Here is the chemistry syllabus and the list of recommended books. The books recommended by me are marked in bold.

With lots of love and care

Ved Scientist

C 101 **Chemistry - I**

Structure and Bonding

Nature of bonding in aliphatic, alicyclic, aromatic and heterocyclic compounds. Aromaticity in benzenoid and non-benzenoid compounds. Dipole moment. Resonance. Inductive and Field effects, Hyperconjugation, Steric inhibition of resonance. Structural effects on acidity and basicity. (9)

Stereochemistry

Conformational analysis of acyclic and cyclohexane systems, decalins and monosaccharides, Anomeric effect. E and Z nomenclature. Introduction of terminologies such as erythro, threo, □.□, exo, endo, epimers.

Optical isomerism with one and two chiral centres. Fischer, Newmann, Saw-horse projection formulae. Optical isomerism in compounds without an asymmetric atom. Racemic modifications. Importance of chirality in drug synthesis and bioactivity. Introduction to asymmetric synthesis. (12)

Reactive Intermediates

Introduction to structure, formation, stability and reactions of carbocations, carbanions, free radicals, radical anions, radical cations, arynes, carbenes and nitrenes. (9)

Substitution and Elimination Reactions

Electrophilic aromatic substitution. Nucleophilic aliphatic substitutions: S_N1, S_N2, S_Ni reactions. Neighbouring group participation. Nucleophilic aromatic substitution. Free radical substitutions (both aliphatic and aromatic).

Eliminations: E1, E2, E1CB reactions; Elimination vs. Substitution. (12)

Recommended Books (Text)

1. **Advanced Organic Chemistry: Reactions, Mechanisms and Structure, J. March, Wiley Interscience, 2007.**
2. **Organic Chemistry, T.W.G. Solomons and C.B. Fryhle, John Wiley, 8th Edn., 2007.**
3. **Organic Chemistry, R. J. Morrison and R. N. Boyd, 6th Edn., Pearson, 2007.**
4. **A Guidebook to Mechanism in Organic Chemistry, P. A. Sykes, Longman Scientific, 1986.**
5. **Stereochemistry of Carbon Compounds, E. L. Eliel, Tata McGraw Hill, 2007. (books by D. Nasipuri or by Subrata Sen Gupta are also good.)**
6. Reactive Intermediates, C. J. Moody and G.H. Whitham, Oxford Science Publications, 2002.

7. Organic Chemistry, J. Clayden, N. Greeves, S. Warren and P. Wothers,
Oxford Univ. Press, 2008.

CL 101 **Chemistry Laboratory**

(1) Element detection and characterization of organic compounds.

(2) Crystallisation :

Activity –I :Purification of known compounds by appropriate solvent (One known compound + number of different solvents).

Activity II: Purification of unknown solid by appropriate solvents.

Activity III : Separation of 2 component mixture and purification of impure compounds by appropriate solvents.

(3) TLC

Activity I: Selection of solvent for TLC (known compound/unknown compound).

Activity II : Separation of compounds using TLC (e.g. o- and p- nitroaniline separation using appropriate solvent system-Diethyl ether; hexane (10:90, 20:80 and 30:70).

Activity III: Separation of components present in Turmeric powder extract (alcohol) or spinach extract using TLC and column chromatography (silica columns at microscale level can be prepared or 10 mL syringe can be used).

(4) Distillation

Separation of a binary mixture by distillation.

Determination of Melting Point.

(5) Organic Synthesis

(a) Preparation of 2-iodobenzoic acid or preparation of methyl orange (involving diazotization).

(b) Synthesis of dibenzalacetone (Aldol condensation)- identification of product by TLC (and Melting point)

(c) Isolation of eugenol from clove oil and identification of functional group present (functional group through qualitative test).

(This can be extended to experiments such as distillation of clove oil from cloves, and then separation of eugenol from clove oil).

(6) Sugar hydrolysis using polarimeter.

As a part of the laboratory work, the following activities will also be included : Use of chemical data base (from Merck or CRC Handbook); use of ISIS/Chemdraw or any other software for drawing structures and indicating mechanisms; use of models for drawing various projections.

Recommended 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.

C 201 **Chemistry - II**

Thermodynamics

Laws of thermodynamics; Thermochemistry; Joule-Thompson Effect; entropy, Helmholtz and Gibbs free energies, Maxwell Relations, partial molar quantities, chemical potential, Gibbs-Duhem equation.

Phase equilibria: Thermodynamic treatment of multi-component systems. The ideal solution, vapour-liquid equilibrium, Raoult's law, Henry's law, colligative properties.

Atomic and molecular systems at finite temperatures (Maxwell-Boltzmann statistics), Connection between microscopic and macroscopic properties (E, heat capacity). (10)

Equilibrium constant and its relation with free energy changes, variation of chemical equilibrium constant with temperature and pressure, vant' Hoff equation, applications of Gibbs-Helmholtz equation. (5)

Electrochemistry

Arrhenius theory of electrolytic dissociation; Conductance of electrolytes in solution; Ionic conductance, transference number, applications of conductance measurements.

Chemical Cells and Electromotive Force: Types of Electrodes and electrode reactions, Electrode potential, Standard Electrode potentials, Electrochemical cells, EMF and chemical cell reactions, Free energy, enthalpy and entropy changes of cell reactions; Concentration cells with and without liquid junction, liquid junction potential, salt bridges, applications of EMF measurements: equilibrium constants and associated thermodynamic parameters. (10)

Chemical Kinetics

Rate laws for first, second and third order reactions, reversible, parallel and consecutive reactions, steady state approximation, temperature dependence of the rates of chemical reactions, Collision theory, qualitative concepts of transition state theory, enzyme kinetics (Michaelis-Menten equation), unimolecular reactions, an introduction to fast reactions. (9)

Atoms and molecules

Atomic structure, concept of atomic orbitals and wave functions, many electron atoms, spin and Pauli principle. Bonding in homo and heteronuclear diatomic molecules; ionic character, dipole moments, molecular polarizability. (6)

Recommended Books (Text)

1. **Physical Chemistry, I. Levine, Tata McGraw Hill, 5th Edn., 2007.**
2. **Physical Chemistry : A Molecular Approach, D. A. McQuarrie and J. D.**
3. **Simon, University Science Books, 1997.**
4. **Physical Chemistry, G. M. Barrow, McGraw Hill, 5th Edn., 2007.**
5. **Chemical Kinetics, K.J. Laidler, 3rd Edn., Harper and Row, 1987.**

Reference

6. Physical Chemistry, R. S. Berry, S. A. Rice and J. Ross, Oxford Univ. Press, 2nd Edn., 2000.
7. General Chemistry, D. A. McQuarrie and P. A. Rock, W. H. Freeman & Co., 3rd Edn., 1991.
8. Physical Chemistry, R. J. Silby and R. A. Alberty, Wiley, New York, 3rd Edn., 2000.
9. Chemical Kinetics: A Study of Reaction Rates in Solution, K. A.
10. Connors, VCH Publications, 1990.

CL- 201 Chemistry Laboratory

1. Determination of Critical Solution Temperature (CST) of Phenol-Water system. Study the effect of added impurity (NaCl) on CST.
2. Determine the solubility of oxalic acid (benzoic acid) in water at different temperatures. Calculate the heat of solubilization (ΔH).
3. Determine the distribution coefficient of I2 between water and an immiscible organic solvent (Benzene, CHCl3), and determination of the equilibrium constant for the reaction : $I_2 + I^- \rightleftarrows I_3^-$ using partition method.

4. (i) Standardise the pH meter. (ii) Titrate a solution of strong acid against a strong base using the pH meter.

5. Estimate carbonate and bicarbonate in the supplied mixture by pH titration.
6. Determine the standard redox potential of Cu^{2+}/Cu (Zn^{2+}/Zn) in aqueous medium at 25oC .

7. Estimate Fe2+ concentration in the supplied solution by potentiometric titration using standard K2Cr2O7 solution.
8. (i) Calibrate the conductometer by using standard KCl solution.
   (ii) Titrate a solution of a strong acid; weak acid; and a mixture of the two acids, conductometrically, against a standard alkali.
9. Determine the dissociation constant of acetic acid.
10. Determine the solubility product of PbCrO4 (BaSO4).
11. Verify the relationship : $\Lambda = \Lambda 0 - S\ C1/2$ for strong uni-univalent electrolyte.
12. Study the kinetics of acid catalysed hydrolysis of methyl acetate in the presence of HCl and H2SO4. Determine the order with respect to [acid], and compare the strengths of the two acids.

C 301 Basic Inorganic Chemistry

Peridocity, Molecular Structure and Bonding, Chemical Forces

Peridoic Table, Perodicity, Trends and anomalies, Relativistic effects; A review of Lewis Structures including formal charges; VSEPR model; Molecular symmetry, point groups and introduction to Character Tables; Molecular orbital theory of homo- and hetero-nuclear diatomic molecules; Chemical forces: strong and weak forces.
(11)

Acids and Bases

Brønsted acidity, gas phase proton acidities, aqueous acidity, concept of pK_a of proton acids, hydroxyl acids, oxo acids, structure of acids with relation to hydrogen bonding; Lewis acids; Hard and Soft acids and bases; Acids and bases in aprotic solvents (6)

Oxidation and Reduction

Reduction potentials; Redox half reactions; Redox stability in water; Representation of electrode potential data diagrammatically. Latimer-Frost Diagrams. (4)

Solid State

Close packing, structures of metals, rationalization of structures of ionic solids; energetics of ionic bonding, defects in solids; perovskites; high T_c superconductors (6)

Ligands and Transition Metal Complexes

Different types of ligands; Structures and isomerism of transition metal complexes; Bonding in transition metal complexes – valence bond, crystal field, M.O. theories, effects of d-orbital splitting; Organometallic compounds: Effective Atomic Number (EAN), metal-carbonyls, metal-olefin complexes; Reactions of organometallic

compounds: Addition, Dissociation, Oxidation addition, insertion, Reductive elimination.
Introduction to catalysis, Ziegler-Natta, a few examples of homogeneous catalysis. (12)

Introduction to Chemistry of f-block Elements

Special features of f-block elements, lanthanide contraction, coordination number, structures, and simple reactions. (3)

Recommended Books

(1) **Inorganic Chemistry- Principles of Structure and Reactivity, J.E. Huheey, E. A. Keiter, R.L. Keiter and O. K. Medhi, Pearson Education, 2007.**

(2) Concise Inorganic Chemistry, J. D. Lee, 4th Edn., ELBS, 1991.

(3) Advanced Inorganic Chemistry, F. A. Cotton, C. A. Murillo, and M. Bochmann, Wiley Interscience, 2001.

(4) Inorganic Chemistry, D. F. Shriver and P. W. Atkins, Oxford University, 1999.

(5) Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications, A. Vincent, John Wiley, 2001.

Reference

(1) Chemistry of the Elements, N. N. Greenwood and A. Earnshaw, 2nd Edition, Elsevier, 2005.

(2) Chemistry, J. McMurry, R. C. Fay, 4th Edition, Pearson Education, 2005.

(3) Group Theory and Chemistry, D. M. Bishop, Dover Publications, New York, 1973.

(4) **Chemical Applications of Group Theory, F. A. Cotton, John Wiley and Sons, 2003.**

C 302 Chemical Thermodynamics
Equilibrium and Non-equilibrium Systems

Surfaces

Thermodynamics of surfaces and interfaces, surface tension, vapour pressure; surface films on liquids, Gibbs adsorption equation; adsorption of gases on solids: Freundlich, Langmuir and BET adsorption isotherms; determination of surface areas; colloids. (11)

Electrochemistry

Debye-Huckel theory of electrolytes; ionic strength principle, activities of ions and activity coefficients.
Applications of EMF measurements: equilibrium constant, thermodynamic parameters,
potentiometric titrations; basic principles of ion-selective membrane electrodes, batteries. Bioelectrochemistry. (11)

Transport Processes
Thermal conductivity, viscosity, diffusion and sedimentation.
Electrical Conductivity : Debye-Huckel-Onsager theory of electrolytic conductance, ion association in electrolytic solution. (10)

Nonequilibrium Thermodynamics
Conservation equations, linear transport processes, Onsager reciprocity relations, continuity and diffusion equations, steady states. (10)

Recommended Books

1. Physical Chemistry, I. Levine, Tata McGraw Hill, 5th Edn., 2007.
2. Physical Chemistry of Surfaces, A. W. Adamson and A. P. Gast, John Wiley and Sons, Inc., 1997.
3. Modern Electrochemistry, J.O'M. Bockris and A. K. N. Reddy, Springer, 2006.
4. Physical Chemistry, R. S. Berry, S. A. Rice and J. Ross, Oxford Univ. Press, 2nd Edn., 2000.
5. Thermodynamics of Irreversible Processes, R. Haase, Dover Publications, 1990.

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C 303 Quantum Mechanics - I
Basic Principles and Applications to Atomic Systems

Origin of quantum mechanics
Historical perspective, The photoelectric effect, Wave-particle duality, electron diffraction, black body radiation, uncertainty principle. (5)

Wave Functions
Concepts of wave function, operators, eigen values and eigen functions, commutation relations.
Introduction to linear algebra and matrix representation of operators. (6)

Basic postulates of quantum mechanics

Time dependent Schrödinger equation, Stationary states, time independent Schrodinger equation, concept of quantization. (6)

Simple exactly solvable systems

Particle in one dimensional box and extensions to two and three dimensions,

One dimensional harmonic oscillator, Rigid rotor, Angular momentum, concept of space quantization. (9)

Applications to atomic systems

Hydrogen atom, orbitals, shapes of orbitals, radial distribution function, electron spin. (8)

Many electron atoms

Helium atom and many electron wave functions, concept of screened nuclear charge, spin orbitals, Pauli Exclusion Principle and Slater determinants to represent many-electron wave functions. Introduction to variational and perburbation methods. (8)

Recommended Books

1. Quantum Chemistry, I. N. Levine, 5th Edn., Pearson Education, 2003.

2. Introduction to Quantum Chemistry, R. K. Prasad,

3. Molecular Quantum Mechanics, P. W. Atkins and R. S. Freidman, 3rd Edn.,
Oxford University Press, 1997.

4. Quantum Chemistry, D. A. Mcquarrie and J. D. Simon, Viva Books, New Delhi, 1998.

5. Physical Chemistry : A Molecular Approach, D. A. Mcquarrie and J. D. Simon, Viva Books, New Delhi, 1998.

6. Elementary Quantum Chemistry, F. L. Pilar, McGraw-Hill Book Company, New York, 1968.

7. Introduction to Quantum Chemistry, A. K. Chandra, Tata McGraw Hill, 1997.

CL 301 Chemistry Laboratory

1. Identification of unknown mixtures containing 4 radicals (CO_3^{2-}, SO_3^{2-}, SO_4^{2-}, S^{2-}, NO_3^-, NO_2^-, Cl^-, Br^-, I^-, PO_4^{3-}, Na^+, K^+, Mg^{2+}, Ca^{2+}, Ba^{2+}, Sr^{2+}, Al^{3+}, Cr^{3+}, Fe^{3+}/Fe^{2+}, Co^{2+}, Ni^{2+}, Mn^{2+}, Zn^{2+}, Cd^{2+}, Hg^{2+}, Pb^{2+}) by dry and wet tests.
2. Standardisation of sodium thiosulphate solution and volumetric estimation of Cu(II) iodometrically.

3. Standardization of potassium permanganate solution and volumetric estimation of Fe(II) and Fe(III) in a mixture.
4. Preparation of standard potassium dichromate solution and estimation of Fe(II) by dichromate.
5. Volumetric estimation of thiocyanate (Volhard titration).
6. Volumetric estimation of Zn(II), Ca(II) and Mg(II) by EDTA titration.
7. Gravimetric estimation of Nickel(II).
8. Gravimetric estimation of Zinc(II).
9. Estimation of calcium using oxalic acid and $KMnO_4$.
10. Estimation of total manganese content in pyrolusite.

Recommended Books

(1) G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denny, Vogel's Text Book of Qualitative Chemical Analysis, 5th Edn. , ELBS, 1991.
(2) G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denny, Vogel's Text Book of Quantitative Chemical Analysis, 5th Edn. , ELBS, 1991.

CL 302 Electronics Laboratory

12 turns (once every week)

1. Use of CRO.
2. Characteristics of a zenner diode and setting up a power supply using a zenner diode.
3. Transistor characteristics and current gain.
4. Operational and differential amplifier.
5. Filtering and phase shifting networks.
6. Stephan's constant.

C 401 Organic Chemistry – I

Reduction (with special emphasis on mechanism, stereochemistry and selectivity wherever necessary)

Catalytic Hydrogenation ; Reduction by Metal Hydrides; Metal reductions in solution, using Na, K, Zn, Sn;
Miscellaneous Reductions : Wolff-Kishner reduction, Rosenmund reduction, Diimide reduction, reductions with low valent titanium species, trialkyltin hydride, DIBAL, Trialkylsilanes. (6)

Oxidation (with special emphasis on mechanism, stereochemistry and selectivity wherever necessary)

Oxidation with chromium [(including pyridinium chlorochromate (PCC) and pyridinium dichromate (PDC)] and manganese compounds.
Oxidation with peracids and peresters.

Miscellaneous oxidising agents: Oppenauer oxidation; Swern oxidation; use of lead tetraacetate, $Hg(OAc)_2$, HIO_4, ceric ammonium nitrate, phenyliodosoacetate; singlet oxygen molecules.
Prevost, Ag_2CO_3 / celite, oxidations using sulfur and selenium based reagents. (6)

Halogenation (with special emphasis on mechanism, stereochemistry and selectivity wherever necessary)
Reaction with carbon-carbon double bonds; halogenation of carbonyl compounds; substitution of halogen at benzylic and allylic carbon-hydrogen bonds. (5)

C – C bond formation (with special emphasis on mechanism, stereochemistry and selectivity wherever necessary)
Acyloin, aldol, Stobbe, Claisen, Knovenagel, benzoin, Dieckman, Wittig (with Wittig-Horner modification). Diels-Alder and ene reactions, Reformatsky, acetoacetic and malonic ester synthesis; enamine, Michael and Mannich reactions; cyclopropanation including Simmons-Smith reaction; Robinson annulation.
(10)

Acylation (with special emphasis on mechanism, stereochemistry and selectivity wherever necessary)
Acylation of active methylene compounds; acylation of olefins and aromatic systems. (4)

Molecular Rearrangements (with special emphasis on mechanism, stereochemistry and selectivity wherever necessary)
Mechanistic and stereochemical aspects of Pinacol, Benzilic acid, Favorskii, Wolff, Curtius, Schmidt, Lossen, Beckman, Dienone-phenol, Fries, Demyanov, Baeyer-Villiger, Wagner-Merwein Rearrangements. 6)

Application of New Methods in Organic Synthesis (with special emphasis on mechanism, stereochemistry and selectivity wherever necessary)
Baker's yeast, DDQ, LDA (lithium diisopropyl amide); Phase transfer catalysts; Crown ethers, polymer-supported reagents; microwave induced organic synthesis; application of ultra-sound in organic synthesis. (5)

Recommended Books

1. **Modern Methods of Organic Synthesis, W. Carruthers and I. Coldham,**
Cambridge University Press, 2006.
2. Organic Synthesis, M. B. Smith, McGraw-Hill , New York, 2000.
3. Advanced Organic Chemistry: Reactions, Mechanisms and Structure,

J. March, Wiley Interscience, 2007.
4. **Organic Synthesis : Special Techniques, V. K. Ahluwalia and R. Aggarwal, Narosa Publications, 2001.**
5. **Organic Chemistry, F. A. Carey and R. J. Sundberg, Kluwer Academic Publishers, 4th Edn., 2005.**

C 402 Main-Group and Organometallic Chemistry

Basic Characterization techniques of main-group and organometallic compounds (NMR, Mass, IR) (5)

1.Representative chemistry of main group elements

a. Organometallic chemistry of lithium and magnesium: synthesis, structures and reactivity.
b. Chemistry of boron: Boranes, bonding in boranes, topology of boranes, synthesis and reactivity, Carboranes and metallacarboranes. New Lewis acids based on boron; polymer-supported Lewis acids.
c. Chemistry of Aluminum: Aluminum alkyls. Use of aluminum alkyls in polymerization of olefins.
d. C_{60} and carbon nanotubes: discovery, preparation and selected reactions.
e. Chemistry of Silicon: Organosilicon compounds, Silicates and aluminosilicates. 14)

2.Unusual compounds of main group elements

Chemistry of multiple bonding: Multiple bonding in heavier main-group elements. Unusual compound of main group elements: (i) Si=Si, Si≡Si, P=P double bond, Bi-Bi double bond. Synthesis, Structure and reactivity. Controversies.

a. Chemistry of low valent compounds: Synthesis, Structure and bonding models and reactivity examples of Al(I), Si(II) low valent compounds.
b. Inorganic rings and polymers. Cyclo and heterocyclophosphazenes and the polymers derived from them. Polysilanes. Borazine and boron nitride.
c. Chemistry of halogens and noble gases-recent trends. CFC's and ozone layer. (6)

3.Organometallic chemistry

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

c. Applications of organometallics in organic synthesis:

C-C bond coupling reactions (Heck, Sonogoshira, Suzuki etc). Reduction reactions using transition metal hydrides; asymmetric hydrogenation. (17)

Recommended Books

1. Organometallics: A Concise Introduction, C. Elschenbroich and A. Salzer, 3rd Edn. 1999.

2. Chemistry of the Elements, N. N. Greenwood and A. Earnshaw, 2nd Edn., Elsevier, 2005.

3. Modern Inorganic Chemistry, W. L. Jolly, McGraw Hill, New York, 2nd Edn., 1991.

4. Concepts and Models of Inorganic Chemistry, B. Douglas, D. McDaniel and J. Alexander, John Wiley, New York, 3rd Edn., 1993.

5. **Organometallic Chemistry of the Transition Metals, R. H. Crabtree, Wiley, New York, 1988.**

C 403 **Statistical Mechanics**
Basic Principles and Applications

Basic assumptions, concept of microscopic and macroscopic states, ensembles and averages. Calculation of distribution functions in canonical ensemble and the canonical partition function. Relations between the canonical partition function and thermodynamic functions. Calculations in other ensembles like micronanonical and grand canonical ensembles. (12)

Calculations of partition functions and thermodynamic properties for ideal systems of monatomic and diatomic molecules. Calculations of fluctuations and equivalence of ensembles. (7)

Calculation of heat capacity of solids, Einstein and Debye theories, study of chemical equilibrium in terms of partition functions (4)

Quantum Statistics: Maxwell-Boltzmann, Bose-Einstein, and Fermi-Dirac statistics. Systems of Fermions and Bosons in weak and strong degenerate limits.
(7)

Classical Statistical Mechanics, partition functions as integrals over phase space coordinates, Systems of interacting particles, imperfect gases, concept of radial distribution functions of liquids and applications to ionic solutions using Debye-Huckel theory. (6)

Non-equilibrium Statistical Mechanics: Onsager regression hypothesis and fluctuation-dissipation theorem, calculations of transport coefficients like diffusion, conductivity.
(6)

Recommended Books

1. **Physical Chemistry : A Molecular Approach, D. A. Mcquarrie and J. D. Simon, Viva Books, New Delhi, 1998.**
2. Statistical Mechanics, D. A. McQuarrie, University Science Books, 2nd Edn., 2000.
3. Introduction to Modern Statistical Mechanics, D. Chandler, Oxford Univ. Press, 1987.
4. Statistical Thermodynamics of Non-Equilibrium Processes, J. Kaizer, Springer, 1st Edn., 1987.
5. Statistical Physics II: Non-Equilibrium Statistical Mechanics, R. Kubo, M. Toda and N. Hashitsume, Springer, 2003.

CL 401 **Chemistry Laboratory**

(1) Calibration of absorption measurements on a spectrophotometer, using potassium chromate and copper(II) sulphate solutions.
(2) Verification of Beer-Lambert Law, using $KMnO_4$ solution.
(3) Study of the equilibrium : $Fe^{3+}(aq) + NCS^- \leftrightarrow Fe(NCS)^{2+}(aq)$ by absorption measurement on a spectrophotometer, and determination of the equilibrium constant.
(4) Study of the pH dependence of the UV-Visible spectrum of 4-nitrophenol and determination of its pK_{OH} by spectrophotometric method.
(5) Estimation of Co^{2+} spectrophotometrically as $[Co(NCS)_4]^{2-}$.
(6) Estimation of Fe^{2+} spectrophotometrically as tris(orthophenanthroline)iron(II).
(7) Identification of functional group in an unknown organic compound by UV-Visible and IR spectroscopy.
(8) Turbidimetry : Determination of SO_4^{2-}.
(9) Determination of stability constant of a complex by pH titration.
(10) Dimerization of benzoic acid by Partition Method.

Books Recommended

2. G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denny, Vogel's Textbook
3. of Quantitative Chemical Analysis, 5th Edn., ELBS, 1991.
4. (2) R. M. Silverstein, G. C. Bassler and T. C. Morrill, Spectrometric
5. Identification of Organic Compounds, 6th Edn., Wiley, 1998.
6. (3) R. L. Shriner, C. K. F. Hermann, T. C. Morrill, D. Y. Curtin and R. C.
7. Fuson, The Systematic Identification of Organic Compounds, John Wiley, 8th Edn., 2004.

CL 402 Biomolecular Chemistry Laboratory

1. Estimation of acid strength in a citrus fruit.
2. Determination of purity of chymotrypsin from the enzyme kinetics.
3. Identification of sugars in fruit juices using TLC.
4. Determination of titration curves of amino acids.
5. Estimation of carbohydrates by the anthrone method.
6. Determination of the free amino acid end group of some proteins, using Sanger's reagent.
7. Determination of the iodine number of a fat.

Recommended Book

1. An Introduction to Practical Biochemistry, D. T. Plummer, Tata McGraw Hill, 2000.

C 501 Organic Chemistry - II

Introduction to Natural Products
Terpenes (mono- , di- , and sesquiterpenes); alkaloids and steroids with special emphasis on biogenesis, structural elucidation of α-pinene, abscisic acid, papaverine, morphine, cholesterol. (8)

Monosaccharides
Structure and nomenclature; synthesis, reactions of monosaccharides (isomerization, glycoside formation, hydrazones and osazones, alditols by reduction, oxidation and oxidative cleavage); protective groups for monosaccharides; synthesis of monosaccharide derivatives. (6)

Polysaccharides
Nomenclature, properties and three dimensional structures; structure determination (degradations, physical methods). (3)

Peptides and Proteins
Amino acids (structures, ionization and polarity); separation and detection of amino acids; chemical synthesis of amino acids; peptides; three-dimensional structures of peptides and proteins; analysis of peptides and proteins; synthesis of peptides. (8)

Nucleic Acids
Components of nucleic acids; nucleosides and nucleotides; structures of nucleic acids; biological functions of nucleic acids; structure determination of nucleic acids; chemical synthesis of nucleic acids; methods of replication; sequencing of nucleic acids. (8)

Steroids
Lipids; structure and nomenclature of steroids; structure and biological activities of steroids; chemical properties of steroids; synthesis of steroids (selected examples). (5)

Antibiotics
Structure and nomenclature; properties of β-lactams; microbial production of penicillins; chemical modification of penicillins. (4)

Recommended Books

1. Chemistry of Biomolecules : An Introduction, R. J. Simmonds, Royal Society of Chemistry, 1992.
2. **Organic Chemistry, Vol. II, I. L. Finar, ELBS, 1990.**
3. **Organic Synthesis, M. B. Smith, McGraw Hill, 1994.**
4. Chemistry of Natural Products, S. V. Bhat, B. A. Nagasampagi and M. Sivakumar, Narosa Publications, 2005.

5. Bioactive Natural Products, D. S. Bhakuni and D. S. Rawat, Anamaya Publishers, 2005.

C 502 Molecular Spectroscopy and Group Theory

Introduction
Interaction of light with matter, transition moments and transition probabilities, Einstein's coefficients, oscillator strength, Beer-Lambert law, Absorbance, Born-Oppenheimer approximation, potential energy curves and vibrational and rotational energy levels, Frank-Condon principle. (6)

Group Theory
Definition of a group and basic theorems, molecular symmetry groups and classes, Great orthogonality theorem, Matrix representation of groups, irreducible representations and Character Tables. (8)

Symmetry Properties
Symmetry properties of wave functions, orbitals as basis sets for irreducible representations, symmetry adapted linear combinations. Symmetry and normal modes of vibration. Symmetry and selection rules for allowed transitions between rotational, vibrational and electronic levels. (8)

Microwave and Infrared Spectroscopy
Rotational spectra of diatomic and simple polyatomic molecules, Stark effects, vibrational spectra of diatomic molecules, simple harmonic oscillator and anharmonic corrections, selection rules, fundamental and overtone bands, Isotope effects, vibrational spectra of organic molecules and functional groups. (8)

Raman Spectroscopy
Concept of anisotropic polarizability and Raman spectra. Selection rules from symmetry considerations. (3)

UV-Visible Spectroscopy
Molecular electronic spectra, photophysical processes, fluorescence, phosphorescence, spectroscopy of conjugated double bonds, lasers. (3)

Magnetic Resonance Spectroscopy (NMR)
Nuclear spin states in presence of a magnetic field, energy gap and transition. chemical shifts, spin-spin interactions. (4)

Analysis of Spectra of Simple Molecules. (2)

Recommended Books

1. **Chemical Applications of Group Theory, F. A. Cotton, John Wiley, 3rd Edn., 2003.**

2. **Fundamentals of Molecular Spectroscopy, C. N. Banwell and E. M. McCash,Tata McGraw Hill, 1995**
3. **Molecular Spectroscopy, G. M. Barrow, McGraw Hill, 1985**.
4. Spectra of Atoms and Molecules, P. F. Bernath, Oxford Univ. Press, 2005.

C 503 Chemical Rate Processes

Transport Properties
Kinetic theory of gases, effusion, thermal conductivity and viscosity, olecular motion in liquids, diffusion**.** (8)

Rate Laws and Chain Reactions
Revision of phenomenological kinetics laws: 1^{st}, 2^{nd} and 3^{rd} order reactions, methods of determining the order of chemical reactions; chain reactions, photochemical reactions; catalysis.
(8)

Fast Reactions
Study of fast reactions by flash photolysis, flow techniques, relaxation methods, salt and solvent effects on reactions in solutions. (10)

Kinetics of Oscillatory Reactions. (3)

Chemical Reaction Dynamics
Collision Theory and Reaction Dynamics; reaction cross section and rate constant; brief idea of Molecular Beam Scattering; concept of potential energy surfaces, transition state theory including its statistical mechanical treatment. Phenomenological theories of unimolecular reactions (Lindemann, Hinshelwood). Statistical mechanical theories of unimolecular reactions (RRKM). (13)

Recommended Books

1. **Physical Chemistry, I. Levine, Tata McGraw Hill, 5th Edn., 2007.**
2. **Physical Chemistry : A Molecular Approach, D. A. McQuarrie and J. D. Simon, University Science Books, 1997.**
3. **Chemical Kinetics and Dynamics, J. I. Steinfeld, J. S. Francisco and W. L. Hasse, Prentice Hall, 1999.**
4. Chemical Dynamics in Condensed Phases: Relaxation, Transfer and Reactions in Condensed Molecular Systems, A. Nitzan, Oxford Univ. Press, 2006.

Reference

1. Basic Chemical Kinetics, H. Eyring, S. H. Lin and S. M. Lin, John Wiley, New York, 1980.
2. **The World of Physical Chemistry, K. J. Laidler, Oxford University Press, Oxford, 1993.**

CL 501 **Chemistry Laboratory**
(Organic Synthesis and Analysis)

1. (i) Separation of organic compounds from a mixture containing two components, and identification of the individual ones by analytical methods.
   (ii) Application of UV-VIS / IR spectroscopy for the characterization of organic compounds / functional groups.
2. Synthesis of organic compounds / drugs :
   (i) preparation of anthranilic acid.
   (ii) preparation of aspirin.
   (iii) preparation of benzilic acid from benzaldehyde.
   (iv) preparation of p-bromoaniline from acetanilide.
3. Estimation of Phenol / Aniline using BrO_3^- + Br^- mixture.
4. Estimation of keto group (by iodoform reaction).
5. Determination of saponification value of an oil (ester of a long chain fatty acid).
6. Beckmann Rearrangement (Benzophenone oxime → Benzanilide).
7. Fischer Indole synthesis (Phenylhydrazone → Phenylindole).
8. Purification of organic compounds by adsorption chromatography.

Recommended Books

(1) G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denny, Vogel's Textbook of Quantitative Chemical Analysis, 5th Edn., ELBS, 1991.
(2) **R. M. Silverstein, G. C. Bassler and T. C. Morrill, Spectrometric Identification of Organic Compounds, 6th Edn., Wiley, 1998.**
(3) R. L. Shriner, C. K. F. Hermann, T. C. Morrill, D. Y. Curtin and R. C. Fuson, The Systematic Identification of Organic Compounds, John Wiley, 8th Edn., 2004.

CL 502 **Chemistry Laboratory**
(Inorganic / Physical / Theoretical)

1. Kinetics of Persulphate and Iodide reaction; influence of inert salt .
2. Synthesis of nitritopentaamminecobalt(III) nitrate, and study of the kinetics of its isomerisation to nitropentaamminecobalt(III).

3. Kinetics of acid catalyzed iodination of acetone; the effect of $[H^+]$, $[I_2]$, $[I^-]$, [acetone] variation.
4. Separation of Co(II) and Ni (II) in a mixture by anion exchange chromatography and their quantitative estimation.
5. Analysis of complex materials: alloys / ores (brass, iron ore, chromite)
6. Adsorption of acetic acid on activated charcoal and verification of Freundlich/Langmuir adsorption isotherm.
7. To construct the phase diagram for a three-component system (chloroform – acetic acid – water).
8. Phenol-water system: consolute temperature, effect of salt concentration.
9. Determination of partial molar volume of a solute in solution.
10. Some computer-aided experiments in Theoretical Chemistry (MO Methods in Chemistry).

Recommended Books

(1) R. C. Das and B. Behera, Experimental Physical Chemistry, Tata McGraw-Hill, 1983.
(2) A. Findlay and J. A. Kitchener, Practical Physical Chemistry, 8th Edn., Longmans, 1967.

C-601 Coordination Chemistry

Symmetry

Symmetry Elements, Symmetry Operations, Point Groups, Symmetry Representations, Applications of symmetry to Molecular Orbital diagrams of simple molecules (examples: H_2O, BeH_2, BF_3 ($\sigma + \pi$). Assignment of symmetry representations of d-orbitals for specific geometries. Various geometries of coordination compounds and different types of isomerism. (9)

Theories of bonding

CFT (including Jahn-Teller). Effects of ligand field (spectrochemical series, enthalpies of hydration, spinel structures. Shortcomings of CFT. MO theory of coordination complexes (5)

Spectroscopy of transition metal complexes

Russell-Sanders coupling term symbols, electronic spectra (Orgel; Tanabe-Sugano diagrams) and EPR spectra. (8)

Magnetism of transition metal complexes

Curie law. Para-, ferro, anti-ferro and ferri, magnetic beh (4)

Reaction mechanisms of transition metal complexes

Substitution (Kinetic effects: labile vs inert) and electron-transfer reactions (Outer-sphere, Self-exchange; Inner-sphere). (4)

Bio-inorganic chemistry

Basic principles (why specific metal ions are present in certain proteins/enzymes):

Heme proteins, types, structure and function (including mechanism of function): Hemoglobin, myoglobin, Cytochrome C, Cytochrome P450, Catalases, Peroxidases.

Non-Heme Proteins: Hemeerythrin, Ribonucleotide reductase, Methanol monooxygenase

(a) Iron-Sulfur Proteins: Ruberodoxin, Ferredoxin; (b) DNA / RNA : Ribozymes (9)

Transition metal based supramolecular structures

Ligand design and applications. (3)

Recommended Books

1. **Inorganic Chemistry- Principles of Structure and Reactivity, J.E. Huheey, E. A. Keiter, R.L. Keiter and O. K. Medhi, Pearson Education, 2007.**
2. **Advanced Inorganic Chemistry, F. A. Cotton, C. A. Murillo, and M.Bochmann, Wiley Interscience, 2001.**
3. **Inorganic Chemistry, D. F. Shriver and P. W. Atkins, Oxford University Press, 1999.**
4. **Chemical Applications of Group Theory, F. A. Cotton, John Wiley, 3rd Edn 2003.**
5. Molecular Symmetry and Group Theory, R. L. Carter, John Wiley and Sons, 1998.
6. **Supramolecular Chemistry: Concepts and Perspectives, J. M. Lehn, VCH, 1995.**
7. Principles of Bioinorganic Chemistry, S. J. Lippard and J. M. Berg, Panima Publications, New Delhi, 1997.
8. Reaction Mechanisms of Inorganic and Organometallic Systems, R. B.

Jordan, Oxford Univ. Press, 2nd Edn., 1991.

Reference

1. Bioinorganic Chemistry, Asim K. Das, Allied Books, Kolkata, 2004.
2. **Concise Inorganic Chemistry, J. D. Lee, 4th Edn., ELBS, 1991.**
3. Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications, A. Vincent, John Wiley, 2001.
4. Mechanisms of Inorganic Reactions, F. Basolo and R. G. Pearson, Wiley, 2nd Edn., 1967.
5. Inorganic Reaction Mechanisms, M. L. Tobe and J. Burgess, Wesley Longmans, 1st Edn., 1999.

C 602 Quantum Mechanics – II
Chemical Bonding and Electronic Structure of Molecules

Introduction to chemical bonding: Covalent bond, ionic bond, metallic bond, weak intermolecular forces, Review of basic principles of quantum mechanics, atomic structure, variation and perturbation methods. (6)

Electronic structure of diatomic molecules, Born-Oppenheimer approximation, H_2^+ ion, molecular orbitals of ground state and excited states of H_2^+ (LCAO-MO), homo and heteronuclear diatomic molecules, electronic term symbols, valence bond theory of diatomic molecules, comparison of valence bond and molecular orbital theories. Term Symbols for diatomic molecules. (11)

Self-consistent Field Methods: Hartree-Fock theory of atoms and molecules, post-Hartree-Fock theories, configuration interaction wave functions. (6)

Electronic structure of polyatomic molecules. SCF-MO treatment of closed shell systems and applications to molecules (H_2O, NH_3, CH_4) ; Potential energy surface and equilibrium geometry, molecular vibrational frequencies. Brief introduction to density functional theory. (9)

Virial theorem and chemical bonding. The Hellman-Feynman theorem. (4)

Semi-empirical and molecular mechanics treatment of molecules, Huckel molecular orbital theory for conjugated organic molecules and its applications to ethylene, butadiene, benzene; delocalization energy and stability. (6)

Recommended Books

1. **Modern Quantum Chemistry: Introduction to Advanced Electronic Structure, A. Szabo and N. S. Ostlund, Dover, 1996.**
2. Molecular Quantum Mechanics, P.W. Atkins and R.S. Friedman, Oxford University Press, 3rd Edn., 1997.
3. Quantum Chemistry, I. N. Levine, 5th Edn., Pearson Education, 2000

C 603 Physical Methods in Chemistry

Infrared Spectroscopy: Introduction. Identification of functional groups, hydrogen bonding etc., metal ligand vibrations. (2)

Nuclear Magnetic Resonance Spectroscopy: Introduction. Application of ^{1}H and ^{13}C NMR spectroscopy including COSY, NOESY, NOE techniques in the structural determination of complex organic systems. Application in conformational analysis. Multinuclear NMR of various inorganic and organometallic compounds.
(9)

Ultraviolet Spectroscopy: Introduction. Studies of conjugated and extended conjugated systems etc. Woodward rules. Electronic spectra of transition metal complexes. (2)

Mass Spectrometry: Basic concepts. Fragmentation and rearrangements (including McLafferty rearrangement) of different classes of organic molecules. Isotope effects etc. ESI-MS, MALDI-TOF techniques. (5)

Structural elucidation by joint application of UV, IR, NMR and mass spectrometry. (3)

Electron Spin Resonance Spectroscopy: A brief review of theory. Analysis of ESR spectra of systems in liquid phase, radicals containing single set, multiple sets of protons, triplet ground states. Transitionmetal ions. Rare earth ions, ion in solid state. Double resonance stechniques: ENDOR in liquid solution, ENDOR in powers and non-oriented solids. Biological applications: Substrate free radical, flavins and metal free flavin proteins, photosynthesis, Heme proteins, Iron-sulfur proteins, spin labels. (6)

Mossbauer Spectroscopy: Basic physical concepts, spectral line shape, isomer shift, quadrupole splitting, magnetic hyperfine interaction. Interpretation of Mossbauer parameters of ^{57}Fe, ^{99}Ru, ^{101}Ru, ^{195}Pt, ^{193}Ir and ^{110}Sn. Some special applications: Solid state reactions, thermal decomposition, ligand exchange, electron transfer, isomerism, surface studies and biological applications. (2)

X-Ray Photo-Electron Spectroscopy: Physical concepts. Application to determine atomic charges, oxidation numbers, catalyst surface structures and in some cases molecular structures. (2)

Fluorescence spectroscopy: Fluorescence energy transfer and its applications to measurement of distances in molecules. (2)

Magnetism: Introduction to Magnetism. Origin of diamagnetism. Paramagnetism: Van Vleck formula and its approximated forms, Curie law. Magnetic susceptibility, orbital quenching and spin-only moment. Magnetic exchange interactions in coordination compounds: ferrimagnetism and antiferromagnetism. Bulk magnetic properties and ferromagnetism. Molecule-based magnetic materials: organic magnets and single molecule magnets. (6)

Electrochemistry: Heterogeneous electron transfer and concept of capacitive and faradic current. Cyclic voltammogram. Instrumentation: three-electrode potentiometer and electrodes. Measurements and analyses of the voltammograms. Differential pulse voltammetry and coulometry. Application of cyclic voltammetry in inorganic and organic chemistry. (3)

Recommended Books

1. Physical Methods in Chemistry, R. S. Drago, 2nd Edn., Saunders, 1992.

2. Introduction to spectroscopy, Pavia, Lampman and Criz.

3. Carbon-13 Nuclear Magnetic Resonance Spectroscopy, G. C. Levy, R. L. Lichter and G. L. Nelson, Wiley, 1980.

4. NMR Spectroscopy - An Introduction, H. Gunther, John Wiley, 1980.

5. Basic One- and Two-Dimensional NMR Spectroscopy, H. Friebolin, VCH, 1991.

6. Spectroscopic Methods in Organic Chemistry, D. H. Williams and I. Fleming, 4th Edn., 1988.

7. Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Morrill, John Wiley, New York, 5th Edn., 1991.

8. Interpretation of Mass Spectra, F. W. McLafferty, 1980.

9. Electron Paramagnetic Resonance: Elementary Theory and Practical Applications, J. A. Weil, J. R. Bolton and J. E. Wertz, Wiley Interscience, New York, 1994.

10. Principles of Fluorescence Spectroscopy by Joseph R. Lackowicz 3rd edition.

CL 601 **Chemistry Laboratory**

(1) Synthesis of a few inorganic complexes of first row transition elements, analysis of their metal contents and study of their spectral and magnetic properties.
   (a) Preparation of nitrite- and nitropentaamminecobalt (III) chlorides.
   (b) Preparation of hexamminecobalt (III) chloride and aquapentaammine- cobalt (III) chloride.
   (c) Preparation of cis- and trans- potassium dioxalatodiaquachromate (III).
   (d) Preparation of hexamminenickel(II) chloride, and estimation of Ni(II) in the complex by gravimetric and volumetric procedures.

(2) Analysis of ore (estimation of aluminium content in bauxite).

(3) Synthesis of carbonatopentamminecobalt(III) and study of the kinetics of decarboxylation, effects of salt and solvent.
   i. (a Stopped Flow Spectrophotometer is required; alternatively, a rapid mixing attachment for a spectrophotometer will suffice).

(4) Photolysis of an inorganic complex [tris-(oxalato) iron(III)].

(5) Photochemical reaction : Fe(II) + thionine.

(6) Synthesis of trans-(dichloro) cobalt (III) chloride; analysis of cobalt and study of its kinetics of solvolysis in aqueous medium.

(7) Determination of the rate constant for the redox reaction between ethanol and Cr(VI).

CL 602 **Chemistry Laboratory**

(1) Kinetics of bimolecular hydrolysis reaction of methyl acetate in aqueous alkaline medium; effect of salt concentration.

(2) Kinetics of Hg(II) catalysed aquation of chloropentaamminecobalt(III); the effect of salt concentration. (This reaction can be studied at 20 – 40^{o}C spectrophotometrically in the presence and absence of Hg(II) to get the activation parameters which can throw light on the mechanistic aspects).

(3) Devise an oscillatory chemical reaction (B-Z reaction), using $KBrO_3$, KBr, malonic acid, H_2SO_4, and the redox indicator ferroin).

(4) Surface tension of water using capillary rise method.

(5) Critical micelle concentration (CMC) : sodium dodecyl sulphate a. (SDS), hexadecyl trimethylammonium bromide (HTAB).

(6) Viscosity of ethanol-water mixture using Ostwald viscometer.
(7) Kinetics of the reaction of hydrogen peroxide with iodide.

Recommended Books

(1) R. C. Das and B. Behera, Experimental Physical Chemistry, Tata McGraw-Hill, 1983.
(2) A. Findlay and J. A. Kitchener, Practical Physical Chemistry, 8th Edn., Longmans, 1967.

ELECTIVE COURSES IN CHEMISTRY [ES]

Solid State Chemistry

Introduction

Space lattice, Crystal point groups, space group, stereographic projections, packing in solids; crystal structures of representative systems: silicates and zeolites; cements, glasses, quasicrystals, nanostructures. (5)

Crystal Defects

Perfect and imperfect crystals; thermodynamics of defect formation; types of defects : point defects, line defects, plane defects; Schottky and Frenkel defects; thermodynamics of Schottky and Frenkel defect formation; crystal classifications; Madelung constant and lattice energy. (6)

Techniques

X-ray diffraction, Electron microscopy (SEM, TEM, AFM), Thermal techniques (TG, DTA, DSC), Spectroscopic techniques (Mossbauer, IR, UV-VIS) and Physical property measurement techniques (Magnetic moments-VSM /SQUID, Electrical resistivity – Two / Four probe methods and thermal conductivity, Optical band gap, XPES, XAS). (9)

Electronic Structure of Solids

Free Electron model; metals, semiconductors and insulators; doped semiconductors; solid state ionics; intrinsic and extrinsic semiconductors; p-n junction. (8)

Critical Phenomena

Phase transitions (Order-disorder, Martensite-austenite, Spinoidal decompositions); liquid crystals; structure-property relations (magnetic, electrical, superconductivity, optical and thermal).

Powder synthesis by conventional and modern chemical methods, reactivity of solids, decomposition mechanisms, powder processing (sintering and diffusion processes), tailoring of solids, special methods for single crystal growth and thin film depositions. (10)

Superconductivity

General aspects of superconductivity; effects of magnetic field; BCS Theory; oxide superconductors. (4)

Recommended Books

1. **Solid State Chemistry and Its Applications, A. R. West, John Wiley, 1987.**
2. **Understanding solids, Richard Tilley**
3. Solid State Chemistry, L. Smart and E. Moore, Chapman and Hall, 1992.
4. Principles of the Solid State, H. V. Keer, Wiley Eastern Ltd., 1994.
5. The Electronic Structure and Chemistry of Solids, P. A. Cox, Oxford University Press, 2005.

Surface Chemistry

Surface Phenomena

Surface tension and surface free energy; bubbles and drops; Young-Laplace equation and Kelvin equation; Solid-Liquid , Solid-gas and liquid-liquid interfaces. (6)

Adsorption Phenomena

Adsorption on solids : Gibbs, Langmuir, Freundlich, Frumkin, Temkin and BET adsorption isotherms; estimation of surface area of adsorbents. Adsorption on porous solids; chemisorption of gases on metals and semiconductors; kinetics of adsorption processes; heterogeneous catalysis, catalysis by metals; semiconductors and solid acids. (12)

Techniques

Characterisation of solid surface structure and composition, using electron microscopy : SEM, XPS, XRF, Auger spectroscopy (6)

Electrical Phenomena at Interfaces

Electrical double layer; Stern layer; electrokinetic phenomena : zeta potential, electrophoresis, electroosmosis, streaming potential, sedimentation potential; electrocapillarity; thermodynamics of lectrocapillary effect. (6)

Micelles

Surface active agents; classification of surface active agents; micellization; critical micellar concentration (CMC); factors affecting the CMC of surfactants; thermodynamics of micelle formation; structure and dynamics of micelles; reverse micelles; micellar catalysis of reactions; emulsions: formation of emulsions, factors determining emulsion stability; microemulsions. (12)

Recommended Books

1. Adsorption and Catalysis by Solids, D. K. Chakravarty, Wiley Eastern,
   1. 1990.
   2. Characterisation of Solid Surfaces, F. P. Kane and G. B. Larrabee (Eds.), Plenum, 1978.
   3. **Physical Chemistry of Surfaces, A. W. Adamson and A. P. Gast , John Wiley and Sons, Inc., 1997.**
   4. Surfactants in Solution, Vol. 2, K. L. Mittal and B. Lindman (Editors), Plenum, 1982.
   5. Surfactants, T. F. Tadros (Editor), Academic Press, London, 1984.

Advanced Organic Chemistry (Organic Synthesis)

Principles of Retrosynthetic Analysis
Linear and convergent synthesis; synthesis under steric control; regio- and stereoselective synthesis; basic synthetic methods. (6)

Methodolgies for the Construction of 3-7 membered rings, medium and large rings
Applications in natural product synthesis. (5)

Methodologies for the Construction of 3-7 membered Heterocyclic Rings Applications in organic synthesis. (5)

Methodologies for the Construction of Linear Acyclic Molecules
Applications in the synthesis of selected natural products. (5)

Asymmetric Synthesis
Asymmetric synthesis using chiral auxilliaries, chemical and enzymatic resolutions, and catalysis. (4)

Organic Synthesis using Organometallic Chemistry.
Chemistry of Pd, Si, Ti, Sn, Cu, Ru, Rh. (6)

Supramolecular Chemistry, Combinatorial Chemistry (5)

Miscellaneous
Green Chemistry, glycobiology, synthetic aspects using domino reactions.Principles of atom economy with examples; templated and solid supported organic synthesis; ultrasound, microwave mediated organic synthesis. (6)

Recommended Books

1. **The Logic of Chemical Synthesis, E. J. Corey and R. Cheng, Wiley, 1989.**
2. Classics in Total Synthesis, K.C. Nicolaou and E.J. Sorensen, VCH, 1996.
3. Classics in Total Synthesis II, K.C. Nicolaou and R. Snyder, VCH, 2003.
4. **Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg, Kluwer Academic Publishers, 4th Edn., 2005.**
5. **Supramolecular Chemistry: Concepts and Perspectives, J. M. Lehn, VCH, 1995.**

Physical Organic Chemistry

Pericyclic Reactions

Conservation of orbital symmetry, and Woodward and Hoffmann rules. Cycloadditions, Electrocyclizations, Sigmatropic rearrangements, and Chelotropic reactions. Orbital overlap effects in chemical processes. (7)

Stereoelectronic Effects in Organic Chemistry

Acetals, Esters, Amides and related functions. Reactions at sp^3, sp^2, and sp carbons. Examples in synthesis and biological processes. Felkin-Ahn model, Houk model, Cieplak model, EFOE model, and Cation-complexation model as applied to π-Facial selectivity. (10)

Reactive Intermediates

Carbonium ions, carbanions, and radicals (formation, rearrangement, and further reactions in reference to Baldwin' rules for ring-closure). (5)

Chemical Equilibria and Chemical Reactivity

Correlation of reactivity with structure, Hammett equation, substituent constants and reaction constants. (4)

Chemical Kinetics and Isotope Effects

Various types of catalysis and isotope effects. Importance in the elucidation of organic reaction mechanisms. (4)

Electron Transfer Reactions

Theoretical basis, Examples of photo-induced and chemically-induced electron transfer reactions (PET and CET). (3)

Organic Photochemistry

Energy and electronic spin states, Spectroscopic transitions, photophysical processes, fluorescence and phosphorescence, energy transfer and electron

transfer, and properties of excited states, Representative photochemical reactions of carbonyl compounds, olefins, and aromatic compounds. (6)

Miscellaneous

$A^{(1,2)}$ and $A^{(1,3)}$ strain, Captodative effect, Hammond's postulate, Curtin-Hammett principle, and thermodynamic and kinetic control of reactions. (3)

Recommended Books

1. **Physical Organic Chemistry, N. S. Isaacs, ELBS, 1990.**
2. Modern Physical Organic Chemistry, E. V. Anslyn and D. A. Dougherty,
1. California Univ. Science Books, 2006.
2. The Physical Basis of Organic Chemistry, H. Maskill, Oxford Univ. Press, 1986.
3. Mechanism and Theory in Organic Chemistry, T.H. Lowry and K.S. Richardson,Harper Collins Publishers, 1987.
4. **Stereolectronic Effects in Organic Chemistry, P. Deslongchamps, Pergamon,1983.**

Chemistry of Organometallic Compounds

Newer aspects of organometallics derived from different elements such as Pd, Cu, Ti, Rh, Ru, Mo, Ni, Fe, Sn, Si, B, Mg, Ce, and their applications in organic synthesis. (20)

Mechanism, stereochemistry, chemo-, regio-, and stereo- (including enantio-) selectivities using reagents derived from the above-mentioned elements in oxidation, reduction, C-C, and C-hetero bond formations. (15)

Applications in organic synthesis, including natural product synthesis. (7)

Recommended Books

1. **.Organometallic Chemistry of the Transition Metals, R. H. Crabtree, Wiley, New York, 1988.**
2. **Organometallics: A Concise Introduction, C. Elschenbroich and A. Salzer, 3rd Edn. 1999.**
3. Concepts and Models of Inorganic Chemistry, B. Douglas, D. McDaniel and
4. J. Alexander, John Wiley, New York, 3rd Edn., 1993.

Chemistry of Natural Products

Synthesis of selected natural products: Biosynthetic, retrosynthetic and chiral synthetic aspects of natural products. (21)

Natural products such as chrysanthemic acid, grandisol, prostaglandins, tricyclcopentanoids, six-membered natural products including steroids, zoapatnol. (21)

Recommended Books

1. Classics in Total Synthesis, K. C. Nicolaou and E. J. Sorenson, VCH, 1996.
2. Chemistry of Natural Products, S. V. Bhat, B. A. Nagasampagi and M. Sivakumar, Narosa Publications, 2005.
3. Bioactive Natural Products, D. S. Bhakuni and D. S. Rawat, Anamaya Publishers, 2005.
4. The Way of Synthesis, T. Hudlicky and J. W. Reid, Wiley VCH, 2007.

Computation in Chemistry

Elements of Numerical Methods and Computer Programming

Geometry optimization, Self Consistent Field calculations and correlated methods, Basis set, Frequency analysis, Population analysis, Global and local descriptors. (15)

Molecular Dynamics (MD) Simulation

Different types of classical equations of motions, Various numerical algorithms, Periodic boundary conditions and minimum image convention, Potential truncation and shifted-force potentials, Force calculations.

Monte Carlo (MC) simulation: Random numbers, Evaluating integrals using random numbers, Importance sampling, Metropolis algorithm, Smart MC techniques.

Analysis of simulated trajectories: Estimation of various distribution functions and transport properties of simulated model systems. (27)

Recommended Books

1. Computer Simulation of Liquids, M. P. Allen and D. J. Tildesley, Oxford Univ.Press, 1989.
2. Understanding Molecular Simulations, D. Frenkel and B. Smit, Academic Press, 2001.
3. Computer Oriented Numerical Methods, V. Rajaram, Prentice Hall, 2004.

Advanced Quantum Theory of Atoms and Molecules

Approximate Methods

Variational principle; LCAO approximation; Huckel Theory; Time-independent perturbation theory.
Many electron atoms: Orbital approximation, Slater determinant; Hartree-Fock self-consistent field theory; Slater type orbitals.
Angular momentum of many-particle systems. Spin orbital interaction; LS and JJ coupling. Spectroscopic term symbols for atoms. (21)

Molecules and Chemical Bonding

Born-Oppenheimer approximation, MO and VB theories illustrated with H_2 molecule; Spectroscopic term symbols for diatomics; Directed valence and hybridization in simple polyatomic molecules.

Elementary treatments of scattering and density functional theories, conceptual density functional theory based global and local reactivity descriptors. (21)

Recommended Books

1. **Modern Quantum Chemistry: Introduction to Advanced Electronic, Structure, A. Szabo and N. S. Ostlund, Dover, 1996.**
2. **Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedman, Oxford University Press, 3rd Edn., 1997.**
3. **Quantum Chemistry, I. N. Levine, 5th Edn., Pearson Education, 2000**
4. Density Functional Theory of Atoms and Molecules, R. G. Parr and Y. Weitao, Oxford University Press, 1994.

Chemical Dynamics

Transport Properties

Kinetic theory, Brownian motion; transport coefficients from time correlation function formalism; transport in solids and electrolyte solutions. (10)

Gas Phase Reaction Dynamics

Dynamics of bimolecular collisions, scattering processes, crossed molecular beams, long-lived collision complexes; adiabatic and non-adiabatic processes.

Some insight into the mechanisms of the gas phase reactions of CH_3I and I_2 (Br_2) with alkali metals. (10)

Dynamics of chemical reactions in condensed phases

Interactions between reactive molecules; hard sphere collision theory; transition state theory; Kramer's theory of reactions in solution; linear free energy relationships; unimolecular reactions; proton and electron transfer reactions; diffusion controlled reactions; Marcus theory; hydrated electron : detection, decay, and reactions with inorganic and organic substrates; biomolecular reactions; chaos in reaction-diffusion systems and fractal dimensions; nonlinear chemical dynamics. (22)

Recommended Books

1. Basic Concepts for Simple and Complex Liquids, J. L. Barrat and J. P. Hansen, Cambridge Univ. Press, 2003.
2. Chemical Dynamics in Condensed Phases, A. Nitzan, Oxford Univ. Press, 2006..
3. **Introduction to Statistical Mechanics, D. Chandler, John Wiley, 1985.**
4. Chemical Kinetics and Dynamics, J. I. Steinfeld, J. S. Francisco, W. L. Hasse, Prentice Hall, 2nd Edn., New Jersey, 1999.
5. Fast Reactions, D. N. Hague, Wiley Interscience, London, 1971.

Reference

1. Non-equilibrium Statistical Mechanics, R. Kubo, Springer, 1991.
2. Basic Chemical Kinetics, H. Eyring, S. H. Lin and S. M. Lin, John Wiley, New York, 1980.
3. **Physical Chemistry : A Molecular Approach, D. A. McQuarrie and J. D.Simon, University Science Books, 1997.**

Molecular Photochemistry

Introduction to Photochemistry

Photochemical reactions; comparison of thermal and photochemical activation; molecular electronic absorption spectra; molecular electronic emission spectra; radiationless transitions; Jablonski diagram: Franck-Condon principle, spin states and their interconversion, Kasha's rule; spin orbit

coupling, energy transfer processes, donor-acceptor complexes; excimers and exciplexes. (10)

Photochemical Laws

Laws of photochemistry; general characteristics; quantum yield and its measurements; fluorescence and phosphorescence; static and dynamic quenching; Stern-Volmer analysis; excited state life time measurements. (8)

Excited States

Energy and geometry of the excited states; excited state pK of acids and bases; study of selected photochemical reactions of alkenes, ketones, benzene, nitro compounds; sensitized photochemical reactions, photo oxidation, heterocyclic chromophores. (10)

Pericyclic Reactions

Pericyclic, electrocyclic, and cycloaddition reactions; Woodward-Hoffman rules; sigmatropic rearrangements. (6)

Photochemistry of Coordination Complexes

Brief introduction to photochemistry of inorganic anions and coordination complexes. (4)

Applied Photochemistry

Photochemistry of vision; photosynthesis; photochromism; bioluminescence; photoluminescence. (4)

Recommended Books

1. **Fundamentals of Photochemistry, K. K. Rohatgi Mukherjee, Wiley Eastern Ltd., 1978.**
2. Modern Molecular Photochemistry, N. J. Turro, University Science Books, 1991.
3. **Molecular Fluorescence, B. Valeur, Wiley-VCH, 2002.**
4. **Principles of Molecular Photochemistry: An Introduction, N. J. Turro, V. Ramamurthy, J. C. Scaiano, University Science Books, 2008.**
5. Organic Reactions and Orbital Symmetry, T. L. Gilchrist and R. C. Torr, Cambridge University Press, 1978.
6. Essentials of Photochemistry, A. Gilbert and J. Baggot, Blackwell Scientific Publications, 1992.

Bioinorganic Chemistry

Principles of Bioinorganic Chemistry

Justification of why certain protein/enzyme contains a particular metal ion. (2)

Heme Proteins: Types, function and mechanisms
Myoglobin, Hemoglobin, Cytochrome c, Cytochrome P450, Peroxidases (Horseradish Peroxidase, Chloroperoxidase), Catalase, Cytochrome c Oxidase.
*For each protein/enzyme, a 'good' model system should be discussed. (5)

Iron-Sulfur Proteins: Types, function and mechanisms
Rubredoxin, Ferredoxins, Aconitase
*For each protein/enzyme, a 'good' model system should be discussed. (3)

Non-Heme Proteins: Types, function and mechanisms
Mononuclear Systems (Catechol-1,2-Dioxygenases, Transferrin, Ferretin, Superoxide Dismutase, Isopenicillin–N-Synthase)
Dinuclear Systems (Hemerythrin, Ribonucleotide Reductase, Methane Monooxygenase, Purple Acid Phosphatases)
*For each protein/enzyme, a 'good' model system should be discussed. (6)

Copper Proteins (Type I, II, and III): Types, function and mechanisms
Blue Copper Proteins; Hemocyanin, Tyrosinase, Catechol Oxidase; Superoxide Dismutase; Ascorbase Oxidase, Laccase; galactose oxidase
*For each protein/enzyme, a 'good' model system should be discussed. (5)

Molybdenum Enzymes: Types, function and mechanisms
Oxo-Transfer Enzymes; Xanthine Oxidase; Nitrogenase
*For each protein/enzyme, a 'good' model system should be discussed. (5)

Manganese: Photosynthesis (Photosystem I and Photosystem II); function and mechanisms
*For each protein/enzyme, a 'good' model system should be discussed. (4)

Zinc Enzymes: Function and mechanisms
Hydrolytic Enzymes (Carbonic Anhydrase; Carboxy Peptidase A; Alkaline Phosphatase)
*For each protein/enzyme, a 'good' model system should be discussed. (4)

DNA/RNA: Types, function and mechanisms
DNA nicking enzymes; DNA Polymerase; Ribozymes

*For each protein/enzyme, a 'good' model system should be discussed. (4)

Environmental and Medicinal Aspects

Acid-rain; Green-house Effect.

Radiopharmaceuticals; Photo-Dynamic Therapy; Anti-Tumor Drugs (*cis*-Platin, Carboplatins; Bleomycins); ion-pumps

*For each protein/enzyme, a 'good' model system should be discussed. (4)

Recommended Books

1. **Principles of Bioinorganic Chemistry, S. J. Lippard and J. M. Berg, Panima**

Publications, New Delhi, 1997.

2. Bioinorganic Chemistry, Asim K. Das, Allied Books, Kolkata, 2004.

3. Specific Review Articles to be collected from Internet.

Single Crystal X-ray Structure Determination

Origin of X-rays, filters, monochromators, sealed tube, rotating anode and synchroton radiation, safety considerations. (2)

Crystals and their properties- direct and reciprocal lattice, planes, indices, concept of unit cell, Bragg's law in direct and reciprocal lattices. (5)

Primitive and non-primitive lattices, point and space groups, equivalent positions, systematic absences and space group determination, occupancy factors. 10)

Theory of structure factors, Argand diagram and its use, Lorentz and polarization corrections, absorption corrections, absolute scale of intensities; unit cell determination, data collection parameters, data reduction, phase problem and structure solution by Patterson and direct methods. (15)

Structure refinement techniques, presentation and interpretation of structural data, examination of CIF file and critical evaluation of a structure. (5)

Errors and pitfalls, twinning and disorder, Renninger effect, extinctions, anomalous scattering and its use. (5)

Recommended Books

1. 1 Single Crystal X-Ray Structure Data, G.U. Stout and L.H. Jenson, Springer, 1992.

2. Structural Inorganic Chemistry, A. F. Wells, Clarendon Press, 1986.

Supramolecular Chemistry

Introduction

Multidisciplinary nature, complementarity in biology, non-covalent interactions in design and synthesis of molecular assembly (electrostatic, hydrogen bonding, π -π stacking, dispersion and induction forces, hydrophobic or solvophobic effects).

Design Principles

Chelate and macrocyclic effects, characterizing supramolecular systems, structural, kinetic and thermodynamic information.

Synthesis of Macrocycles

High dilution technique, coordination template effects, Cation binding and de-metallation; porphyrins, corrins, crown ethers, cryptands, spherands, sepulchrates, siderophores, calixarenes.

Anion Binding

Properties of anions; receptor design principles, recognition by electrostatic, hydrogen bonding; Lewis acidic hosts interactions and combinations of interactions, expanded porphyrins, amide functionalized metallo compounds, cyclophanes, electrostatics and hydrophobicity. Simultaneous cation and anion binding; cascade approach, ion pairs, and zwiterions binding.
Neutral guest binding: hydrogen bond receptors, chiral recognition. Hydrophobic effect: recognition in water, solvent effect, cyclodextrins, calixarenes, metallo receptor for nucleic acid bases, boronic acid receptors for sugars.

Self -Assembly

π-electron donor-acceptor systems- Catenanes and rotaxanes, transition metal directed assemblies, molecular macrocycles and boxes: locked and unlocked molecular boxes, ladders and grids.
Hydrogen bond directed assemblies: Rosettes and ribbons, peptide nanotubes, self-replicating molecular systems, anion directed assemblies

Recommended Books

1. D. J. Cram and J. M. Cram, Container Molecules and their Guests, Monographs in Supramolecular Chemistry, Ed. J. F. Stoddart, The Royal Society of Chemistry, Cambridge, 1994.
2. **J. M. Lehn, Supramolecular Chemistry : Concepts and Perspectives, VCH,**

Weinheim, 1995.
3. Comprehensive Supramolecular Chemistry, Ed. J. L. Atwood, J. E. D.
Davies, D. D. MacNicol, F. Vogtle, vols. 2 and 3, Elsevier Science, Oxford, 1996.
4. Supramolecular Chemistry of Anions, Ed. A. Bianchi, K. Bowman-James, E. Garcia-Espana, John Wiley and Sons, New York, 1997.
5. Supramolecular Chemistry, P. D. Beer, P. A. Gale and D. K. Smith, Oxford University Press, 1999.

Nuclear and Radiochemistry

Introduction to Nuclear Science
Radioactivity, (α, β, γ) decay of nuclei, half life, radioactive series, nuclear mass and stability, isotopes.
Nuclear reactions : fission and fusion; radionuclides in nature, cosmic rays, absorption of nuclear radiation, nuclear structure. (12)

Measurement Techniques
Detection of nuclear radiations and measurement techniques, energetics of nuclear radiations and particle accelerators. (5)

Radiation Effects on Matter
Interaction of radiation with matter, radiation effects on solids, radiation biology and radiation protection. (5)

Radioactive Tracers
Radiocarbon dating, activation analysis, medical applications, probing chemical reaction mechanisms. (11)

Cosmic Radiations and Elementary Particles (3)

Production of Radionuclides
Trans Uranium Elements. (2)

Thermonuclear Reactions, Nuclear Power Generation. (2)

Behaviour of Radionuclides in the Environment (2)

Recommended Books

1. Radiochemistry and Nuclear Chemistry, G. R. Choppin, J. Rydberg and Jan-Olov Liljenzin, Elsevier, 3rd Edn., 2008.

3. Modern Nuclear Chemistry, W. D. Loveland, D. Morrissey and G. T. Seaborg, John Wiley and Sons, Inc., 2006.
2. A Text Book of Nuclear Chemistry, A. Singh and R. Singh, Campus Books International, 2005.

ELECTIVE COURSES IN CHEMISTRY

(For Students opting for subjects other than Chemistry)

Semester-III [EO-I] **Catalysis**

Principles and Applications

Catalyst
Definition, the basis of catalytic action, catalysis and equilibrium constant, auto catalysis, negative catalysis (inhibition). (3)

Homogeneous Catalysis
Homogeneous catalysis in gas phase and in solution ; acid-base catalysis, the Bronsted catalysis law, general and specific catalysis. (6)

Enzyme Catalysis
A model of reaction scheme, Michaelis -Menten Equation, enzyme active site, catalysis of hexokinase in the phosphorylation of glucose, reversible hydration of carbon dioxide by carbonic anhydrase, turn-over number, competitive inhibition in enzyme catalysis. (10)

Adsorption
Adsorption of gases on solids, physisorption and chemisorption, heat of adsorption: adsorption isotherms : Langmuir, Freundlich, and BET; catalyst active sites; Kinetics of adsorption and desorption; Surface tension: films on a liquid surface, Gibbs adsorption equation and surface excess. (10)

Heterogeneous Catalysis
Oxidation of CO on Pt , Pd; Decomposition of ammonia on tungsten surface. Amphiphilic molecules and their reorganisation in solution : micelles, micellar catalysis. (6)

Catalysis by Organometallic Compounds
Hydrogenation of olefins, hydroformylation reaction, synthetic gasoline, polymerisation reaction (Zeigler –Natta catalyst). (4)

Chain reactions
Gas phase reactions (hydrogen-bromine); free radical polymerization reactions. (3)

Books Recommended

1. **Physical Chemistry, G. M. Barrow, 4th Edn., McGraw-Hill, 1979.**
2. **Physical Chemistry - A Molecular Approach, D. A. McQuarrie and J. D. Simon, University Science Books, Sausalito, California, 1997.**
3. **Physical Chemistry, Engel and Reid, Pearson Education, 2006.**
4. **Inorganic Chemistry- Principles of Structure and Reactivity, J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, Pearson Education, 2007.**

Reference

(1) **Physical Chemistry of Surfaces, 6th Edn., A. W. Adamson and A. P. Gast, Wiley Interscience, 1997.**

(2**) Physical Chemistry, I. N. Levine, Pearson Education, 2007.**

(3) Concise Inorganic Chemistry, J. D. Lee, 4th Edn., ELBS, 1991.

(4) Basic Inorganic Chemistry, 2nd Edition, F. A. Cotton and G. Wilkinson John Wiley, 1987.

Semester-IV [EO-II]

Inorganic Chemistry

Trends in the Periodic Table

Periodicity in properties – ionization potential, electron affinity, ionic radii, electro negativity, General properties of *s*- and *p*-block elements and their compounds. (8)

Chemistry of *p*-block and *d*-block elements

Preparation, properties and uses of halogens and hydrogen halides, oxides and oxyacids of chlorine; hydride, oxides and oxy acids of nitrogen, sulphur and phosphorous.

Survey of transition elements : electronic configuration, oxidation states, complex compounds, preliminary ideas on spectral and magnetic and redox properties, shapes of molecules (VSEPR theory). (15)

Rare gases

Isolation, properties, uses and their important compounds. (3)

Introduction to general role of metals (Iron, Copper, Zinc) in some biological processes. (6)

Nuclear Chemistry

Nuclear reactions and their characteristics, radioactivity, detecting and measuring radioactivity, radioactive decay rates, nuclear stability, energy changes during

nuclear reactions, nuclear fission and fusion, nuclear transmutation, biological effects of radiation; Some applications of Nuclear Chemistry: Dating with radioisotopes, medical uses – therapeutic and imaging procedures. (10)

Recommended Books

(1) **Concise Inorganic Chemistry, J. D. Lee, 4th Edition, ELBS, 1991**.

(2) Inorganic Chemistry by Huyeeh

(3) Basic Inorganic Chemistry, Second Edition, F. A. Cotton, G. Wilkinson and P. G. Gans, John Wiley & Sons, 1987.

(4) Chemistry, J. McMurry and R. C. Fay, 4th Edition, Pearson Education, 2004.

Semester-V [EO-III]

Chemistry of Reactive Intermediates

Charged Species

Carbocations : Generation, structure and stability; direct detection; classical and non-classical carbocations; typical carbocation rearrangements. (5)

Carbanions : Generation, structure and stability; carbanions as nucleophiles; 1, 2 - anionic shifts. (5)

Neutral Species

Carbenes : Generation, structure and stability; singlet and triplet states; cyclopropanation; reactions involving carbenes. (8)

Nitrenes : Generation, structure and stability; C – H bond insertions and aziridine formation; rearrangement of acyl nitrenes (Hoffmann, Curtius). (8)

Free Radicals : Generation, structure and stability; spin trapping; radical coupling mechanisms of some known free radical reactions. (8)

Arynes (Benzynes) : Generation, structure and stability; the benzyne mechanisms; addition and rearrangement reactions. (8)

Recommended Books

1. Carbenes, Nitrenes and Arynes, T. L. Gilchrist and C. W. Reese, Nelson, London, 1969.

Semester-VI [EO-IV] Photochemistry

Photophysical and Photochemical processes

Introduction; excitation and the excited states; laws of photochemistry : Grotthus-Draper's Law, Einstein's law of photochemical equivalence; quantum yield. Jablonski diagram: Franck-Condon principle, Kasha's rule, spin states and their interconversion, spin orbit coupling, energy transfer processes, static and dynamic quenching, Stern-Volmer analysis. (8)

Bimolecular Photophysical Processes

Thermodynamics and kinetics of excited state bimolecular interactions; excimers and exciplexes, fluorescence quenching, photoinduced electron transfer, radiative and nonradiative resonance energy transfer processes; coulombic and exchange mechanisms, photosensitization. (9)

Fluorescence Spectroscopy

Characteristics of excitation and emission spectra; basic theories involving various fluorescence spectral parameters: intensity and lifetime, transition energy and its solvent dependence; fluorescence anisotropy.
Introduction to fluorescence probing techniques. (8)

Photochemistry of Carbonyl Compounds

Norrish Type – I and Type – II reactions; hydrogen abstraction reactions; Paterno-Buchi reaction; photochemistry of α, β- unsaturated carbonyl compounds; photo-reduction and photo-oxidations; photochemistry of alkenes, dienes and aromatic compounds; dye-sensitized photo-oxygenations. (11)

Applied Photochemistry

Photochemistry in nature and applied photochemistry; photochemical reactions in the atmosphere; chemistry of vision. (6)

Recommended Books

1. **Fundamentals of Photochemistry, K. K. Rohatgi Mukherjee, Wiley Eastern Ltd., 1978.**
2. Modern Molecular Photochemistry, N. J. Turro, University Science Books, 1991.
3. **Molecular Fluorescence, B. Valeur, Wiley-VCH, 2002**.
4. Principles of Molecular Photochemistry: An Introduction, N. J. Turro, V. Ramamurthy, J. C. Scaiano, University Science Books, 2008.
5. Organic Photochemistry, J. M. Coxon and B. Halton, Cambridge Univ. Press, 1974.
6. Molecular Reactions and Photochemistry, C. H. Depuy and O. L. Chapman, Prentice Hall of India.
7. Photochemistry and Pericyclic Reactions, J. Singh and J. Singh, New Age International Publishers, 2003.

***() Refers to number of lectures**