Metal Chelate Compounds. Prentice-Hall : N. Y. (1952).
3. Ringbom, A. Complexation in Analytical Chemistry Wiley: New York (1963).
4. Hartley, F. R. , Burgess, C. & Alcock. , R. M. Solution Equilibria Prentice-Hall : Europe (1980).
5. Beck, M. T. Chemistry of Complex Equilibria van Nostrand Reinhold: New York (1970).
6. Rossotti, F. J. C. & Rossotti, H. The Determination of Stability Constants McGraw Hill: London (1961).
7. Lippard, S.J. Progress in Inorganic Chemistry, Vol. 18, 3rd Ed. Wiley-Interscience (1991).
8. Lehn, J. M. Supramolecular Chemistry: Concepts & Perspectives Wiley-VCH (1995)..
9. Balzani, V. Photochemistry of Coordination Compounds Academic Press (1970)..
10. Desiraju, G. R. , Ed. Perspectives in Supramolecular Chemistry, Vol.2: Crystal Engineering and Molecular Recognition Wiley: Chichester (1995).
11. Atwood, J. L. & Steed, J. W. Supramolecular Chemistry: A Concise Introduction John Wiley & Sons (2000).
12. Adamson, A. W. & Fleischauer, P. D. (Eds.) Concepts of Inorganic Photochemistry, Wiley: New York (1975).

Subject: - Organic Chemistry - I

Course A: Organic Stereochemistry

Molecular symmetry and chirality: Symmetry operations and symmetry elements, point group classification and symmetry number.

Stereoisomerism: Classification, racemic modification, molecules with one, two or more chiral centres; Configuration nomenclature, D L, R S and E Z nomenclature. Axial and planar chirality and helicity (P & M); Stereochemistry and configurations of allenes, spiranes, alkylidine, cycloalkanes, adamantanes, catenanes, biphenyls (atropisomerism), bridged biphenyls, ansa compounds and cyclophanes.

Topicity and prostereoisomerism: Topicity of ligands and faces and their nomenclature; Stereogenicity, chirogenicity, and pseudoasymmetry, stereogenic and prochiral centres.

Simple chemical correlation of configurations with examples, quasiracemates.

Cyclostereoisomerism: Configurations, conformations and stability of cyclohexanes (mono-, di- and tri-substituted) cyclohexenes, cyclohexanones, halocyclohexanones, decalins, decalols and decalones.

Asymmetric induction: Cram's, Prelog's and Horeau's rules; Dynamic stereochemistry (acyclic and cyclic), Qualitative correlation between conformation and reactivity, curtin-Hammett Principle.

Molecular dissymmetry and chiroptical properties. Linear and circularly polarised lights, circular birefringence and circular dichroism, ORD and CD curves, Cotton effect.The axial haloketone rule, octant diagrams, helicity, and Lowe's rule. Application of ORD and CD to structural and stereochemical problems.

Course B: Study of Reactive Intermediates

A review of reaction mechanisms including methods of determination.

Linear free energy relationships and their applications (Hammett equation and modifications).

Carbocations: Classical and non-classical, neighbouring group participation, ion-pairs, molecular rearrangements in acyclic, monocyclic and bicyclic systems, stability and reactivity of bridge-head carbocations.

Carbanions: Generation, structure and stability, ambident ions and their general reactions; HSAB principle and its applications.

Radicals: Generation, structure, stability and reactions, cage effects; radical-cations & radical-anions.

Carbenes: Formation and structure, reactions involving carbenes and carbenoids.

Nitrenes: Generation, structure and reactions of nitrenes.

Nucleophilic aromatic substituion; Benzynes, SNAr and SRN1 mechanisms; Ipso effect.

Recommended Texts:

1. Carey, F. A. & Sundberg, R. J. Advanced Organic Chemistry, Parts A & B, Plenum: U.S. (2004).
2. Eliel, E. L. Stereochemistry of Carbon Compounds Textbook Publishers (2003).
3. Finar, l. L. & Finar, A. L. Organic Chemistry,Vol. 2, Addison-Wesley (1998).
4. Finar, l. L. Organic Chemistry Vol. 1, Longman (1998).
5. Lowry. T. H. & Richardson, K. S. Mechanism and theory in Organic Chemistry Addison-Wes!ey Educational Publishers, Inc. (1981).
6. Nasipuri, D. N. Stereochemistry of Organic Compounds: Principles & Applications South Asia Books (1994).
7. March, J. Advanced Organic Chemistry John Wiley & Sons (1992).

Subject: Physical Chemistry-I

Quantum Chemistry

Postulates of quantum mechanics, Linear and Hermitian operators, Commutation of operators and Uncertainty Principle.

Differential equations, partial differential equations, series solutions and special functions, linear vector spaces, transformation of coordinate matrix, representation of operators, eigen value problem orthonormal sets, Fourier and Laplace transforms.

Some exactly soluble problems: Particle in a box and ring, Concept of degeneracy and Jahn-Teller distortion.

Simple harmonic oscillator problem and its solution using series solution or factorization method. Calculation of various average values using ladder operators and recursion relations of Hermite polynomials.

Angular momentum operators, Eigenvalues and eigen functions, Ladder operators, rigid rotator and hydrogen atom: Complete solution, Radial distributions, Virial theorem.

Approximate methods: First order time-independent perturbation theory for non-degenerate states, Variation theorem and variational methods, Use of these methods illustrated with some examples (particle in a box with a finite barrier, anharmonic oscillator, approximate functions for particle in a box and hydrogen atom).

Ground and excited state of helium atom. Pauli's Exclusion principle. Many-electron atoms. Concept of spin and determinantal wave functions. Qualitative treatment of Hartree theory and Hartree-Fock SCF procedure.

Chemical bonding: Born-Oppenheimer approximation. Variational treatment of hydrogen molecule ion. Valence bond and MO (LCAO) treatment of hydrogen molecule. Comparison of the MO and VB treatments

and their equivalence limit. Configuration Interaction. Extension of MO theory to other systems- Homonuclear and heteronuclear diatomics, polyatomics. Walsh diagrams for dihydrides, linear and bent triatomics.

HMO method and its applications: π-Electron approximation, Hückel Molecular Orbital Theory of conjugated systems. Calculation of properties- Delocalization energy, electron density, bond order, alternant and nonalternant hydrocarbons. Pairing theorem. Electronic and ESR spectra. Effect of substituents on spectra. Reactivity and electrocyclic ring closures.

Recommended Texts:

1. Lowe, J. P. & Peterson, K. Quantum Chemistry Academic Press (2005).
2. McQuarrie, D. A. Quantum Chemistry Viva Books Pvt. Ltd.: New Delhi (2003).
3. Mortimer, R. G. Mathematics for Physical Chemistry 2nd Ed. Elsevier (2005).
4. Pilar, F. L. Elementary Quantum Chemistry 2nd Ed., Dover Publication Inc.: N.Y. (200 1).
5. Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry 8th Ed., Oxford University Press (2006).
6. Levine, I. L. Quantum Chemistry 5th Ed, Prentice-Hall Inc.: New Jersey (2000).
7. Engel, T. & Reid, P. Physical Chemistry Benjamin-Cummings (2005).
8. McQuarrie, D. A. & Simon, J. D Physical Chemistry: A Molecular Approach 3rd Ed., Univ. Science Books (2001).
9. Silbey, R. J., Alberty, R. A. & Bawendi, M. G. Physical Chemistry 4th Ed. Wiley (2004).

Subject: - Green Chemistry

Introduction to Green Chemistry
The need of Green Chemistry, principles of Green Chemistry

What is Green Chemistry? Need for Green Chemistry. Goals of Green Chemistry. Limitations/ Obstacles in the pursuit of the goals of Green Chemistry

Designing a Green Synthesis using these principles; Prevention of Waste/ byproducts; maximum incorporation of the materials used in the process into the final products , Atom Economy, calculation of atom economy of the rearrangement, addition, substitution and elimination reactions.

Prevention/ minimization of hazardous/ toxic products reducing toxicity. risk = (function) Hazard × exposure; waste or pollution prevention hierarchy. Green solvents– supercritical fluids, water as a solvent for organic reactions, ionic liquids, fluorous biphasic solvent, PEG, solventless processes, immobilized solvents and how to compare greenness of solvents.

Energy requirements for reactions – alternative sources of energy: use of microwaves and ultrasonic energy. Selection of starting materials; avoidance of unnecessary derivatization – careful use of blocking/protecting groups.

Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; catalysis and green chemistry, comparison of heterogeneous and homogeneous catalysis, biocatalysis, asymmetric catalysis and photocatalysis.

Prevention of chemical accidents designing greener processes, inherent safer design, principle of ISD "What you don't have cannot harm you", greener alternative to Bhopal Gas Tragedy (safer route to carcarbaryl) and Flixiborough accident (safer route to cyclohexanol) subdivision of ISD, minimization, simplification, substitution, moderation and limitation. Strengthening/ development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

Future Trends in Green Chemistry

Oxidation reagents and catalysts; Biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions; co crystal controlled solid state synthesis (C2S3); Green chemistry in sustainable development.

Recommended Texts:

1. Ahluwalia, V.K. & Kidwai, M.R. New Trends in Green Chemistry, Anamalaya Publishers (2005).
2. Anastas, P.T. & Warner, J.K.: Green Chemistry - Theory and Practical, Oxford University Press (1998).
3. Matlack, A.S. Introduction to Green Chemistry, Marcel Dekker (2001).
4. Cann, M.C. & Connely, M.E. Real-World cases in Green Chemistry, American Chemical Society, Washington (2000).
5. Ryan, M.A. & Tinnesand, M. Introduction to Green Chemistry, American Chemical Society, Washington (2002).
6. Lancaster, M. Green Chemistry: An Introductory Text RSC Publishing, 2nd Edition, 2010.

Subject: - Analytical Chemistry - I

Introduction: Introduction to Analytical Chemistry and its interdisciplinary nature. Concept of sampling. Importance of accuracy, precision and sources of error in analytical measurements. Presentation of experimental data and results, from the point of view of significant figures.

Analysis of soil: Composition of soil, Concept of pH and pH measurement, Complexometric titrations, Chelation, Chelating agents, use of indicators

(a) Determination of pH of soil samples.

(b) Estimation of Calcium and Magnesium ions as Calcium carbonate by complexometric titration.

Analysis of water: Definition of pure water, sources responsible for contaminating water, water sampling methods, water purification methods.
(a) Determination of pH, acidity and alkalinity of a water sample.
(b) Determination of dissolved oxygen (DO) of a water sample.

Analysis of food products: Nutritional value of foods, idea about food processing and food preservations and adulteration.
(a) Identification of adulterants in some common food items like coffee powder, asafoetida, chilli powder, turmeric powder, coriander powder and pulses, etc.
(b) Analysis of preservatives and colouring matter.

Chromatography: Definition, general introduction on principles of chromatography, paper chromatography, TLC etc.
(a) Paper chromatographic separation of mixture of metal ion (Fe^{3+} and Al^{3+}).
(b) To compare paint samples by TLC method. Ion-exchange: Column, ion-exchange chromatography etc. Determination of ion exchange capacity of anion / cation exchange resin (using batch procedure if use of column is not feasible).

Analysis of cosmetics: Major and minor constituents and their function
(a) Analysis of deodorants and antiperspirants, Al, Zn, boric acid, chloride, sulphate.
(b) Determination of constituents of talcum powder: Magnesium oxide, Calcium oxide, Zinc oxide and Calcium carbonate by complexometric titration.

Recommended Texts:

1. Willard, H.H., Merritt, L.L., Dean, J. & Settoe, F.A. Instrumental Methods of Analysis. 7th Ed. Wadsworth Publishing Co. Ltd., Belmont, California, USA, 1988.
2. Skoog, D.A. Holler F.J. & Nieman, T.A. Principles of Instrumental Analysis, Cengage Learning India Ed.
3. Skoog, D.A.; West, D.M. & Holler, F.J. Fundamentals of Analytical Chemistry 6th Ed., Saunders College Publishing, Fort Worth (1992).
4. Harris, D. C. Quantitative Chemical Analysis, W. H. Freeman.
5. Dean, J. A. Analytical Chemistry Notebook, McGraw Hill.
6. Day, R. A. & Underwood, A. L. Quantitative Analysis, Prentice Hall of India.
7. Freifelder, D. Physical Biochemistry 2nd Ed., W.H. Freeman and Co., N.Y. USA (1982).
8. Cooper, T.G. The Tools of Biochemistry, John Wiley and Sons, N.Y. USA. 16 (1977).
9. Vogel, A. I. Vogel's Qualitative Inorganic Analysis 7th Ed., Prentice Hall.
10. Vogel, A. I. Vogel's Quantitative Chemical Analysis 6th Ed., Prentice Hall.
11. Robinson, J.W. Undergraduate Instrumental Analysis 5th Ed., Marcel Dekker, Inc., New York (1995).

MASTER OF SCIENCE (CHEMISTRY) – SECOND SEMESTER

Second Semester			
S. No.	Name of Subject	Credits	Total Marks
1	Inorganic Chemistry - II	4	100
2	Organic Chemistry - II	4	100
3	Physical Chemistry - II	4	100
4	Retro Synthesis	2	100
5	Analytical Chemistry II	2	100
6	Lab-II	6	100
Total		22	

Subject: - Inorganic Chemistry – II

Course A: Group Theory and its Applications

Molecular symmetry: Symmetry elements and symmetry operations, definition of group and its characteristics, subgroups, classes, similarity transformation.

Products of symmetry operations, equivalent atoms and equivalent symmetry elements ,relations between symmetry elements and operations, classes of symmetry operations. Point groups and classification.

Symmetry: Optical activity and dipole moment.

Representation of groups. Reducible and irreducible representations. The Great Orthogonality theorem. Character tables, position vector and base vector as basis for representation.

Wavefunctions as bases for irreducible representations (p- and d-orbitals). Direct product .Vanishing integral.

Russell-Saunders coupling for dn states. Splitting of one-electron levels in an octahedral environment. Correlation diagram. The method of descending symmetry, selection rules.

Spectral transition probability, vibronic coupling. Non-centrosymmetric complexes. Polarization of allowed transitions.

Symmetry: Infrared and Raman Spectroscopy.

SALCs, projection operators. Illustrative examples.

Hybridization and its applications. Hybrid orbitals as Linear Combinations of Atomic Orbitals. Selected examples. MOs using Group Theory principles

Symmetry and chemical reactions.

Course B: Chemistry of d-and f-block elements :

Term-symbols, Russel-Saunders states. Crystal field theory and splitting in Oh, Td, D4h and C4v systems, Orgel and Tanabe-Sugano diagrams, determination of Dq and Racah parameters, oxidation states and electronic absorption spectra of complex ions. Spectrochemical series and effects of covalency, nephelauxetic series, magnetic properties of transition metal complexes and lanthanides, metal-metal bonds, cluster compounds of d-block elements. poly-oxo metallates of Ru, Os, Mo. Structure and bonding in complexes containing π-acceptor ligands. Relativistic effects affecting the properties of heavier transition elements..

Recommended Texts:

1. Cotton, F. A. Chemical Applications of Group Theory Wiley Interscience: N.Y (1990).
2. Jaffe, H. H. & Orchin. M. Symmetry in Chemistry Dover Publications (2002).
3. Hatfield, W. F. & Palmer, R. A. Problems in Structural Inorganic Chemistry W. A. Benjamin, Inc .:NY (1971)
4. Hatfield. W. E. & Parker, W. E. Symmetry in Chemical Bonding & Structure C. E. Merrill Publishing co.: USA (1974).
5. Bishop, D. M. Group Theory and Chemistry, Clarendon Press: Oxford, U.K. (1973).
6. Shriver, D. F., Atkins, P. W. & Langford, C. H. Inorganic Chemistry, 2nd Ed., Oxford Univ. Press (1998)
7. Purcell. K. F. & Kotz. J, C Inorganic Chemistry. W B. Saunders and Co.: N. Y. (1985).
8. Wulfsberg, G. Inorganic Chemistry Univ. Science books: USA (2000); Viva Books: New Delhi.
9. Sutton, D. Electronic Spectra of Transition Metal Complexes McGraw-Hill.' New York (1968).
10. Mabbs. F. E. & Machin. D. J. Magnetism and Transition Meta/ Complexes Chapman and Hall : U.K. (1 973).
11. Drago, R. S. Physical Methods in Chemistry, W. B. Saunders Co.: U.K. (1977).

Subject – Organic Chemistry – II

Course A: Spectroscopy

PMR: Natural abundance of 13C, 19F and 31P nuclei; the spinning nucleus, effect of external magnetic field. precessional motion and frequency, Energy transitions, Chemical shift and its measurements. Factors influencing chemical shift, anisotropic effect; Integrals of protons. Spin-spin coupling, splitting theory. Magnitude of coupling constant; Simple, virtual and complex spin-spin coupling; Chemical and magnetic equivalence. Proton exchange, factors affecting the coupling - First and non-first order spectra; Simplification of complex spectra (solvent effect, field effect, double resonance and lanthanide shift reagents) and NOE experiments (NOESY, HOESY, ROESY, etc.). Applications of PMR in structural elucidation of simple and complex compounds.

CMR: Resolution and multiplicity of 13C NMR. 1H-decoupling, noise decoupling, broad band decoupling; Deuterium, fluorine and phosphorus coupling; NOE signal enhancement, off-resonance, proton decoupling, Structural applications of CMR. DEPT and INEPT experiments; Introduction to 2D-NMR; COSY, HMQC and HETEROR spectra.
ESR: Derivative curves, hyperfine splitting, g-values, ESR spectra of simple molecules.

MASS: Theory, instrumentation and modifications; Unit mass and molecular ions; Important terms- singly. doubly/multiple charged ions, metastable peak, base peak, isotopic mass peaks, relative intensity, FTMS, etc.; Recognition of M+ ion peak; Ionization methods (El, CI and FAB), General fragmentation rules: Fragmentation of various classes of organic molecules, including compounds containing oxygen, sulphur, nitrogen and halogens; α-,β-, allylic and benzylic cleavage; McLafferty rearrangement; ESI, APCI and MALDI, etc.
Combined problems on UV, IR, NMR and MASS

Course B: Methods in Organic Synthesis

Organosilicone Compounds: Preparation and applications in organic synthesis; Applications of Pd(0) and Pd(II) complexes in organic synthesis- Stille, Suzuki and Sonogashira coupling, Heck reaction and Negishi coupling.

Preparation and applications of lithium organocuparates.
Reductions: Stereochemistry, stereoselection and mechanism of catalytic hydrogenation and metal-liquid ammonia reductions.

Hydride transfer reagents: Sodium borohydride, sodium cyanoborohydride, lithium aluminium hydride and alkoxy substituted LAH reducing agents, DIBAL; Applications of hydroboration (reductions, oxidations and cabonylations): diborane, diisoamylborane, thexylborane, 9-BBN, isopinocamphenyl and diisopinocamphenyl borane.

Homogeneous hydrogenations: Mechanisms and applications using Rh, Ru and other metal complexes.
Oxidations: Scope of the following oxidising reagents with relevant applications and mechanisms: DDQ, SeO_2, $Tl(NO_3)_3$ Sharpless epoxidation.

Recommended Texts:
1. Carruthers, W. Modern Methods of Organic Synthesis Cambridge University Press (1971).
2. Kemp. W. Organic Spectroscopy 3rd Ed., W. H. Freeman & Co. (1991).
3. Silverstein, R M., Bassler, G. C & Morrill, T. C. Spectroscopic Identification of Organic Compounds John Wiley & Sons (1981).
4. March, J. Advanced Organic Chemistry John Wiley & Sons (1992).

Subject: - Physical Chemistry-II

Statistical mechanics and thermodynamics:

Fundamentals: Concept of distribution. Thermodynamic probability and most probable distribution. Canonical and other ensembles. Statistical mechanics for systems of independent particles and its importance in chemistry. Types of statistics: Maxwell-Boltzmann. Bose-Einstein and Fermi-Dirac statistics. Idea of microstates and macrostates. Thermodynamic probability (W) for the three types of statistics. Derivation of distribution laws (most probable distribution) for the three types of statistics. Lagrange's undetermined multipliers. Stirling's approximation, Molecular partition function and its importance. Assembly partition function.

Applications to ideal gases: The molecular partition function and its factorization. Evaluation of translational, rotational and vibrational partition functions for monatomic, diatomic and polyatomic gases. The electronic and nuclear partition functions. Calculation of thermodynamic properties of ideal gases in terms of partition function. Statistical definition of entropy. Ortho- and para-hydrogen, statistical weights of ortho and para states, symmetry number. Calculation of equilibrium constants of gaseous solutions in terms of partition function, perfect gas mixtures.
Einstein theory and Debye theory of heat capacities of monatomic solids.
Third law of thermodynamics, Residual entropy.
Electrochemistry: Solutions: Activity coefficients and ion-ion interactions. Physical significance of activity coefficients, mean activity coefficient of an electrolyte and its determination. Derivation of the Debye-Huckel theory of activity coefficients (both point ion size and finite ion size models). Excess functions.

Kinetics:
Theories of reaction rates: Collision theory. Potential energy surfaces (basic idea). Transition state theory (both thermodynamic and statistical mechanics formulations). Theory of unimolecular reactions, Lindemann mechanism, Hinshelwood treatment, RRKM model (qualitative treatment).
Solution kinetics: Factors affecting reaction rates in solution. Effect of solvent and ionic strength (primary salt effect) on the rate constant. Secondary salt effects.

Macromolecules: Concepts of number average and mass average molecular weights. Methods of determining molecular weights (osmometry, viscometry, sedimentation equilibrium methods). Theta state of polymers. Distribution of chain lengths. Average end-to-end distance.

Recommended Texts:
1. McQuarrie, D. A. Statistical Mechanics Viva Books Pvt. Ltd.: New Delhi (2003).
2. Nash, L. K. Elements of Statistical Thermodynamics, 2nd Ed., Addison Wesley ( ] 974).
3. Laidler. K. J. Chemical kinetics 3rd Ed., Benjamin Cummings (1997).
4. Billmeyer. F.W. Textbook of Polymer Science 3rd Ed. Wiley-Interscience: New York (1984).
5. Atkins. P. W. & Paula. J. de Atkin's Physical Chemistry 8th Ed., Oxford University Press (2006).
6. McQuarrie. D. A. & Simon. J. D. Physical Chemistry: A Molecular Approach 3rd Ed., Univ. Science Books

Subject: - Retro Synthesis

Introduction: General Aspects of Retrosynthetic Analysis, Disconnection Versus Interconversion of the Functional Group, Retrosynthesis and Asymmetric Synthesis, Interconversion of Functional Groups, and C–H Acidity. Interconversions of Oxygenated Functional Groups, Acidity of C–H Bond, Stabilization of Carbanions, Organic Synthesis and the Environment

Retrosynthetic Analysis of the Compounds with One Functional Group: Disconnection of Carbinols, Disconnection of Alkenes, Examples of the Wittig Reaction on the Industrial Scale, Disconnection of

Ketones, Disconnection of Dialkyl Ketones, Alkyl Aryl Ketones and Diaryl Ketones, Interconversion of the Nitro Group, Nitroalkanes as Building Blocks

Stereoisomers and Stereoselective Reactions: ["Departure into Third Dimension"]: Retrosynthesis and Stereochemical Aspects of Synthetic Reactions, Basics of Stereoselective Reactions, Topological Relation and Stereoselectivity, Stereoselective Processes and Kinetic Control, Reaction Stereochemistry, More About Enantioand Diastereoselectivity, Examples of Asymmetric Syntheses, Hydrogenation of the C=O Bond Catalyzed by Chiral Organometallic Complexes, Hydrogenation of the C=N Bond Catalyzed by Chiral Organometallic Complexes, Asymmetric Alkylation of Stabilized Carbanion

Disconnection with Participation of Two Functional Groups: Match and Mismatch of Charges in Bifunctional Molecules, 4.3 1,3-Dioxygenated Pattern (1,3-CO), 1,3-Hydroxycarbonyl Compounds, 1,3-Dicarbonyl Compounds, Concept of Hard and Soft Acids and Bases (HSAB), 1,5-Dicarbonyl Pattern (1,5-CO), From Retrosynthesis to Robinson Annulation, Vinyl Ketones via the Mannich Reaction.

Illogical Disconnections with Participation of Two Groups: 1,2-Dioxygenated Pattern (1,2-CO), Illogical Nucleophiles, Three-Membered Heterocyclic Rings, Illogical Electrophiles, 1,2-Dihidroxy Pattern, Vicinal Diols, 1,4-Dioxygenated Pattern (1,4-CO), 1,4-Dicarbonyl Compounds, 1,4-Hydroxy Carbonyl Compounds. 1,6-Dicarbonyl Pattern (1,6-CO)

Recommended Texts:]

1. Stuart Warren, Organic synthesis, the disconnection approach, John Wiley & sons, 1992.
2. Vitomir Sunjic, Vesna Petrovik, Organic Chemistry from Retrosynthesis to Asymmetric Synthesis, Springer, 2015
3. Carey FA, Sundberg RJ (2007) Advanced organic chemistry. Part B. Reactions and synthesis, 5th edn. Springer, Berlin
4. Smith JG (2011) Organic chemistry, the Diels-Alder reaction, 3rd edn. McGraw-Hill, New York

Subject: - Analytical Chemistry II

X-ray Diffraction: Principles and applications of powder and single crystal X-ray Diffraction (XRD)

Thermal methods: Principles and application of Thermogravimetry (TG), Differential Thermal Analysis (DTA) and Differential Scanning Calorimetry (DSC)

Surface Science: Adsorption and Desorption isotherms, Particle size analysis (PSA) and Pore size distribution (PSD)

Chromatography: Gas Chromatography (GC) and High Performance Liquid Chromatography (HPLC)

Electron Microscopy: Transmission Electron Microscopy (TEM) and Scanning Electron Microscopy (SEM)

Recommended Texts:

1. Instrumental Methods of Chemical Analysis - H Kaur, Pragati Prakashan
2. Introduction to Thermal Analysis: Techniques and Applications - M.E. Brown, Springer
3. Introduction to instrumental Analysis - R.D. Braun, McGraw Hill.

MASTER OF SCIENCE (CHEMISTRY) – THIRD SEMESTER

Third Semester			
S. No.	Name of Subject	Credits	Total Marks
1	Inorganic Chemistry – III	4	100
2	Organic Chemistry – III	4	100
3	Physical Chemistry – III	4	100
4	Special paper – I (any one) 1. Organometallic Chemistry of Transition Metals 2. Stereochemistry and Photochemistry 3. Electrochemistry	4	100
5	Elective paper (any two) 1. Chemistry Application of Group Theory 2. Medicinal Chemistry 3. Material Chemistry 4. Photoinorganic Chemistry 5. Fuel and Combustion Technology 6. Environmental Chemistry	2 2	100 100
6	Lab - (Special Paper)	2	100
	Total	**22**	

Subject Name: INORGANIC CHEMISTRY - III

Course A: Inorganic Reaction Mechanisms

Mechanisms of substitution reactions of tetrahedral, square planar, trigonal bipyramidal, square pyramidal and octahedral complexes. Potential energy diagrams, transition states and intermediates, isotope effects, Berry's pseudo rotation mechanism, factors affecting the reactivity of square planar complexes, Swain-Scott equation, Trans effect and its application to synthesis of complexes.

Molecular rearrangement processes: Electron transfer reactions (outer and inner sphere) HOMO and LUMO of oxidant and reluctant, chemical activation. Precursor complex formation and rearrangement, nature of bridge ligands , fission of successor complexes, Two-electron transfers, Synthesis of coordination compounds using electron transfer reactions, mixed valence complexes and internal electron transfer.

Course B: Catalysis and Bio-inorganic Chemistry

Transition metal ion catalysts for organic transformations and their application in hydrogenation (using symmetric and chiral organometallic catalysts), isomerization, olefin oxidation, carbonylation and polymerization reactions. Role of metal ions in biological systems. Toxic metal ions and their detoxification, chelation therapy/chelating agents in medicine. Recent advances in cancer chemotherapy using chelates. Biological nitrogen fixation. Natural and synthetic oxygen carriers. Na-K, ATPase or sodium pump. Futuristic aspects of organo transition metal complexes as catalysts and in bio-inorganic chemistry.

Recommended Texts:

1. Katakis, D. & Gordon, G. Mechanism of Inorganic Reactions John Wiley & sons: N.Y.(1987).

2. Langford, H. &.Gray, H. B. Ligand Substitution Processes W. A. Benjamin: N. Y. (1966).

3. Tobe, M & Wadington, F.C.Ed., Inorganic Reaction Mechanisms Thomas Nelson: London (1973).

4. Hughes, M. N. The Inorganic Chemistry of Biological Processes, 2nd Ed., Wiley (1981).

5. Masters, C. Homogeneous Transition Metal Catalysis Chapman & Hall (1981).

Subject Name: ORGANIC CHEMISTRY - III

Course A: Photochemistry & Pericyclic Reactions

Photophysical processes: Jablonskii diagram, energy pooling, exciplexes, excimers, photosensitization, quantum yield, solvent effects. Stern-Volmer plot, delayed fluorescence, etc.

Photochemistry of alkenes: cis-trans isomerizatlon, non-vertical energy transfer; photochemical additions; reactions of 1, 3- , 1, 4- and 1, 5-dienes; dimerizations.

Photochemistry of carbonyl compounds: Norrish type I & II reactions (cyclic and acyclic); α, β-unsaturated ketones; β, γ -unsaturated ketones; cyclohexanones (conjugated); cyclohexadienones (cross-conjugated & conjugated); Paterno-Buchi reactions, photoreductions.

Photochemistry of aromatic compounds: Isomerizations, skeletal isomerizations, Dewar and prismanes in isomerization. Singlet oxygen reactions: Photo Fries rearrangement of ethers and anilides; Barton reaction, Hoffman-Loefller-Freytag reaction.

Pericyclic reactions: Electrocyclic, cycloaddition, sigmatropic and chelotropic reactions: General Orbital Symmetry rules, Frontier Orbital approach, PMO approach, Correlation diagrams for different svstems, Hückel-Mobius approach, General pericyclic selection rule and its applications, 1,3-dipolar additions, Ene reaction.

Course B: Chemistry of Life Processes

Introduction to metabolic processes: Catabolism and anabolism, ATP- currency of biological energy, energy rich and energy poor phosphates, role of NADH, NADPH, $FADH_2$, TPP, coenzyme A, lipoic acid and biotin.

Carbohydrate metabolism: Glycolysis, fate of pyruvate under anaerobic conditions, citric acid cycle, oxidative phosphorylation (electron transport system), gluconeogenesis, C_4 pathway, pentose phosphate pathway and photosynthesis.

Fatty acid metabolism: Even chain and odd chain (saturated and unsaturated) fatty acids, ketone bodies, fatty acid anabolism, calorific values of food.

Protein metabolism and disorders: Degradation of amino acids (C_3, C_4, C_5 family), urea cycle, uric acid and ammonia formation.

Proteins (structure and functions): Primary, secondary, tertiary and quaternary structures. Enzymes, active sites, allosteric sites and mechanisms of their actions, e.g. chymotrypsin, carboxypeptidase, lipases, etc.

Nucleic acids: Chemical and enzymatic hydrolysis, structure and functions of DNA, RNA (m-RNA, t-RNA, r-RNA), an overview of gene expression (replication, transcription and translation), genetic code (origin, Wobble hypothesis and other important features), genetic errors, carcinogenesis and recombinant DNA technology.

Recommended Texts:

1. Carey, F.A. & Sundberg, R. J. Advanced Organic Chemistry, Parts A & B, Plenum: U.S. (2004).

2. Horspool, W. M. Aspects of Organic Photochemistry Academic Press (1976).

3. Lowry, T. H. & Richardson, K. S. Mechanism and Theory in Organic Chemistry Addison-Wesley Educational Publishers, Inc. (1981).

4. March, J. Advanced Organic Chemistry John Wiley & Sons (1 992).

5. Marchand, A. P. & Lehr, R. E. Pericyclic Reactions Academic Press (1977).

6. Stryer, L. Biochemistry 4th Ed., W. H. Freeman & Co. (1995).

7. Sykes. P. A Guidebook to Mechanism in Organic Chemistry 6th Ed., Prentice-Hall (1996)

8. Zubay. S. Biochemistry Addison-Wesley (1983).

Subject Name: PHYSICAL CHEMISTRY - III

Spectroscopic methods: Characterization of electromagnetic radiation. Born-Oppenheimer approximation. Heisenberg's Uncertainty Principle. Basic elements of spectroscopy. Time dependent perturbation. Einstein coefficients. Lambert-Beer's law. Integrated absorption coefficients. Transition dipole moments and general selection rules based on symmetry ideas.

Atomic spectra: Characterization of atomic states. Microstate and spin factoring methods. Hund,s rules. Derivation of spin and orbital selection rules (based on recursion relations of Legendre polynomials). Spectra of complex atoms. Zeeman and Stark effects. Atomic photoelectron spectroscopy.

Introduction to molecular spectroscopy: Rotational spectroscopy of diatomic molecules based on rigid rotator approximation. Determination of bond lengths and/ or atomic masses from microwave data. Effect of isotopic substitution. Non-rigid rotator. Classification of polyatomic molecules. Energy levels and spectra of symmetric top molecules and asymmetric top molecules. First order Stark effect.

Vibrational spectroscopy: Normal coordinate analysis of homonuclear and heteronuclear diatomic molecules. Extension to polyatomic linear molecules. Derivation of selection rules for diatomic molecules based on Harmonic oscillator approximation. Force constants and amplitudes. Anharmonic oscillator. Overtones and combination bands.

Dissociation energies from vibrational data. Vibration-rotation spectra, P, Q and R branches. Breakdown of the Born-Oppenheimer approximation. Nuclear spin effect.

Symmetry of normal coordinates. Use of Group Theory in assignment of spectra and selection rules for simple molecules.

Raman spectroscopy: Stokes and anti-Stokes lines. Polarizability ellipsoids. Rotational and Vibrational Raman spectroscopy. Selection rules. Polarization of Raman lines.

Electronic spectroscopy: Diatomic molecules. Selection rules. Breakdown of selection rules. Franck-Condon factors. Dissociation energies. Photoelectron spectroscopy of diatomic (N_2) and simple polyatomic molecules (H_2O, formaldehyde). Adiabatic and vertical ionization energies. Koopmans' theorem.

Polyatomic molecules. Oscillator strengths. Use of Free Electron Model, HMO theory and Group theory for polyenes and carbonyl compounds (formaldehyde). Qualitative ideas of solvent effects- viscosity, polarity, hydrogen bonding.

Excited states: Deactivation. Jablonskii diagram. Fluorescence and phosphorescence and factors affecting these. Calculation of excited state life-times from absorption data. Quenching of fluorescence, Stern-Volmer equation.

NMR spectroscopy: Larmor precession. Mechanisms of spin-spin and spin-lattice relaxations and quantitative treatment of relaxation. Quantum mechanical treatment of the AB system. Selection rules and relative intensities of lines.

Principles of Mossbauer spectroscopy: Isomer shifts. Quadrupole and Nuclear Zeeman splittings. Applications in structure determination.

Diffraction Methods: Atomic scattering factors. Scattering by a small crystal. Direct and reciprocal lattice. Miller indices. Bragg's law and Laue's equations. Structure factors. Systematic absences for different types of unit cells (primitive, face-centred, body - centred, side-centred) and application to some common metal and metal salt structures (rock salt, zinc blende). Space groups. Glide planes and screw axes. Structure determination for organic crystals like naphthalene. Fourier series.

Patterson's functions. Heavy atom method. Comparison of X-ray method with electron and neutron diffraction methods.

Recommended Texts:

1. Hollas. J. M. Modern Spectroscopy 4th Ed., John Wiley & Sons (2004).

2. Barrow. G. M. Introduction to Molecular Spectroscopy McGraw-Hill (1962).

3. Brand. J. C. D. & Speakman. J. C. Molecular Structure: The Physical Approach 2nd Ed., Edward Arnold: London (1975).

4. Chang. R. Basic Principles of Spectroscopy McGraw-Hill, New York, N.Y. (1970).

5. Moore, W. J. Physical Chemistry 4th Ed., Prentice-Hall (1972)

6. Warren, B. E. X-Ray Diffraction Dover Publications (1990)

7. Bacon, G. E. Fifty Years of Neutron Diffraction Hilger (1987)

Subject Name: ORGANOMETALLIC CHEMISTRY OF TRANSITION METALS

Inorganic π Acid Ligands: Dioxygen and dinitrogen, nitrosyl, tertiary phosphines and arsines as ligands.

Complexes of π donor ligands: Transition metal alkenyls, alkynyls, carbenes and carbines

Complexes of unsaturated molecules: Preparation, bonding and structure of alkene, alkyne, allyl, dienyl and trienyl complexes; reactions with special reference to organic synthesis

Transition metal compounds in catalysis: Hydrogenation, hydroformylation and polymerization; Wacker Process

Transition metal Compounds with M-H bonds: Metal hydrides (classical and nonclassical). Agostic interaction. Application of NMR in studying hydrido complexes

Recommended Texts:

1. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 6th Ed. (1999) John Wiley & Sons, NY.

2. J.E. Huheey, Keiter and Keiter, Inorganic Chemistry,

3. R. H. Crabtree, the Organometallic Chemistry of Transition Metals, John Wiley.

4. Ch. Elschenbroich and A. Salzer, Organometallics, VCH.

5. J.P. Collman, L.S. Hegedus, J.R. Norton and R.G. Finke, Principles and Applications of Organotransition metal Chemistry, Univ. Sci. Books, Mill Valley. California.

Subject Name: STEREOCHEMISTRY AND PHOTOCHEMISTRY

Stereochemistry:

Enantioselcetive synthesis with chiral non racemic reagents and catalysts: Hydroboration with chiral boranes (IPCBH2), (IPC)2BH, Carbonyl group reduction with chiral complex hydride (BINAL-H, Chiral oxazaborolidines), Chiral organometal complex –(-)DAIB; 3-exo-dimethylamino isoborneol. Enantioselective epoxidation of alkene: Sharpless epoxidation, enantioselective hydrogenation with [Rh(DIPAMP)]+. Diastereoselective synthesis:Aldol reactions (Chiral enolate & Achiral Aldehyde and Achiral enolate and chiral aldehyde).

Optical Activity in absence of chiral carbon: Biphenyls and Allenes and Atropisomerism.

Conformation: Conformational analysis of decalines and cyclohexene.

Photochemistry:

(a) Introduction and Basic Principles of Photochemistry: Absorption of light by organic molecules, properties of excited states, mechanism of excited state processes and methods of preparative photochemistry.

(b) Photochemistry of alkenes and related compounds: Isomerization, Di-β-methane rearrangement and cycloadditions.

(c) Photochemistry of aromatic compounds: Ring isomerization and cyclization reactions.

(d) Photochemistry of carbonyl compounds: Norrish type-I cleavage of acyclic, cyclic and α, β unsaturated carbonyl compounds, Norrish type-II cleavage. Hydrogen abstraction: Intramolecular and intermolecular hydrogen abstraction, photoenolization. Photocyclo-addition of ketones with unsaturated compounds: Paterno-Buchi reaction, photodimerisation of α, β unsaturated ketones, rearrangement of enones and dienones, Photo-Fries rearrangement

Rearrangements: Sommelet-Hauser, Favorskii, rearrangements. Hofmann-Loffler-Freytag reaction, Barton reaction and Shapiro reaction.

Recommended Texts:

1. M.B. Smith and J. March, March's Advanced Organic Chemistry-Reactions, Mechanisms and Structure, 5th Edition (2001), John Wiley & Sons, New York.

2. D. Nasipuri, Stereochemistry of Organic Compounds, 2nd Edition (1994), Wiley Eastern Ltd., New Delhi.

3. J. Aube and R. E. Gawley, Principles of Asymmetric Synthesis.

4. E.L. Eliel, S.H. Wilen and L.N. Mander, Stereochemistry of Organic Compounds, Wiley Interscience, New York (2004).

5. Paul de Mayo, Molecular Rearrangements, Vol.I & II, Interscience Publishers, New York (1963).

6. John D. Coyle, Introduction to Organic Photochemistry, John Wiley and Sons, New York (1986).

7. C.H. Depuy and O.L. Chapman, Molecular Reactions and Photochemistry, 2nd Edition (1988), Prentice-Hall of India (P) Ltd., New Delhi.

8. F.A. Carey and R.J. Sundberg, Photochemistry in Advanced Organic Chemistry, Chapter 13, Part A, 3rd Edition (1990), Plenum Press, New York.

9. N. J. Turro, Modern Molecular Photochemistry, University Science Books, Sausalito (1991).

Subject Name: ELECTROCHEMISTRY

Activity coefficient and ionic migration in electrolyte solutions: Quantitative treatment of Debye- Hückel theory of ion-ion interaction and activity coefficient, applicability and limitations of Debye-Hückel limiting law, its modification for finite-sized ions, effect of ionsolvent interaction on activity coefficient. Debye-Hückel-Onsagar (D-H-O) theory of conductance of electrolyte solution, its applicability and limitations. Pair-wise association of ions (Bjerrum and Fuoss treatment), modification of D-H-O theory to account for ion-pair formation, determination of association constant (KA) from conductance data.

Electrical double layer at metal/electrolyte interface: Thermodynamics of double layer, electrocapillary equation, determination of surface excess and other electrical parameter selectrocapillarity, excess charge capacitance, and relative surface excesses. Metal/ water interaction-contact adsorption, its influence on capacity of interface, complete capacitypotential curve, constant capacity region hump. Specific adsorption.

Electrode kinetics: Multistep reactions- a near equilibrium relation between current density and over potential, Concept of rate determining step. Determination of reaction order. Stoichiometric number, and transfer coefficient. Electrocatalysis-comparison of electrocatalytic activity. Importance of hydrogen evolution reaction and its mechanism.

Electrochemical techniques: Impedance technique-its application for studying electrode kinetics and corrosion. Rotating disc electrode (RDE): Application of measurement of electrochemical rate constant.

Recommended Texts:

1. Modern Electrochemistry, Vol. 1 & 2A and 2 B, J.O'M. Bockris and A.K.N. Reddy,Plenum Press, New York (1998).

2. Electrochemical Methods: Fundamentals and Applications; A.J. Bard and L.R. Faulkner, 2nd edition (2001), John Wiley & Sons, New York.

Subject Name: CHEMICAL APPLICATIONS OF GROUP THEORY

Group Theory in Chemistry: Classification of Groups; Matrix representation of symmetry elements and point groups, matrices of C3v and C4v point groups, transformation matrices; Structure of character tables, determination of symmetry species for translations and rotations.

Chemical Applications of Group theory:

IR and Raman Spectroscopy: Brief introduction to molecular vibrations; selection rules for fundamental vibrational transitions, symmetry of normal modes of molecules, Infrared and Raman activity of some typical molecules (molecules of C2v, C3v, C4v, D2h, D3h, D4h, Td and Oh point groups

Crystal Field Theory: Splitting of levels and terms in chemical environment, construction of energy level diagrams, selection rules and polarizations.

Molecular Orbital Theory: Introduction, transformation properties of atomic orbitals; hybridization schemes for bonding, hybrid orbitals as LCAOs; Molecular Orbital Theory for some typical ABn types (n = 2, 3, 4, 6) of molecules (H_2O, NH_3 and BH_3)

Electronic Spectra: General considerations, typical examples from tetrahedral and octahedral systems, Orgel energy level diagrams.

Recommended Texts:

1. F. A. Cotton, Chemical Applications of Group Theory, 3rd Edn. (1999), John Wiley & Sons, New York.

2. G. L. Miessler and D. A. Tarr, Inorganic Chemistry, 2nd Edn. (1999), Prentice Hall International Inc., London.

3. K. Veera Reddy, Symmetry and Spectroscopy of Molecules, New Age International Pvt. Ltd., New Delhi (1999).

Subject Name: MEDICINAL CHEMISTRY

UNIT- I

Introduction to Medicinal Chemistry

Definition, History and development of medicinal chemistry.

Physico-Chemical factors and Biological activity: Introduction; Physicochemical properties in relation to biological action - Ionization, Solubility, Partition Coefficient, Hydrogen bonding, Protein binding, Chelation, Optical and Geometrical isomerism; factors governing ability of drugs to reach active site; dissociation constants; isosterism and bio-isosterism.

Drug metabolism principles, Factors affecting drug metabolism including stereo chemical aspects.

Drug Design: Introduction, procedures followed in development of new drugs design, concepts of lead compound and lead modification, concepts of analogues & prodrugs , structure-activity relationship (SAR).

Combinatorial Chemistry:

Concept and applications of combinatorial chemistry: solid phase and solution phase synthesis.

Brief introduction; classification - chemical and pharmacological; synthesis of selected members; mode of action; relevant SAR of following classes of compounds (Unit II to Unit VI):-

UNIT-II

Non-Steroidal Anti-Inflammatory Drugs (NSAID): Salicylates, Indomethacin, Diclofenac Sodium, Ibuprofen.

UNIT-III

Antibiotics and Anti-infective Drugs:

Antibiotics: Penicillin: penicillin G, Penicillin V, Amoxycillin, Chloramphenicol, Cephalosporin, Tetracycline and Streptomycin.

Local anti-infective drugs: Introduction and general mode of action of Nalidixic Acid derivatives, Quinoloine derivatives.

UNIT-IV

Central Nervous System Depressant:

General anesthetics: Inhalation anesthetics; Intravenous anaesthetics; Basal anesthetics.

Local anesthetics: Esters, amides, Quinoline & Iso-quinoline analogues.

Central Nervous System Stimulants: Xanthine derivatives; Analeptics and miscellaneous CNS stimulants.

UNIT-V

Antineoplastic agents: Alkylating agents; Antimetabolites, Antibiotics

UNIT-VI

Diuretics:

Mercurial Diuretic & Non-mercurial diuretics (Thiazides, Carbonic-anhydrase inhibitors, miscellaneous sulphonamides diuretics).

Books Recommended:

1. An Introduction to Medicinal Chemistry, Graham L. Patrick.
2. Medicinal Chemistry: Principles and Practice Edited by F.D. King.
3. Textbook of Organic Medicinal and Pharmaceutical Chemistry, Edited by Charles O. Wilson, Ole Gisvold, Robert F. Doerge.
4. Introduction to Medicinal Chemistry, Alex Gringuage.
5. Principles of Medicinal Chemistry, William O. Foye, Thomas L. Lemice and David A. Williams.
6. Introduction to Drug Design, S.S. Pandeya and J. R. Dimmock, New Age International.
7. Burger's Medicinal Chemistry and Drug Discovery, Vol-1to VI, Ed. M.E. Wolff, John Wiley.
8. Goodman and Gilman's Pharmacological Basis of Therapeutics, Mc Graw-Hill.
9. The Organic Chemistry of Drug Design and Drug Action, R.B. Silverman, Academic Press.
10. Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley.

Su

bject Name: MATERIALS CHEMISTRY

Introduction: Materials and their classification, inorganic and organic materials.

Inorganic materials: Design and synthesis of inorganic materials, requirements and constraints, combination properties of composites, functional materials, active materials; solid state reactions for synthesis of inorganic materials: ceramic methods, precursor method and sol-gel synthesis, physical and chemical vapour depositions; carbides, nitrides, structural and functional ceramics, intermetallics; intrinsic and extrinsic properties: electrical, optical and magnetic properties; ceramic superconductors, magnetic ceramics.

Organic materials: Molecular electronics: molecular materials for electronics and molecular scale electronics: Molecular properties, molecular arrangement and molecular interactions, piezoelectric and pyroelectric organic materials; molecular magnets based on transition metal complexes and organic ferromagnets, organic non-linear optical materials: photochromic organic materials and their classes; conducting polymers: polyacetylene, polypyrrole, polyaniline and polythiophene; conductive change transfer materials: TTFTCNQ, metal–dithiolate systems, fullerenes. Langmuir-Blodgett films, molecular electronic logic and architectures.

Nanomaterials:

Recommended Texts:

1. P.J. Vander Put, Inorganic Chemistry of Materials, Plenum Press, New York, 1998.

2. M.C. Petty, M.R. Bryce and D. Bloor, Editors An Introduction to Molecular Electronics, Edward Arnold, London 1995

Subject Name: PHOTOINORGANIC CHEMISTRY

Photochemistry of Transition Metal Complexes: Photoreactions of complexes of Cr(III) and Co(III), photo-aquation, photo-substitution and photo-racemization Photochemistry of Ru(bpy)32+ and its application as photocatalyst for photo-splitting of water, photooxidation of 2-propanol and photo-reduction of carbon dioxide, cyanide bridged triruthenium(II) bipy complexes as antenna. Photochemistry of diisocyanide bridged diimers of Rh(I). Applications of quenching and sensitization techniques in the identification of reactive state in coordination complexes. Photochemistry of Transition Metal Carbonyls and Europium complexes.

Recommended Texts:

1. D. M. Roundhill, Photochemistry and Photophysics of Metal Complexes, Plenum Press, New York and London (1994).

2. G. J. Ferraudi, Elements of Inorganic Photochemistry, John Wiley & Sons (1988).

3. V. Balzani and V. Carassiti, Photochemistry of Coordination Compounds, Academic Press, London (1970).

4. O. Horvath and K.L. Stevenson, Charge Transfer Photochemistry of Coordination Complexes, VCH Publishers Inc. (1993)

Subject Name: FUEL AND COMBUSTION TECHNOLOGY

Introduction: History of solid, liquid and gaseous fuels, Production, present scenario and consumption pattern of fuels, Fundamental definitions, properties and various measurements techniques.

Solid Fossil Fuel (Coal): Coal classification, composition and basis, Coal mining, Coal preparation and washing, Combustion of coal and coke making, Coal liquefaction, Coal gasification

Liquid Fossil Fuel (Petroleum): Exploration of crude petroleum, Evaluation of crude, Distillation: Atmospheric distillation and Vacuum distillation, Secondary processing: (a) Cracking, Thermal cracking, Visbreaking, Coking, Catalytic cracking (b) Reforming of naphtha (c) Hydrotreatment, dewaxing and deasphalting, Refinery equipments, Petroleum refining techniques, Desulfurization of petroleum fuels.

Gaseous Fuels: Natural gas and LPG, Producer gas, Water gas, Hydrogen, Acetylene, Other fuel gases

Combustion Technology: Fundamentals of thermochemistry, Combustion air calculation, Calculation of calorific value of fuels, Adiabatic flame temperature calculation, Mechanism and kinetics of combustion, Flame properties, Combustion burners, Combustion furnaces, Internal combustion engines

Recommended Texts:

1. Fuels and Combustion, Samir Sarkar, 3rd. ed Universities Press.

2. Modern Petroleum Refining Processes, B.K. Bhaskar Rao, 4th ed., Oxford & IBH Publishing Co. Pvt. Ltd.

3. Modern Petroleum Technology, Vol 1, Upstream, Ed. by Richard A. Dave, IP, 6th ed., John Wiley & Sons. Ltd.

4. Modern Petroleum Technology, Vol 2, Downstream, Ed. by Alan G. Lucas, IP, 6th ed., John Wiley & Sons. Ltd.

5. Combustion, Irvin Glassman, 2nd ed., Academic Press.

6. Fuels Combustion and Furnaces, John Griswold, Mc-Graw Hill Book Company Inc.

7. Petroleum Refinery Engineering, W.L. Nelson, 4th ed. Mc-Graw Hill Book Company.

Subject Name: ENVIRONMENTAL CHEMISTRY

Introduction to Environmental Chemistry: Concept and scope of environmental chemistry, Environmental terminology and nomenclatures, Environmental segments, The natural cycles of environment (Hydrological, Oxygen, Nitrogen)

Atmosphere: Regions of the atmosphere, Reactions in atmospheric chemistry, Earth's radiation balance, Particles, ion and radicals in atmosphere; Chemistry of ozone layer.

Hydrosphere: Complexation in natural water and waste-water, Micro-organisms in aquatic chemical reactions, Eutrophication, Microbiology mediated redox reactions.

Lithosphere: Inorganic and organic components in soil, acid-base and ion-exchange reactions in soil, micro and macro nutrients, nitrogen pathways and NPK in soil.

Chemical Toxicology: Toxic chemicals in the environments, Impact of toxic chemicals on enzymes, Biochemical effects of arsenic, cadmium, lead, mercury, carbon monoxide, nitrogen oxides, sulphur oxides.

Air Pollution: Particulates, Aerosols, SOx, NOx, COx and hydrocarbon, Photochemical smog, Air-quality standards

Water Pollution: Water-quality parameters and standards: physical and chemical parameters, Dissolved oxygen, BOD, COD, Total organic carbon, Total nitrogen, Total sulfur, Total phosphorus and Chlorine, Chemical speciation (Pb, As, Hg)

Recommended Texts:

1. G.W. Vanloon, S.J. Duffer, Environmental Chemistry - A Global Perspective, Oxford University Press (2000).

2. F.W. Fifield and W.P.J. Hairens, Environmental Analytical Chemistry, 2nd Edition (2000), Black Well Science Ltd.

3. Colin Baird, Environmental Chemistry, W.H. Freeman and Company, New York (1995).

4. A.K. De, Environmental Chemistry, 4th Edition (2000), New Age International Private Ltd.,New Delhi.

5. Peter O. Warner, Analysis of Air Pollutants, 1st Edition (1996), John Wiley, New York.

6. S.M. Khopkar, Environmental Pollution Analysis, 1st Edition (1993), Wiley Estern Ltd., New Delhi.

7. S.K. Banerji, Environmental Chemistry, 1st Edition (1993), Prentice-Hall of India, New Delhi.

Subject Name: PRACTICAL CHEMISTRY SPECIAL PAPER

INORGANIC CHEMISTRY

1. (a) Synthesis and structural characterization (IR, electronic spectra and magnetic susceptibility) of $[Ni(py)_4(NCS)_2]$.

(b) Synthesis of a series of Ni(II) complexes (with ligands of varying ligand field strength), electronic spectral interpretation and calculation of various ligand-field parameters.

2. Synthesis and structural characterization (IR, Electronic spectra) of the cis- and transisomers of $[Co(en)_2Cl_2]$

3. Synthesis and characterization (IR and PMR & CMR) of $[Al(acac)_3]$

4. Synthesis, purification by sublimation and structural characterization (IR and electronic spectra) of ferrocene.

5. Acetylation of ferrocene and separation of the acetyl derivative by column chromatography.

ORGANIC CHEMISTRY

1. Separation and identification of organic mixtures containing up to three components.

2. Preparation of organic compounds involving several stages, characterization of intermediates and final products by IR and NMR spectroscopy.

3. Techniques of organic chemistry: Special practical's involving steam distillation, photo-isomerization and thin layer chromatography etc.

4. Quantitative analysis of (i) sulphur and (ii) nitrogen.

PHYSICAL CHEMISTRY

1. Kinetics of decomposition of benzene diazonium chloride.

2. Conductometric study of the kinetics of saponification of ethyl acetate.

3. Determination of transport numbers of Cu^{2+} and SO_4^{2-} by Hittorf's method.

4. Conductometric titration of triple mixture ($HCl+NH_4Cl+KCl$) with (i) NaOH and (ii) $AgNO_3$.

5. Analysis of halide mixture by differential potentiometry.

6. Conductometric titration of a polybasic acid.

7. Verification of the Nernst law of electrode potential.

8. Determination of band-gap of a semiconductor.

9. Ternary phase diagram of water, benzene, and acetic acid.

10. Determination of molecular weight of a macromolecule by viscometry.

11. Half-life periods of a source containing two radionuclides.

12. Electrochemical Impedance study of metal/solution interface.

13. Cyclic Voltammetry of the $[Fe(CN)_6]^{3-}/[Fe(CN)_6]^{4-}$ system.

Subject Name: SUMMER TRAINING

Summer training at any Industry/ National Laboratory/ University/ Institution

MASTER OF SCIENCE (CHEMISTRY) – FOURTH SEMESTER

Fourth Semester			
S. No.	Name of Subject	Credits	Total Marks
1	Computers in Chemistry	2	100
2	Special paper – II(any one) 1. Bio-Inorganic Chemistry 2. Chemistry of Natural Products 3. Quantum Chemistry	4	100
3	Special paper – III(any one) 1. Structural Methods in Inorganic Chemistry 2. Application of Spectroscopy to Structural Analysis 3. Statistical Mechanics	4	100
4	Special paper – IV(any one) 1. Inorganic Rings, Chains, and Clusters 2. Reagents and Organic Synthesis 3. Chemical Kinetics	4	100
5	Project + Training	8	100
	Total	**22**	

Subject Name: COMPUTERS IN CHEMISTRY

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mputer programming in FORTRAN.

Computer application in Chemistry: Development of small computer codes involving simple formulae in chemistry, such as van der Waals equation, pH titration, kinetics, radioactive decay. Evaluation of lattice energy and ionic radii from experimental data. Linear simultaneous equations to solve secular equations within the Hückel theory. Elementary structural features such as bond lengths, bond angles, dihedral angles etc., of molecules extracted from a database such as Cambridge database.

Use of computer programmes: Execution of linear regression, X-Y plot, numerical integration and differentiation as well as differential equation solution programmes. Monte Carlo and Molecular dynamics. Programmes with data preferably from physical chemistry laboratory.

Representation of molecules: Cartesian and Internal Assesment Coordinates; Geometry Optimization (Newton-Raphson), vibrational frequencies; ionization potential and electron affinities of molecules. BO

approximation, potential energy surface, SCF theory, Gaussian basis sets, Basic idea of Molecular Mechanics and force field; Molecular dynamics: basic concept, Verlet and Velocity-Verlat algorithm; Basic ideas of structure–activity relationship. Introduction to popular softwares (like Gaussian, GAMESS, MOPAC).

Recommended Texts:

1. Computational Chemistry by A. C. Norris, John Wiley

2. Numerical Recipes in FORTRAN/C by W. H. Press, S. A. Teukolsky, W. T. Vetterling and B. P. Flannery, Cambridge University Press, 2nd Ed. 1996.

3. Fortran 77 and Numerical Methods by C. Xavier, New Age International, 2002.

4. Introduction to Computational Chemistry by Frank Jensen

5. Essentials of Computational Chemistry: Theories and Models by C. J. Cramer

6. Molecular Modeling: Principles and Applications by A. R. Leach, 2nd Ed. Pearson Education: England, 2001

7. Computational Chemistry Workbook by T. Heine, J-O. Joswig and A. Gelessus

Subject Name: INORGANIC CHEMISTRY SPECIALIZATION: - BIO-INORGANIC CHEMISTRY

Role of alkaline earth metal ions in biological systems: (i) Catalysis of phosphate transfer by Mg^{2+} ion, (ii) Ubiquitous regulatory role of Ca^{2+} in muscle contraction

Iron, copper and molybdenum proteins with reference to their oxygenation and oxidase activity: (i) Anti-oxidative functions: cytochrome P-450, catalases and peroxidases, (ii) Nitrate and nitrite reduction: NO_3 and NO_2 reductase, (iii) Electron transfer: cytochromes; blue copper proteins and iron-sulfur proteins and their Synthetic models, (iv) molybdo-enzymes – molybdenum cofactors: molybdenum-protien Complexes, (v) Nitrogen fixation through metal complexation, nitrogenase, (vi) Photosynthesis (PS-I and PS-II).

Metalloenzymes: Urease, Hydrogenase, and Cyanocobalamine

Interaction of metal complexes with DNA: DNA probe and chemotherapeutic agents

Iron storage and transport proteins: Ferritin, Transferritin and Hemosiderin

Recommended

Tex

ts:

1. M. N. Hughes, *Inorganic Chemistry of Biological Processes*, 2nd Ed.(1981), John-Wiley & Sons, New York.

2. W. Kaim and B. Schwederski, *Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, An Introduction and Guide*, Wiley, New York (1995).

3. S. J. Lippard and J. M. Berg, *Principles of Bioinorganic Chemistry*, University Science Books, (1994).

4. I. Bertini, H. B. Grey, S. J. Lippard and J. S. Valentine, *Bioinorganic Chemistry*, Viva Books Pvt. Ltd., New Delhi (1998)

Subject Name: ORGANIC CHEMISTRY SPECIALIZATION: - Chemistry of natural products

Steroids:

Introduction, Occurrence, nomenclature, basic skeleton, spectral properties, Stereochemistry, isolation, synthesis, structure determination, reactions & Biosynthesis of steroids.
Bile acids, steroid hormones and corticosteroids.

Haemoglobin, chlorophyll and phthalocyanines:

Introduction, degradation products of Haemoglobin; spectral properties and synthesis of porphyrins.

Chlorophyll: introduction, structure, degradation products of chlorophyll.

Phthalocyanines: Introduction, preparation & structure of phthalocyanines.

Vitamins: Introduction to vitamin B complex, vitamin B1,B2,B12,Pantothenic acid, Folic acid, Biotins, Pyridoxine.
Vitamin E and K group.

Carotenoids:
Introduction; Geometrical isomerism, Characterization and biosynthesis of carotenoids.
Anthocyanins:

Recommended Texts:

1. Nitya Anand, J.S. Bindra and S. Ranganathan, *Art in organic synthesis*,2nd ed.(1970),Holden Day,San Francisco.
2. S .W .Pelletier, *Chemistry of Alkaloids*, Van Nostrand Reinhold Co. New York (1970).
3. I.L. Finar,*Organic Chemistry*,Vol.II,5th ed.(1975),Reprinted in 1996,ELBS and Longman Ltd, New Delhi.
4. J.W.Apsimon, *Total synthesis of Natural Products* ,Vol. 1-6,Wiely-Interscience Publications,New York,(Vol. 1, 1973).
5. J.S.Bindra and R. Bindra, *Creativity in Organic synthesis,* Academic Press,NY(1975).

Subject Name: PHYSICAL CHEMISTRY SPECIALIZATION: - QUANTUM CHEMISTRY

Fundamentals: Review of classical mechanics, general formulation of quantum mechanics, review of angular momentum, harmonic oscillator problem.

Approximation methods: Stationary perturbation theory for non-degenerate and degenerate systems with examples, time-dependent perturbation theory, radiative transitions, Einstein coefficients.

Many Electron atoms: Electron correlation, addition of angular momenta, Clebesch Gordan series, total angular momentum and spin-orbit interaction.

Group Theory: Review and applications**.**

Ab initio methods for closed shell systems: Review of molecular structure calculations, Hartree-Fock SCF method for molecules, Roothaan-Hartree-Fock method, selection of basis sets. Density functional method: energy as a functional of charge density, Kohn-Sham equations.

Recommended Texts:

1. *Molecular Quantum Mechanics,* P.W. Atkins and R.S. Friedman, 3rd edition (1997), Oxford University Press. Oxford.
2. *Quantum Chemistry,* H. Eyring, J. Walter and G.E. Kimball, (1944) John Wiley, New York.
3. *Quantum Chemistry*, I.N. Levine, 5th edition (2000), Pearson Educ., Inc., New Delhi.

4. Modern Quantum Chemistry: Introduction to Advanced Electronic Structure, A. Szabo and N. S. Ostlund, (1982), Dover, New York.

Subject Name: INORGANIC CHEMISTRY SPECIALIZATION: - STRUCTURAL METHODS IN INORGANIC CHEMISTRY

NMR Spectroscopy: (i) Use of Chemical shifts and spin-spin couplings for structural determination, (ii) Double resonance, and Dynamic processes in NMR, (iii) Decoupling phenomenon, Nuclear Overhauser Effect, DEPT spectra and structural applications in 13C NMR, (iv) Use of Chemicals as NMR auxiliary reagents (shift reagents and relaxation reagents) (v) 1H NMR of paramagnetic substances. (vi) NMR of Metal nuclei.

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

Vibrational Spectroscopy: Applications of vibrational spectroscopy in investigating the stretching and bending modes of molecules (AB3 and AB4 types).

Recommended Texts:

1. E. A. V. Ebsworth, D. W. H. Rankin and S. Cradock, *Structural Methods in Inorganic Chemistry*, 1st Edn.(1987), Blackwell Scientific Publications, Oxford, London.
2. R. S. Drago, *Physical Methods in Chemistry*, International Edition (1992), Affiliated East West Press, New Delhi.
3. R. S. Drago, *Physical Methods in Inorganic Chemistry*, 1st Edn.(1971), Affiliated East West Press, New Delhi.
4. K. Nakamoto, *Infrared and Raman Spectra of Inorganic and Coordination Compounds*, 4th Edn. (1986), John Wiley & Sons, New York.
5. W. Kemp, *Organic Spectroscopy*, 3rd Edn. (1991), Macmillan, London.
6. G. Aruldhas, *Molecular Structure and spectroscopy*, Prentice Hall of India Pvt. Ltd., New Delhi (2001).

Subject Name: ORGANIC CHEMISTRY SPECIALIZATION: - APPLICATION OF SPECTROSCOPY TO STRUCTURAL ANALYSIS

PMR Spectroscopy: Interpretation of spectra, chemical shift, shielding mechanism and anisotropic effects, chemical exchange and chemical shifts in chiral molecules. Spin-spin, spin-lattice relaxations, Spin-spin interactions, naming spin systems, magnitude of coupling constant: Germinal, vicinal and long range couplings. Simplification of Complicated Spectra: Aromatic induced shifts spin decoupling, deuterium exchange, spectra at higher fields. Hindered rotation and rate processes. Nuclear Overhauser effect.

CMR Spectroscopy: General considerations, chemical shift, calculation of approximate chemical shift values, coupling constants. Interpretation of simple CMR spectra. DEPT spectrum. 2 DNMR: COSY, NOESY and HETCOR.

Mass Spectrometry: Introduction, ion production, fragmentation, single and multiple bond cleavage, rearrangements, cleavage associated with common functional groups, molecular ion peak, metastable ion peak, Nitrogen rule and interpretation of mass spectra

Problems: Structure elucidation based on spectroscopic data (IR, UV, NMR and Mass).

Recommended Texts:

1. J. R. Dyer, *Application of Absorption Spectroscopy of Organic Compounds,* Prentice Hall, New Delhi (1978).
2. R.M. Silverstein and F.X. Webster, *Spectroscopic Identification of Organic Compounds*, 6th Edition (2003) John Wiley, New York.
3. D.H. Williams and I.F. Fleming, *Spectroscopic Methods in Organic Chemistry*, 4th Edition(1988), Tata-McGraw Hill, New Delhi.
4. P.Y Bruice, *Organic Chemistry*, 2nd Edition (1998) Prentice – Hall, New Delhi.

Subject Name: PHYSICAL CHEMISTRY SPECIALIZATION: - STATISTICAL MECHANICS

Basic statistical mechanics: Phase space, equal a priori probability, ensemble (canonical, micro-canonical and grand canonical), Liouville theorem, entropy, Gibbs paradox.

Partition function: Rotational, vibrational, translational, electronic and nuclear partition functions, application of partition functions to specific heat of solids and chemical equilibrium.

Bose-Einstein and Fermi-Dirac distributions: Einstein condensation, thermodynamic properties of ideal BE gas, degenerate Fermi gas, application of FD statistics to electron gas in metals.

Fluctuations: Means square deviation and fluctuations in ensembles, concentration fluctuations in quantum statistics.

Recommended Texts:

1. Statistical Mechanics (1988), B.K. Agarwal and M. Eisner, Wiley Eastern, New Delhi
2. Statistical Mechanics (2000), D.A. Mcquarrie, California University Science Books
3. Statistical Mechanics (1996), R. K. Patharia, Butterworth, Heinemann, Elsevier
4. Statistical Mechanics (1962), N. Davidson, Mc Graw Hill Book Co. New York

Subject Name: INORGANIC CHEMISTRY SPECIALIZATION: - INORGANIC RINGS, CHAINS, AND CLUSTERS

Clusters and element-element bonds: Polyhedral boranes: Electron deficiency *vs* sufficiency. Types and IUPAC nomenclature. Wade's polyhedral skeleton electron pair theory (PSEPT). W. N. Lipscomb's styx rules and semi-topological structures of boranes. Equivalent and resonance structures. Wade's vs Lipscomb's methods of studying higher boranes.

Heteroboranes: Types of heteroboranes with special reference to carboranes, structure, bonding and IUPAC nomenclature. Metallaboranes, Metallacarboranes, metal σ and μ bonded borane/carborane clusters. Resemblance of Metallaboranes/ Metallacarboranes with ferrocene and related compounds. Applications of Metallaboranes / Metallacarboranes as drug delivery system. Applications of PSEPT over heteroboranes.

Principle of Isolobility: Development and formulation of the concept of isolobility and its applications in the understanding of structure and bonding of heteroboranes.

Metal Clusters: Metal-metal bonds. Concept of quadrupolar bond and its comparison with a C-C bond; Types of metal clusters and multiplicity of M-M bonds. Simple and condensed metal carbonyl clusters. Applications of PSEPT and Wade's-Mingo's and Lauhr's rule over metalcarbonyl clusters. Metal halide and metal chalcogenide clusters: Bloomington schuffle in dinuclear tungsten clusters.

Heteropoly and Isopoly acids: Structural principles and their applications.

Inorganic Polymers: Classification, Types of Inorganic Polymerization, Comparison with organic polymers, Boron-oxygen and boron-nitrogen polymers, silicones, coordination polymers, sulphur-nitrogen, sulphur-nitrogen-fluorine compounds, - binary and multicomponent systems, haemolytic inorganic systems.

Recommended Texts:

1. F. A. Cotton and G. Wilkinson, *Advanced Inorganic Chemistry*, 6th Edn. (1999), JohnWiley & Sons, New York.
2. James E. Huheey, *Inorganic Chemistry*, 4th Edn. (1993), Addison Wesley Pub. Co., New York
3. N. N. Greenwood and A. Earnshaw, *Chemistry of the Elements*, 2nd Edn. (1997), Butterworth Heinemann, London.

Subject Name: ORGANIC CHEMISTRY SPECIALIZATION: - REAGENTS AND ORGANIC SYNTHESIS

Oxidation : (i) Oxidation with peracids: Oxidation of carbon-carbon double bonds carbonyl compounds, allylic carbon-hydrogen bonds, (ii) Oxidation with selenium dioxide and Osmium tetraoxide, (iii) Oxidation with lead tetraacetate, mercuric acetate (iv) hypervalent iodine

Reagents and Reactions: (i) Gilman's reagent – Lithium dimethylcuprate, (ii) Lithium diisopropylamide (LDA), (iii) Dicyclohexyl carbodiimide (DDC), (iv) 1,3-Dithiane (Umpolung reagent), (v) Peterson's synthesis, (vi) Baker's yeast, (vii) DDQ, (viii) Palladium catalysed reactions, (ix) Woodward and Prevost hydroxylation, (x) Iodotrimethyl silane and (xi) Ionic liquids

Recommended Texts:

1. H.O. House, *Modern Synthetic Reactions*, 2nd Edition (1972), Benjamin/Cummings Publishing Company, California.

2. L.F. Fieser and M. Fieser, *Reagents for Organic Synthesis,* Vol. 1-16 (Vol. 1, 1967), WileyInterscience, New York.

3. M.B. Smith and J. March, *March's Advanced Organic Chemistry – Reactions, Mechanisms & Structure*, 5th ed. (2001), Wiley-Interscience, New York.

4. M. B. Smith, *Organic Synthesis,* McGraw Hill Inc., New York (1995).

5. J. Clayden, N. Greeves, S. Warren, and E. Wothers, *Organic Chemistry,* Oxford Univ. Press, Oxford (2001).
6. P. R. Jenkins, *Organometallic Reagents in Synthesis,* Oxford science Publ., Oxford (1992).

Subject Name: PHYSICAL CHEMISTRY SPECIALIZATION: - CHEMICAL KINETICS

Transition state theory: Application of statistical mechanics to transition state theory, comparison of transition state theory with experimental results, thermodynamic treatment of TST, theories of unimolecular reactions - treatments of: Lindmann, Hinshelwood, Rice Ramsperger- Kassel (RRK), and Rice-Ramsperger-Kassel-Marcus (RRKM).

Reactions in solution: Reaction between ions, effect of solvent (single & double sphere models), interpretation of frequency factor and entropy of activation, influence of ionic strength, salt effect, reactions involving dipoles, influence of pressure on reaction rates in solution.

Molecular collisions: Intermolecular potential and centrifugal barrier, impact parameter, collision cross section and rate, energy threshold, opacity function and reaction cross section.

Experimental probes of reactive collisions: IR chemiluminescence, laser-induced fluorescence. Features of potential energy surfaces (PES), enhancement of reaction.

Molecular beams: Stripping and rebound mechanism.

Dynamics with femtosecond laser techniques: Detection of activated complex.

Recommended Texts:

1. *Reaction Kinetics* (1998), M. J. Pilling and A.P.W, Seakins, Oxford Science Publication, New York
2. *Chemical Kinetics*, 3rd Edition (1967), K.J. Laidler, Harper & Row Publishers, New York.
3. *Kinetics and Mechanism of Chemical Transformation*, Ist Edition (1993), J. Rajaram and J.C. Kuriacose, MacMillan India Ltd., New Delhi.
4. *Modern Liquid Phase Kinetics* (1994), B. G. Cox, Oxford University Press, Oxford.
5. *Molecular Reaction Dynamics and Chemical Reactivity* (1987), R. D. Levine and R. B. Bernstein, Oxford University Press, Oxford.