

MASTER OF SCIENCE IN CHEMISTRY

S.NO.	Name of the subject	Marks
I YEAR		
1.	Organic Chemistry – I	100
2.	Inorganic Chemistry – I	100
3.	Physical Chemistry – I	100
4.	Polymer Chemistry – I	100
5.	Spectroscopy	100
6.	Practical I – Inorganic Chemistry – I	100
7.	Practical II – Organic Chemistry – I	100
8.	Practical III – Physical Chemistry – I	100
II YEAR		
9.	Organic Chemistry – II	100
10.	Inorganic Chemistry – II	100
11.	Physical Chemistry – II	100
12.	General Chemistry – II	100
13.	Analytical	100
14.	Practical IV – Inorganic Chemistry – II	100
15.	Practical V – Organic Chemistry – II	100
16.	Practical VI – Physical Chemistry - II	100

1st - YEAR
Paper – 1
ORGANIC CHEMISTRY – I

UNIT – I

Electron displacements : Inductive and Field effects – mesomeric and hyper conjugative effects – steric inhibition and steric enhancement of resonance. Organic acids and bases – Bronsted and Lewis concepts, influence of inductive, mesomeric and steric effects on strengths of acids and bases.

Organic Reaction Mechanisms: Classification of organic reactions – General methods of investigating reaction mechanism – kinetic and non-kinetic methods, kinetic and thermo dynamic control – principle microscopic reversibility.

UNIT – II

Optical isomerism : chirality – asymmetry – dissymmetry – homotopic – enantiotopic diastereotopic hydrogens – optical isomerism of compounds containing one and more than one asymmetric carbon atoms – projection formula – configuration R.S. notation of absolute configuration optical isomerism of Nitrogen and Sulphur compounds, allenes, spiranes and diphenyls – dissymmetric overcrowded molecules – resolution – racemisation Walden inversion – asymmetric synthesis Cram's rule – Prelog's rule – asymmetric transformation. Geometrical isomerism in carbon – carbon double bond and carbon – nitrogen double bond – E,Z notations – determination of configuration of geometrical isomers.

UNIT – III

Aromaticity : Hückel's rule and MO approach to aromaticity in various carbocyclic systems and charged species – non-aromatic and anti-aromatic systems – absorption spectra and induced ring current.

Chemistry of cyclopropanium cation cyclopentadienyl anion – cycloheptatrienium cation to tropylium cation – annulenes – fulvenes – ferrocene. Organic Reactive Intermediates. Free radicals – formation, structure, detection, stability and reactions. Formation, structure, reactions

and stability of carbocations, carbanions, carbenes, nitrenes, arynes and non-classical carbocations.

UNIT – IV

Organic Photo-chemistry : Photochemical reactions of saturated ketones – Norish type I and II reactions – photoreduction – paterno Buchi reaction – reaction of α, β –unsaturated ketones – Isomerisation – photo rearrangement of cyclohexedone. Photochemistry of simple alkenes cis-trans isomerisation – photochemical oxidations – oxidative coupling – Barton reaction.

Conformational Analysis :

Conformation in open chain system energy consideration – conformation of cyclohexane and its mono, disubstituted derivatives. Effect of conformation on reactivity in acyclic compounds and cyclohexane derivatives.

UNIT – V

Alkaloids and Terpenoids : General methods of structural elucidation and biosynthesis of alkaloids and terpenoids. Structure and synthesis of alkaloids atropine – terpenoids – Zingiberene. Carbohydrates and Polymers. Structure, configuration and conformation of sucrose, maltose, starch and cellulose. Synthetic polymers – addition polymers – stereochemistry of polymers – stereochemical control of polymerisation – Zeigler – Natta catalyst.

Text Books and References:

1. Ferguson, The Modern Structural Theory of Organic Chemistry.
2. I.L. Finar, Organic Chemistry, Vol I and II, ELBS.
3. Pelletier (Ed.) Chemistry of Carbohydrates.
4. Gulhrine and J.Honeyman, An Introduction to the chemistry of Carbohydrates.
5. P.J. Garrat, Aromaticity.
6. E.L. Eliel, Stereochemistry of Carbon Compounds, Tata McGraw Hill – 1962.
7. Coxon and Halton, Organic Photochemistry.
8. w. Billmeyer, A Text Book of Polymer Science, Wiley – Inter-Science, 1984.

9. Jerry March, Advanced Organic Chemistry – Reactions, Mechanisms and Structure,
Fourth Edition, McGraw Hill International Book Company, 1995.

Paper – 2

INORGANIC CHEMISTRY – I

UNIT – I

Plank's Quantum theory, wave particle duality, uncertainty Principle, Operator and observables – postulates of Quantum Mechanics – Schrodinger equation – interpretation of Wave function and expectation (eigen) values. Orthogonality and Normalisation of wave function – principle of super position. Application of Schrodinger wave equation to particle in one dimensional box – three dimensional box.

UNIT – II

Schrodinger equation for hydrogenation, separation of variables, phi-equation, theta equation and radial equation, total wave function, quantum numbers and their significance, shapes of atomic orbitals, Electron spin and Pauli exclusion principle, poly electronic atoms, Inter electron repulsion and its consequences. Energy levels in poly electronic atoms, R-S coupling, spin-orbit coupling, J-J coupling, Microstates and their classification, Term symbols.

UNIT – III

Nature of covalent bond, valence bond Method, concept of resonance and hybridization and bond angles, application to simple molecules, molecular orbital theory, Geometries of the orbitals, symmetry and anti-symmetry of molecular orbitals, construction of molecular orbitals in diatomic molecules molecular orbitals in polar molecules. Ionic bonding, Lattice energy, Born equation and its derivation radius ratio rules, structures of some ionic crystals (Sodium Chloride, Cesium Chloride, Rutile, Wurtzite, Fluorite), hydrogen bonding.

UNIT – IV

Co-ordination chemistry of transition Metal ions. Introduction – nomenclature – stability constraints of complex and their determination (pH metric and spectrophotometric methods). Factors influencing stability. Stabilization of unusual oxidation states. Stereoisomerism of co-ordination complexes – absolute configuration of complexes – stereoselectivity of the conformation of chelate rings.

UNIT – V

Bonding in complex : metal – ligand bond – V.B. theory and its limitations – crystal field theory – splitting of d-orbitals, CFSE evidence for CFSE. Factor affecting splitting, spectrochemical series, site preference, Limitations of CFT, ligand theory, M.O. theory sigma and pi-bonding in complexes. Spectral and magnetic properties of complexes/ Term states for a d-ions in octahedral complexes. Characteristic of d-d transitions. Energy level diagrams of Orgel, Tanabe Sugano – weak field and strong field concepts. Jahn Teller distortion, Nephelauxetic effect, Magnetism : dia, para magnetism, spin only moments of dn-systems.

Text Book and Reference :

1. A.K. Chandra, Introductory Quantum Chemistry, Tata McGraw Hill, 1997.
2. R.K. Prasad, Quantum Chemistry, New Age International, 1993.
3. B.K. Sen, Quantum chemistry, Tata Mc Graw Hill, 1999.
4. E.A.V. Ebsworth, S.rankine and S.Craddock, ELBS, 1991.
5. M.C.Day and J.Selbin, Teoretical Inorganic Chemistry.
6. J.E. Hubblee, Inorganic Chemistry, Addison Wesley, 1993.
7. B.E. Darglas, D.H. Mc Daniel and Alexander, Concepts and Models of Inorganic.
8. F.A. Cotton and G.Wilkinson, advanced Inorganic Chemistry, wiley-Eastern, 1998.
9. L.Pauling, The Nature of the Chemical Bond, 1961.
10. S.F.A. Kettle, Co-ordination compounds.
11. D. Bannerjea, Co-ordination Chemistry, Tata McGraw Hill, 1993.
12. Figgis, Introduction to Ligand Field Theory. Wiley-Eastern, 1976.

Paper – 3
PHYSICAL CHEMISTRY – I

UNIT – I

Thermodynamics : Calculation of adiabatic flame temperature, Maxwell's relations, thermodynamic equations of state, thermodynamics of open systems, partial molal quantities, chemical potential, Gibb's – Duhem equation, variation of chemical potential with temperature and pressure, third law of thermodynamics. Nernst heat theorem, Chemical equilibrium Van't Hoff reaction isotherm, standard free energy change of reactions, variation of equilibrium constant with temperature and pressure.

UNIT – II

Spectroscopy : Origin of molecular spectra, rotational spectra rigid rotator, vibrational, rotational spectra Harmonic oscillator, Fundamentals and overtones, force constant, electronic spectra of diatomic molecules, Frank-Condon principle, transition probability, potential energy curves and their applications. Raman spectra, polarization and polarizability selection rules.

UNIT – III

Group Theory : symmetry operations point groups, identification of point group, reducible and irreducible representation, orthogonality theorem. Construction of C_{2v} and C_{3v} character tables, symmetry selection rules for I.R. and Raman spectra, procedure for determining symmetry of normal modes of vibration hybrid orbitals in non-linear molecules BF_3 , PCl_5 , CH_4 , NH_6 .

UNIT – IV

Solid State Chemistry : Dislocation in solids, Schottky and Frenkel defects, F-centre, electrical properties : Insulators, semiconductors, conductors, superconductors, Band theory of solids, conducting polymers, liquid crystals, fullerenes.

UNIT – V

Potential energy surface – absolute reaction rate theory, ARRT in thermodynamic terms. Significance of entropy and volume of activation. Ionic reaction – salt effect – Kinetic isotopic effect. Fast reactions – stopped flow technique method – Laser flash photolysis, magnetic resonance method. Acid – base catalysis – Bronsted relation – enzyme catalysis – Heterogeneous catalysis : Langmuir – Hinshewood and Ridel – Elay mechanisms.

Text Book and Reference :

1. K.J. Laidlet, Chemical Kinetics, Tata McGraw Hill, 1973.
2. Agarwal, Basic chemical Kinetic, Tata McGraw Hill, 1990.
3. S. Glasstone, An Introduction to Electrochemistry Affiliated, East-West Press, 1971.
4. F.A. Cotton, Chemical Application of Group Theory, Wiley Eastern, 1971.
5. S. Glasstone, Text book of Physical Chemistry, McGraw Hill, 1956.
6. W.J. Moore, Basic Physical Chemistry, Prentice-Hall, 1986.
7. K.V. Raman, Group Theory and its Application to Chemistry, Tata McGraw Hill, 1993.
8. C.N. Banwell, Fundamental of Molecular Spectroscopy, Tata McGraw Hill, 1983.
9. G. Glasstone, Thermodynamics for Chemists, Affiliated East Press, 1947.
10. Gupta, Statistical Thermodynamics, Wiley Eastern, 1986.
11. Rajaram and J.C. Kuriakose, Thermodynamics for students of chemistry, shoban Lal Nagin Chand, 1986.

Text Book and Reference :

1. Text Book of Polymer Science, F.W. Billmeyer Jr. Wiley.
2. Polymer Science, V.R. Gowarker, N.V. Viswanathan and J. Sreedhar, wiley – Eastern
3. Functional Monomers and Ploymers, K.Takemot, Y.Inaki and R.M. Ottanbrite.
4. Contemporary Polymer Chemistry, H.R.Alcock and F.W. Lamber, Prentice Hall.
5. Physics and Chemistry of Polymers, J.M.G. Cowic, Blackie Academic and Professionnal.

Paper – 4

POLYMER CHEMISTRY

UNIT – I

Basic concepts : Monomer, repeat units, degree of Polymerization, Linear, branched and network Polymers. Condensation Polymerization. Addition polymerization : Free radical, cationic and anionic polymerization conditions. Polymerization in homogeneous and heterogeneous systems.

UNIT – II

Coordination Polymerization : Kinetics, mono and bimetallic mechanism of coordination polymers.. Co-polymerization : Block and graft co-polymers, Kinetics of copolymerization. Types of copolymerization. Evaluation of monomer. Reactivity ratio. Rate of Co-polymerization.

UNIT – III

Molecular weight and properties of polymers : Polydispersion – average molecular weight concept, number, weight and viscosity average molecular weights. Measurement of molecular weights. Gel permeation chromatography, viscosity, light scattering, osmotic and ultracentrifugation methods. Polymer structure and physical properties – crystalline melting point T_m . The glass transition temperature. Determination of T_g . Relationship between T_m and T_g .

UNIT – IV

Polymer Processing : Plastics, elastomers and fibers. Compounding processing techniques : calendaring, die casting, rotational casting, film casting, injection moulding extrusion moulding, thermoforming, foaming, reinforcing and fibre spinning.

UNIT – V

Properties of Commercial Polymers : Polyethylene, polyvinyl chlorides, polyesters, phenolic resins, epoxy resins and silicone polymers. Functional polymers – Fire retarding polymers and electrically conducting polymers. Biomedical polymers – contact lens, dental polymers, artificial heart, kidney, skin and blood cells.

Paper – 5

SPECTROSCOPY

UNIT – I

UV and IR Spectroscopy : Ultraviolet – visible spectroscopy – types of electronic transitions – chromophores and auxochroms – factors influencing position and intensity of absorption bands – absorption spectra of dienes, ployenes and α , β – unsaturated carbonyl compounds – woodward – fieser rules.

IR Spectroscopy – vibrational frequencies and factors affecting them – identification of functional groups – intra and inter molecular hydrogen bonding – finger print region – far IR region – metal ligand stretching vibrations.

UNIT – II

^1H NMR Spectra : Nuclear spin – magnetic moments of a nucleus – nuclear spin energy levels in the presence of magnetic fields, basic principles of NMR experiments – CW and FT NMR – ^1H NMR chemical shift and coupling constants – factors influencing proton chemical shifts and vicinal proton – proton coupling constants.

UNIT – III

^{13}C NMR and Two dimensional NMR Spectroscopy : ^{13}C NMR – proton decoupled and off-resonance – ^{13}C NMR spectra – factors affecting ^{13}C chemical shifts – ^{13}C NMR spectra of simple organic molecules – use of INEPT and DEPT methods in assigning ^{13}C signals. Basic principles of two dimensional NMR spectroscopy – HOMOCSY, HETCSY, NOESY.

UNIT – IV

Principles – Measurement techniques (EI, CI, FD FAB, SIMS) – Presentation of spectra data – molecular ions – isotope ions – fragment ions of odd and even electron types – rearrangement ions – factors affecting fragmentation patterns – McLafferty rearrangement.

UNIT – V

Identification of organic compounds using UV, IR, NMR spectroscopy and mass spectrometry – problems.

PRACTICALS

Practical – 1

INORGANIC CHEMISTRY – I

1. Qualitative Analysis

Qualitative Analysis involves the analysis of a mixture containing four cations.

2. Colorimetric estimations.

- Estimation of Iron.
- Estimation of Nickel
- Estimation of Copper.

Practical – 2

ORGANIC CHEMISTRY – I

- Preparation of p-Bromoacetanilide
- Preparation of p-Bromoaniline
- Preparation of Benzoin
- Preparation of Nenzil
- Preparation of S-Benzyl-iso-Thiruonium chloride
- Preparation of Benzpinacol


Organic Mixture Analysis

Analysis if organic mixture contain two components including separation.

Practical – 3

PHYSICAL CHEMISTRY – I

Partition of Co-efficient

- Determination of partition coefficient of iodine between carbon tetracholoride and water.
- Determination of equilibrium constant for the reaction $I_2 +$  I_3

3. Estimation of I ions from a knowledge of the equilibrium constant of the above reaction.

Conductivity Measurements

4. Determination of cell constant of a conductivity cell.

5. A study of variation of equivalent conductance of a strong electrolyte with concentration.

6. Determination of dissociation constant of a weak acid.

7. Conductometric Titrations :

a. Mixture of HCL and acetic acid Vs NaOH.

b. Ammonium chloride Vs NaOH.

c. A solution containing Ba^{2+} ions Vs a solution containing SO_4^{2-} .

Phase Rule

8. Construction of phase diagram for diphenyl-naphthalene system.

9. Determination of composition of a mixture of diphenyl and naphthalene.

Determination Of Molecular weights

10. Determination of molecular weight by cryoscopic method using benzene as solvent.

11. Determination of molecular weight by cryoscopic method using water as solvent.

12. Determination of molecular weights by Rast's Method.

IIND – YEAR
Paper – 6
ORGANIC CHEMISTRY – II

UNIT – I

ADDITION TO CARBON-CARBON MULTIPLE BONDS

Electrophilic and nucleophilic additions, addition to conjugated systems, orientation and reactivity, addition of halogen and nitrosyl chloride to olefins, hydration of olefins and acetylenes, hydroboration, hydroxylation epoxidation, Michael addition, 1,3 dipolar addition, carbenes and their additions, Diels-alder reactions.

UNIT – II

ADDITION TO CARBON-HETERO ATOM MULTIPLE BONDS

Mechanism and reactivity. Mannich, Stobbe, Darzens Glycidic ester condensation, Bensoin condensation, Peterson olefination (silyl Wittig reaction). Strecker synthesis. Wittig. Wittig-Horner, Perkin, Thorpe, Ritter, Prins reactions.

UNIT – III

ELIMINATION REACTIONS

E1, E2, E1cB mechanisms, Orientation of the double bond, Hofmann and Saytzeff rule, competition between elimination and substitution, dehydration and dehydrohalogenation reactions, stereochemistry of E2 eliminations in cyclohexane ring systems, mechanism of pyrolytic eliminations. Chugaev reaction and Cope elimination.

UNIT – IV

MOLECULAR REARRANGEMENTS

A detailed study of the mechanism of the following rearrangements : Nucleophilic, Electrophilic and Free radical rearrangements – memory effects, Migratory aptitudes, Pinacol-Pinacolone, Wagner-Meerwein, Demjanov, Dienone-phenol, Favorski, Baeyer-Villiger, Wolff, Stevens and Von-richter (a few examples in each rearrangement are to be studied), rearrangements involving nitrenes – Hofmann, Curtius, Lossen, and Beckmann.

UNIT – V

OXIDATION AND REDUCTION

Study of the following oxidation reactions with mechanism: Oxidation of alcohols by CrO_3 , DMSO alone, DMSO in combination with DC; acetic anhydride and oxalyl chloride, oxidation of arylmethane, oxidation of methylene alpha to carbonyl, allylic oxidation of olefins, oxidative cleavage of glycols, oxidative cleavage of double by ozonolysis.

Study of the following reduction reactions with mechanism : Reduction of carbonyl compounds by hydrides, selectivity in reduction of 4-ter-butyl cyclohexanone using selectrides, Clemmensen and Wolff Kishner reductions, Birch reduction, MPV reduction.

Text Books :

1. Advanced Organic Chemistry – Reactions, Mechanisms and Structure. Fourth Edition, Herry March, John wiley & Sons (1992).
2. Organic Chemistry, Francis A. Carey, Third Edition, The McGraw_Hill Companies, Inc.
3. Organic Chemistry , Hendrickson, Cram and Hammond, Thord Edition, McGraw Hill Book Company.
4. Organic Reactions and Mechanisms, P.S. Kalsi, Second Edition, New Age International Publishers.
5. Stereochemistry of Carbon Compounds, Ernest L. elite, T.M.H. edition, Tata McGraw Hill Publishing Company.
6. Stereochemistry – Conformation and mechanism, P.S. Kalsi, Wiley Eastern Limited.
7. Stereochemistry and mechanism through solved problems, P. S. kalsi, Second Edition, New Age International Publishers.
8. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International Publishers.
9. Reaction Mechanism in Organic chemistry, S.M. Mukerherji and S.P. Singh, Macmillan.
10. Organic Chemistry, R.T. Morrison and R.N. Boyd, Prestice-Hall.
11. Principles of Organic synthesis, R.O.C. Norman, Second Edition, Chapman and Hall.
12. Organic Reaction Mechanism S.M. Mukherji and S.P.singh, Macmillan India.
13. Physical Organic Chemistry, Neil Issac.

14. Molecular rearrangements, Vol.I, Vol.II, Pane de Mayo.
15. Structure and Mechanism, E.S. Gould.

Paper – 7

INORGANIC CHEMISTRY – II

UNIT – I

CO-ORDINATION CHEMISTRY

Crystal field theory, splitting of d-orbitals under various geometries, Factors affecting splitting, CFSE and evidences for CFSE (Structural and thermodynamic effects). Spectrochemical series, Jahn-Teller distortion, site preferences, limitations of CFT. Evidence for metal-ligand overlap. M.O. theory and energy level diagrams, concept of weak and strong fields, sigma and pi bonding in complex, nephelauxetic effect, magnetic properties of complexes.

UNIT – II

ELECTRONIC SPECTRA OF COMPLEXES

Term symbols for d^n ions, characteristics of d-d transitions and selection rules, weak and strong field limits, Energy level diagrams. Orgel and Tanabe-Sugano diagrams, effect of distortion and spin orbital coupling on spectra. Evaluation of Dq and B value for octahedral complexes of Nickel, Charge transfer spectra.

UNIT – III

SOLID STATE CHEMISTRY

Structure of Solids, comparison of x-ray, neutron and electron diffraction, Structure of NiAs , CdI_2 , perovskite, spinels and inverse spinels, defects in solids, point defects, line defects and surface defects, non-stoichiometric compounds, Use of x-ray powder data in identifying inorganic crystalline solids, details for cubic systems.

UNIT – IV

PROPERTIES OF SOLIDS

Electrical properties of solids, Band Theory, Semiconductor, super conductor, solid state electrolytes. Magnetic properties, dia, para, ferro, antiferro and ferrimagnetism, hysteresis, ferrites, garnets. Optical properties, solid state lasers and Inorganic phosphors. Reactions in solid state and phase transitions, diffusion coefficient, diffusion mechanism, vacancy and

interstitial diffusions, formation of spinels. Solid solution, order-disorder transformations and super structure.

UNIT – V

ANALYTIC TECHNIQUES

Chromatography : Gas, liquid chromatography, principle, retention volumes, carrier gas, columns, preparations, stationary phase, detectors, thermal conductivity, ionization, electron capture applications of GLC.

High performance liquid chromatography : scope, column efficiency, instrumentation, pumping systems, columns, column packing detectors, applications.

Text Books :

1. Inorganic Chemistry, K.F. Purcell and J.C. Kotz. WB Saunders Co., U.S.A (1977)
2. Inorganic Chemistry, J.E. Huheey, Harper and Collins, NY, Fourth Edition (1993)
3. Advanced Inorganic Chemistry – A Comprehensive Text, F.A, Cotton and G.W.wilkinson, John Wiley & sons (1988)
4. B.E. Douglas, D.H Mc Daniels and Alexander, Concepts and Models of Inorganic Chemistry, Oxford IBH (1983)
5. W.U.Malik, G.D. Tuli, R.D, Madan, Selected topics in Inorganic Chemistry, S.Chand & Co., New Delhi (1992)
6. A.R. West, Basic Solid State Chmeistry, John Wiley (1991)
7. W.E. Addison, Structural Principles Principles in Inorganic chemistry, Longman (1961)
8. D.M. Adams, Inorganic solids, John Wiley Sons (1974)
9. Principles of Instrument Methods of Analysis – D.A. Skooig, Sauuders college Publ. III Edition (1985)
10. Indtrumental Methods of Analysis, Willard Merrit, Deace and settle, CBS Publ. VI Edition 1986.
11. Text Books of Qualitative Inorganic Analysis – A.1. Vogel, ELBS III edition, 1986.
12. Fundamentals of analytical Chemistry, D.A. skoog and D.M. West Holt Reihhart & Winston Publication, IV Edition, 1982.

Reference:

1. Instrumental Analysis, G.D. Christian & J.E.O. Reily, Alagan Becon II Edition, 1986.
2. Chemical Instrumentation, H.A., Strobel Addison – Wesley Publ. Co. 1976.
3. Treatise on Analytical Chemistry, Klthoff and Goning (all series)
4. Comphrehensive Analytical Chemistry, Wilson and Wilson Series.
5. Principles of Polarrgraphy, R.C. Kappor and B.S. Agarwal, Wiley Eastern Ltd, Ms 1991.
6. S.F.A. Kettle, Co-ordination Chemistry, ELBS (1973)
7. B.N. Figgis, Introduction to Ligand Fields Interscience. (1996)
8. M.N. Hughes, The Inorganic chemistry of Biological processes, Wiley London (1982).
II Edition.
9. D.Noeholas, Complexes of first row transition elements, (1974)
10. D.F. Shrivvers, P.W. Atkins, CII Langford, Inorganic Chemistry, OUP (1990)
11. M.C. Day and J.Selbin, Theoretical Inorganic Chemistry, Van Nostrand Co., N.Y. (1974)
12. G.S. Manku, Inorganic Chemistry, TMH (1984)
13. A.F. Wells, Structural Inorganic Chemistry, Oxford, V Edition (1984)
14. R. West, solid State Chemistry, John Wiley (1990)

Paper – 8
PHYSICAL CHEMISTRY – II

UNIT – I

CHEMICAL KINETICS – II

- 1.1 Catalysis by enzymes, kinetics of single substrate enzyme catalyzed reactions, effect of substrate concentration. pH and temperature of enzyme catalyzed reactions, inhibition of enzyme catalyzed reactions.
- 1.2 Kinetics of complex reactions, reversible reactions, consecutive reactions, parallel reactions chain reactions, general treatment of chain reaction, chain length, Rice Herzfeld mechanism, explosion limits.

UNIT – II

2.1 STUDY OF KINETICS OF SURFACE REACTIONS

Physical and Chemical absorption, adsorption, isotherms, types of adsorption isotherms, Langmuir adsorption isotherm. BET theory for multilayer adsorption, application of transition state theory to adsorption, measurement of surface area, catalysis by metals and semiconductor oxides. Mechanisms of heterogeneous catalytic reactions, the adsorption coefficient and its significance

2.2 Study of fast reactions

Relaxation methods, temperature and pressure jump methods, stopped flow and flash photolysis methods.

UNIT – III

THERMODYNAMICS – II

- 3.1 Objectives of statistical thermodynamics, concept of thermodynamic and mathematical probabilities, distribution of distinguishable and indistinguishable particles. Maxwell-Boltzmann, Fermi-dirac, Bose-Einstein statistics, comparison and applications, modes of contribution to energy, radiation law.
- 3.2 Partition function, evaluation of translational vibrational and rotational partition functions for mono, diatomic and polyatomic ideal gases, thermodynamic functions in terms of partition

functions, calculation of equilibrium constants from partition functions (isotope exchange and dissociation of diatomic molecules), application of partition functions to heat capacities of ideal gases, heat capacity of solids (Einstein and Debye models).

UNIT – IV

Experiment results of black body radiation – photo effect, Compton effect, quantum mechanical postulates, the Schrödinger equation – the particle in a box (one, two and three dimensional systems), the harmonic oscillator.

UNIT – V

Wave particle duality – de Broglie equation, uncertainty principle. Schrödinger equation for the rigid rotator, the hydrogen atom – setting up the Schrödinger, arriving solution for energy and wave functions. The origin of quantum numbers and their physical significance.

Text Books :

1. Kinetics and Mechanism of Chemical transformations, J. Rajaram and J.C. Kuriacose, MacMillan India Ltd., (1993)
2. Chemical Kinetics, K.J. Laidlar, Harper and Row, New York (1987)
3. Statistical Thermodynamics, M.C. Gupta, Wiley Eastern, New Delhi (1990)
4. Introduction to Thermodynamics of Irreversible process, I. Prigogine, Interscience, New York (1961)
5. Quantum Chemistry, D.A. McQuarrie, University Science Books, Mill Valley, California (1983)

Reference:

1. R.G. Frost and Pearson, Kinetics and Mechanism, Wiley, New York., 1961
2. W.J. Moore and R.G. Pearson, Kinetics and Mechanism 1981
3. C. Capellos and B.H.J. Bielski, Kinetics, Wiley Interscience, New York 1972
4. I. Amdur and G.G. Hammes, Chemical Kinetics, Principles and selected topics, McGraw Hill, New York 1968
5. G.M. Harris, Chemical Kinetics, D.C. Heath and Co., 1966.

Paper – 9

PHOTOCHEMISTRY AND GROUP THEORY

UNIT – I

INORGANIC PHOTO CHEMISTRY

Photo substitution, Photo rector and isomerization process, application of metal complexes in solar energy conversion. Photo voltaic and photogalvanic cells, photo electro chemical cell, photo assisted electrolysis of water, aspects of solar energy conversion.

UNIT – II

ORGANIC PHOTOCHEMISTRY

Fundamental concepts – Jablonski diagram – energy transfer characteristics of photo reactions, Photo reduction and photo oxidation and Photo reactions of carbonyl compounds, Norrish Type I and type-II reactions, Photo chemistry of alkenes, dienes and aromatic compounds – reactions of unactivated centres – Photolytic cyclo – additions and photolytic rearrangements – Photo sensitisation – Photo addition – Barton reactions – Paterno – Buchi reaction.

UNIT – III

Absorption and emission of radiation, Franck – Condon Principle, decay of electronically excited states, radioactive and non-radioactive processes, fluorescence and phosphorescence, Spin forbidden, radioactive transition, internal conversion and inter system crossing, energy transfer Process, excimers and exciplexes, static and dynamic quenching, Stern Volmer analysis Experimental methods, quantum yields and life time measurements, steady state quantum yield and chemical actinometry, Photophysical process and Kinetics of Photochemical reactions, Photo redox, reactions, photo substitution reactions, photo sensitized reactions, photo isomerisation.

UNIT – IV

GROUP THEORY – I

Symmetry elements and symmetry operation, point groups, identification and determination, comparison of molecular symmetry with crystallographic symmetry, reducible and irreducible representations, direct product representation, orthogonality theorem and its consequences, character tables.

UNIT – V

GROUP THEORY – II

Hybrid orbitals in non-linear molecules (examples BF_3 , CH_4 , XeF_4 , PCl_5 and SF_6), determination of representations of vibrational modes in – non-linear molecules such as H_2O , CH_4 , XeF_4 , SF_6 and NH_3 , Symmetry. Selection rules for infra red and Raman Spectra, Electronic Spectra of formaldehyde, application of group theory.

Text Books:

1. F.A. Cotton, Chemical Application of Group theory, 2nd ed, Wiley Eastern (1971).
2. Inorganic Photochemistry, A.W. Adamson.
3. Horspool, Aspects of organic photo chemistry, Academic Press, 1976.
4. K.K. Rahatgi – Mukherjee, Fundamentals, of Photo chemistry, Wiley Eastern, 1978.
5. N.H. Furrow, Molecular Photo Chemistry, W.A. Benjamin. Reading, 1965.

Paper – 10
ANALYTICAL TECHNIQUES

UNIT – I

Gravimetric Analysis:

Formation and treatment of precipitates: co-precipitation, post precipitation and absorption phenomena – Homogeneous precipitation –making – Specific and Selective precipitations.

Volumetric Analysis:

Theory and principles of acid base redox complexometric and precipitation titrations – Titrations in non-aqueous solvents Equilibria in solutions of mono and polyprotic acids – Amino acid titrations.

Treatments of Analytical Data:

Nature of quantitative measurements and treatment of data accuracy and precision – types of errors – Significant figures – mean and standard deviation - rejection of data – comparison of results – F and T tests – regression and correlation.

UNIT – II

Instrumental Methods of Analysis: Instrumentation: Instrumentation in Uv, IR, Raman, NMR and EPR Spectral Methods.

Atomic Absorption Spectroscopy: Principles and applications.

UNIT – III

Electro Analytical Methods:

Principles and applications of potentiometry, Conductometry, electro gravimetry, coulmetry, polarography and cyclic voltametry – amperometric titrations.

Thermal Methods:

Principles and applications of thermo gravimetric and differential thermal analysis.

UNIT – IV

Chromato Graphic Methods of Analysis:

Theory of chromatography – Distribution equilibria –rate of travel – retention time – retention volume – relative retention – Plate theory – rate theory – resolution.

Principles of column, paper, vapor, Thine layer and ion exchange chromatographic methods – Examples for separation and purification using the above methods – Zone electrophoresis and highperformance liquid chromatography.

UNIT – V

Electronics:

Electrical fundamentals, Resistance – Capacitance – inductance impedance – resonance – Electrical circuits – Filters – Semi conductors – devices – Diodes – Transistors – Operational amplifiers – rectifiers – circuits for polarography, coulometry and potentiometry – chemical instrumentation – origin and type of noise optimization of signal to noise ratio.

Computer Programming:

Input and output statements, Transfer and control statements, programming in BASIC only for calculation of equilibrium constants, PH of buffer, Potentio metric titrations and Standard deviation.

Ms Word, Ms-Excel and Internet usage, Ms Power point.

Text Books:

1. Text Book of Quantitative Inorganic Analysis, ELBS, A.I. VOGEL.
2. Instrumental Methods of Analysis, Willard, Merit, Dean and Settle, CBS Puhlishers and Distributors, V1. Edn, 1986.
3. Principles of Instrumental Analysis, D.A. Skog and D.M. West Sounders College, Pub. Co, III ed, 1985.
4. E. Balagurusamy, Programming Inc., TMH New Delhi.

Reference:

1. Analytical Chemistry, J.G. Dick, McGraw Hill, Publishers, 1974.
2. Electronic Principles, Albert Paul, Mahino, TMH Publishers, III edn, 1984.
3. Galen W. Ewing, Instrumental Methods of Chemical Analysis, V Edn. McGraw Hill, N.Y, 1985.

Practical – 4

INORGANIC CHEMISTRY PRACTICAL – II

Part – I

Semimicro qualitative analysis of mixtures containing two common and two rare cations.

The following are the cations to be included : W, Ti, Mo, Tc, Sc, Cr, Th, Be, Zr, V, U and Li.

Part – II

a. Colorimetric analysis : Visual and photometric : determination of iron, nickel, manganese and copper.

b. Preparation of the following :

- i. Potassium trioxalatoaluminate (III) trihydrate
- ii. Trithiourea copper (I) chloride
- iii. Potassium trioxalatochromate (III) trihydrate
- iv. Sodium bis (thiosulphato) cuprate (I)
- v. Tetramminecopper (II) sulphate
- vi. Potassium Tetrachlorocuprate (II)

c. Separation of mixture of two metal ions by paper chromatography.

Practical – 5
ORGANIC CHEMISTRY PRACTICAL – II

1. Identification of components in a two component mixture and preparation of their derivatives. Determination of boiling point/melting point for components and melting point for their derivatives.

II. Preparation :

1. Beta naphthyl methyl ether from beta naphthol
2. S- Benzyl isothiuronium chloride from benzylchloride
3. Beta glucose penta acetate from glucose
4. Ortho-Benzoyl benzoic acid from phthalic anhydride
5. Resacetophenone from resorcinol
6. Para-Nitrobenzoic acid from para nitrotoluene
7. Meta-Nitroaniline from meta dinitrobenzene
8. Methyl orange from sulphanilic acid
9. Anthraquinone from anthracene
10. Benzylhydrol from benzophenone

Reference: Laboratory manual of organic chemistry – B.B. Dey, M.V. Sitaraman

Practical – 6

PHYSICAL CHEMISTRY PRACTICAL – II

Experiments in chemical kinetics, phase rule, chemical equilibrium and Conductivity measurements:

DETAILED OF EXPERIMENTS: Typical list of possible experiments are given.

Experiments of similar nature and other experiments may also be given. The list given is only a guideline. A minimum of 15 experiments have to be performed in a year.

1. Study the kinetics of acid hydrolysis of an ester, determination of the temperature coefficient of the reaction and determination of the activation energy of the hydrolysis of ethylacetate.
2. Study the kinetics of the reaction between acetone and iodine in acidic medium by half life method and determine the order with respect to iodine and acetone.
3. Study of the saponification of ethylacetate by sodium hydroxide conductometrically and determine the order of the reaction.
4. Determination of dissociation of ethylacetate by sodium hydroxide conductometrically and determine the order the reaction.
5. Study the phase diagram for m-toluidine and glycerin system.
6. Construction of phase diagram for a simple binary system (naphthalene-phenanthrene and benzophenone-diphenylamine).
7. Construction of the phase diagram of the three component of partially immiscible liquid systems (DMSO-Water-Benzene; Water-Benzene-Acetic acid; Ethyl alcohol-Benzene-Water; Acetone-Chloroform-Water; Chloroform-Acetic acid-Water).
8. Determination of the equilibrium constant of the reaction between iodine and partition method.
9. Determination of equivalent conductance of a weak acid at different concentrations and verify Ostwald's dilution law and calculation of the dissociation constant of the acid.
10. Determination of equivalent conductivity of a strong electrolyte at different concentrations and examine the validity of the Onsager's theory as limiting law at high dilutions.

11. Conductometric titrations of a mixture of HCL and CH_3COOH against Sodium hydroxide.
12. Compare the relative strength of acetic acid and monochloroacetic acid by conductivity method.