M.SC., CHEMISTRY SYLLABUS

MADURAI KAMARAJ UNIVERSITY

Course structure & Credits Distribution

Sub. Code		Title of the paper	Credit	Internal	External	Total
Core	ECH8C11	Introduction to Organic Reactions	5	25	75	100
Core	ECH8C12	Structure and Bonding	4	25	75	100
Core	ECH8C13	Thermodynamics, Chemical Equilibrium and Electrochemistry	4	25	75	100
Major Elective	ECH8T11/ ECH8T12	1.Medicinal and pharmaceutical Chemistry (OR) 2. Biochemistry	5	25	75	100
Core Practical	ECH8C1P	Inorganic Qualitative and quantitative analyses and Preparations	5	40	60	100
Core	ECH8C21	Stereochemistry and Organic Reactions	4	25	75	100
Core	ECH8C22	Coordination and Organometallic Chemistry	5	25	75	100
Core	ECH8C23	Group Theory and Spectroscopy	4	25	75	100
Major Elective	ECH8T21/ ECH8T22	1. Analytical Chemistry (OR) 2. Industrial Chemistry	5	25	75	100
Core Practical	ECH8C2P	Organic preparation and Qualitative and Quantitative analyses	5	25	75	100
Core	ECH8C31	Organic Spectroscopy and Natural Products	4	25	75	100
Core	ECH8C32	Inorganic Spectroscopy and Nano chemistry	4	25	75	100
Core	ECH8C33	Quantum, Nano and Macromolecular Chemistry	5	25	75	100
Non-Major Elective	ECH8N31/ ECH8N32	1. Computer Applications (OR) 2. Environmental Science	5	25	75	100
Core Practical	ECH8C3P	Conductometric and Potentiometric Titrations and Kinetics, Adsorption and Spectral Measurements	5	40	60	100
Core	ECH8C41	Biomolecules, Rearrangements and Synthetic methods	4	25	75	100
Core	ECH8C42	Nuclear and Analytical Chemistry	4	25	75	100
Core	ECH8C43	Chemical Kinetics, Surface, Biophysical and Photochemistry	4	25	75	100
Major Elective	ECH8T41/ ECH8T42	1. Introduction to Nanoscience (OR) 2. Polymer Chemistry	5	25	75	100
Project	ECH8C4 P	Project/ Review of Recent aspects of Chemistry Project Viva-voce	4	40	60	100
Total			**90**			**2000**

Scheme of Examination (EXTERNAL)

Passing minimum for theory paper (external) – 34 marks
Internal and External put together – 50 marks
Mode of evaluation of Internal Assessment for the theory papers:
Seminar - 5 marks
Assignment - 5 marks
Test - 15 Marks (Three tests: best of two)

PROJECT WORK

1. Each learner can select for his/her research project in any one of the areas of chemistry-in consultation with his/her guide and the Head of the department
2. The project report should be submitted to the Principal through the Head of the Department one week prior to the commencement of the university examinations. If a candidate fails to submit his/her project report on the date presented above, he/she may be permitted to submit the same four days prior to the date of viva-voce examination with a fine as prescribed by the university.
3. Each learner shall submit 2 copies of his/her project report for valuation.
4. The project report shall contain at least 25 pages excluding bibliography and appendices.
5. The project report shall be valued for a total of 150 marks out of which the external examiner and guide share 90 and 60 marks respectively. The sum of marks awarded by both the examiners shall be considered to be the final mark. For the pass in the project the learner shall secure a minimum of 75 marks. If the learner fails to get the minimum pass mark in the project report he/she shall be permitted to resubmit his/her project report once again within a period of 6 months after the publication of the result.
6. For those candidates who have passed in the evaluation of the project there will be a viva-voce examination of the above. The viva-voce carries a minimum of 50 marks and it will be conducted jointly by the guide and the external examiner. The learner should secure a minimum of 25 marks for a pass in the viva-voce examination failing which he/she shall be required to reappear for the same after a month but within a period of 3 months for which he/she will have to pay a fee as prescribed by the University.
7. Further for a pass in this paper as a whole a learner should secure at least 60 marks in project report and viva-voce put together.

ORGANIC CHEMISTRY

SEMESTER I
Introduction to organic reactions

Unit: 1

Electron Displacement:

Inductive and field effects – bond distances – bond energies- delocalized bonds – cross conjugation – rules of resonance – resonance energy – resonance effect – steric inhibition of resonance – Hyper conjugation hydrogen bonding addition compounds EDA complexes – Crown ether complexes – inclusion compounds – effect of structure on the dissociation constants of acids and bases – concept of Hard and Soft acids and bases.

Introduction to Reaction Mechanisms:

Reaction intermediates – free radicals, carbenes, nitrenes, carbanions and carbocation's – formation and stability of reaction intermediates – methods of determination of reaction mechanism – kinetic and thermodynamic control of chemical reactions. Kinetic and non-kinetic methods for determining organic reaction mechanism. Principle of microscopic reversibly – Energy profile diagram – Hammond postulate.

Unit: 2

Aliphatic nucleophilic substitution:

Nucleophilicity and basicity – S_N1 and S_N2 mechanisms – effect of substrate structure – effect of the attacking nucleophiles – effect of the leaving group – effect of the reaction medium – ambident nucleophiles ambident substrates – neighboring group participation of n ,π, and σ electrons – Sni mechanism – nucleophilic substitution at an aliphatic trigonal carbon – nucleophilic substitution at an allylic carbon – nucleophilic substitution at a vinyl carbon.

Aliphatic electrophilic substitution: Electrophilic substitution at saturated carbon – Se1, Se2, and Sei mechanisms.

Unit: 3

Symmetry elements and point group classification:

Concept of chirality, necessary and sufficient conditions for chirality – Relationship between substrate symmetry and chirality. Projection formulae Wedge, Fischer, Sawhorse and Newmann. Optical isomerism due to centre of chirality. Molecules with one stereo genic centre [chiral centre] and molecules with more than one chiral centre. Properties of enantiomers and diastereoisomers. Erythro and threo nomenclature. Configuration – determination of configuration. Cahn Ingold and Prelog system of designation of configuration.

Geometrical Isomerism:

E-Z nomenclature – determination of configuration of geometrical isomers using physical and chemical methods – stereoisomerism in monocyclic compounds [upto six membered ring].

Unit: 4

Aromatic Character:

Aromatic character in benzene, six membered rings, five, seven, eight membered rings- other systems with aromatic sextets – Huckel's rule. Craig's rule - concept of homo aromaticity and anti aromaticity - systems with 2, 4,8 and 10 electrons - system with more than 10 electron –

Alternant and nonalternant hydrocarbons. Chemistry of cyclopentedienyl anion – Fulvene, Azulene, Tropolones, Sydnones and Annulens.

Novel ring system:

Nomenclature of bicyclic and tricyclic systems – chemistry of adamantine, diamantine [congressane], cubane and catenanes.

Unit: 5

Oxidation and Reduction:

Elimination of hydrogen and aromatization reactions catalytic dehydrogenation – mechanism, applications and stereochemical aspects of the following oxidation – reduction reactions: Oxidation reaction involving CrO3, SeO2, OsO4, lead tetraacetate, periodic acid, N-bromosuccinimide, H2O2 – Oppenaver oxidation.

Catalytic hydrogenation:

Reactions involving lithium aluminium hydride triisobutyl aluminohydride, DIBAL and sodium borohydride – Birch reduction – Meerwein – Pondorf - Verely reduction – Wolff-Kishner reduction – Huang – Minlon modification- hydroboration – selectivity in oxidation and reduction.

Reagents in Organic synthesis:

Gilman's reagent [lithium dimethylcuprate], lithium diisopropylamide [LDA], dicyclohexylcarbodiimide, 1,3 trimethylsilyl iodided , tri –n-butyltin hydride, Woodward and Prevost hydroxylation, DDQ, Merrified resin phase transfer catalysts, Peterson's synthesis , Bsker yeast.

SUGGESTED READINGS:

1. P. Sykes, Guidebook to Mechanism in Organic Chemistry, Orient Longman, 1976.
2. Jerry March, Advanced Organic Chemistry, John Wiley & Sons, 4th edn., 2000.
3. E.S Gould , Mechanism and structure in Organic Chemistry, Henry Holt & Co., New York, 1959.
4. J.Shorter, Correlation Analysis in Organic Chemistry, Clarendon Press, Oxford,1973.
5. R.T.Morrison and R.N.Boyd, Organic Chemistry Prentice-Hall, 6th edn.,2001.
6. I.L.Finar , Organic Chemistry , Vol.1 and 2, 5th edn., ELBS,1975.
7. T.H.Lowry and K.S.Richardson, Mechanism and Theory in Organic Chemistry.
8. Reinhard Bruckner,Advanced Organic Chemistry, Reaction Mechanisms, Academic Press,2002.
9. F.A. Carey and R.J. Sundberg, Advanced Organic chemistry, Part B 4th edn., Plenum Publishers,2001.
10. R.O.C. Norman, Organic synthesis, 3rd edn., 1993.
11. W.Carruthers, some Modern Methods of Organic synthesis, Cambridge University Press, 2nd edn., 1982.
12. H.O House, Modern synthetic Reactions, W.A.Benkjamin Inc., California, 2nd edn., 1972.
13. P.S. Kalsi, spectroscopy of Organic Compounds 6th edn., New Age International[P] ltd., 2004.
14. P.Ramesh, Basic Principles of Organic Stereochemistry, Meenu Publications. Madurai, 2005.

SEMESTER II
STEREOCHEMISTRY AND ORGANIC REACTIONS

Unit: 1

STREOCHEMISTRY II

Prochirality and, prosteroisomerism, enantiotopic and diasterotopic ligands and faces and their nomenclature pro –R and pro-S Re and Si faces. Stereospecific and stereoselective reaction. Asymmetric synthesis Cram and Prolog rules. Optical isomers due axial chriality – biphenyls allenes and spiranes. Molecules with planar chirality – paracyclophanes, trans cyclooctene, ansa compounds.

Unit: 2

Conformational analysis

Configurations and conformations – conformations of ethane and n-butane- conformation analysis – stereoelectronic and steric factors- conformation of simple acyclic compounds- conformation of monosubstituted and disubstituted cyclohexanes- correlation of the conformation of acyclic and cyclic systems with their physical and chemical properties – conformational free energy – Curtin Hammett principle Quantitative treatment of mobile system – Eliel –Ro equation – conformations and reactivity of cyclohexamones- conformational analysis of aldohexopyranoses.

Unit: 3

ADDITION TO MULTIPLE BONDS

Electrophilic, nucleophilic and free radical addition to conjugated systems – orientation of the addendum – stereochemical factors in reactions like addition of hydrogen, halogens halides and hypohalous acids, hydroboration and hydroxylation –epoxidation.

Addition to carbonyl groups – mechanism –Aldol condensation – Perkin reaction –Knoevenagel reaction – Mannion reaction –Cannizaro reaction – Benzoin condensation – Claisen ester condensation – Darzen's reaction – Reformatsky reaction – Witting reaction – Grignard reactions.

Addition to α,β-unsaturated carbonyl groups – addition of Grignard reagent to α,β-unsaturated carbonyl compounds – Michael addition – Diels –Alder reaction – addition to carbenes and carbeniods to double and triple bonds.

Esterification of acids and hydrolysis of esters – decarboxylation of carboxylic acids.

ELIMINATION

A-elimination –β-elimination –E1,E2 and E1cB mechanisms – stereochemistry of eliminastion – orientation of the double bond – effect of changes in the substrate, base, leaving group and medium on E1,E2 and E1cB reactions – elimination vs substitution – pyrolytic cis elimination – Bredt's rule.

Unit: 4

TERPENES

Classification of terpenoids structure stereochemistry and synthesis of α-pinene, camphoa, zingiberene, cadinene , α-santinin, abietic acid and squalene.

VITAMINS

Structure and synthesis of Vitamins A, B1, B2, B6, B12 [structural features only], C, E, H and K.

Unit: 5

Aromatic electrophilic substitution- orientation –reactivity – mechanism of nitration, halogenations , Friedel-Craft's reaction and sulphonation – partial rate factors ortho/para ratio – Quantitative treatment of reactivity of the electrophile [the selective relationship] – Aromatic nucleophilic substitution reactions- SnAr, Sn1and benzyne mechanisms.

Quantitative treatment of the effect of structure on reactivity – The Hammen relationship –siginficance of reaction and substitutents constants – application of the Hammett equation in reaction mechanism – limitations and deviations.

SUGGESTED READINGS:

1. E.L. Eliel , S.H. Wilen & L.N.Mandar, Stereochemistry of Carbon Compounds John Wiley & Sons, 2003.
2. V.M.Potapov, Stereochemistry, MIR Publishers, Moscow,1979.
3. I.L.Finar, Organicchemistry, Vol.II, 5th edn., ELBS; 1975
4. D.Nasipuri, Stereochemistry of Organic Compounds, Principles and Applications, New Age International [P]Ltd.,2nd edn., 1994.
5. P.S.Kalsi, Stereochemistry, Conformation and Mechanism , New Age International [P] Ltd., 4th edn.,1997.
6. T.H.Lowry and K. S.Richardson, Mechanism and Theory in Organic Chemistry.
7. Jerry March, Advanced Organic Chemistry, John Wiley & Sons, 4th edn., 2000.
8. E.S.Gould, Mechanism and structure in Organic Chemistry, Henry Holt & Co; New York, 1959.
9. Reinhard Bruckner, Advanced Organic chemistry, Reaction Mechanisms, Academic Press,2002.
10. F.A.Carey and R.J.Sundberg , Advanced Organic Chemistry,Part B 4th edn., Pienum Publlsher, 2001.
11. Paul de Mayo, Chemistry of Terpenoids, Vol, I & II, academic Press.
12. L.Fieser and Mary Fieser,Steroids, Reinhold, 1953.
13. W.Klyne, The Chemistry of Steroids. Methuen & Co; New York, 1965.
14. S.F.Dyke, Chemistry of Vitamins, Interscience Publishers, 1965.
15. SEMESTER III
16. ORGANIC SPECTROSCOPY AND NATURAL PRODUCTS

SEMESTER III
ORGANIC SPECTROSCOPY AND NATURAL PRODUCTS

Unit I: Spectroscopy I

UV Spectroscopy: Principle- absorption spectra of conjugated dienes – α,β- unsaturated carbonyl compounds- Woodward – Fieser rules.

IR Spectroscopy: Molecular Vibrations – Vibrational frequency – factors influencing group frequencies – quantitative studies.

Mass Spectroscopy: Principle – type of ions – base peak – parent ion, metastable and isotopic peaks – fragmentation – general rules – pattern of fragmentation for various classes of compounds – McLafferty rearrangement – Retro Diels –Alder reaction

Unit: 2 Spectroscopy II

^{1}H NMR Spectrocopy : Origin of NMR spectra- chemical shift – spin coupling – coupling constant – first and second order spectra – spin – spin splitting- influence of stereochemical factor on chemical shift of protons –simplification of complex spectra deuterium substitution- spin decoupling - double resonance – shift reagents - Nuclear Overhauser Effect – CIDNP –concept of aromaticity.

^{13}C NMR Spectroscopy : Basic principle of FT technique – Relaxation time – assignment of signals – Off-resonance decoupling – additivity relationship – calculation of chemical shifts for aromatic and aliphatic compounds – DEPT ^{13} C Spectra – $^{13}C^{13}$ correlation COSY , HETCOR , ROESY , NOESY, and TOCSY – Inadequate.

Unit: 3 Chiro optical and Analytical techniques

ORD and CD – Principle – Cotton effect – type of ORD curves – α – haloketone rule – Octant rule – applications to determine the configuration and conformation of simple monocyclic and bicyclic ketones – comparison of ORD and CD.

Chromatographic techniques: Column, TLC, Paper, GLC, HPLC, Exclusion and Ion exchange.

Unit: 4 Steroids

Classification – configuration and conformational aspects of A/B cis and A/B trans steroids – complete chemistry and stereochemistry of cholesterol [includes bile acids], chemistry of ergosterol and Vitamin D_2 – male sex harmones – androsterone and testosterone – female sex harmones – oestrone, equilenin and progesterone – A basic idea about adrenocortical harmones – Cortisone [synthesis not included].

Prostaglandins. General study of prostaglandins - Structures. Chemistry of PGEL and PGF1 α.

Unit :5 Alkaliods and antibiotics

General methods of structural determination – Hofmann, Emde and Von Braun degradations. Structure and synthesis of quinine, papaverine, atropine, narcotine, morphine, reserpine, and lysergic acids

Antibiotics

Definition , classification of antibiotics, structure, stereochemistry and synthesis of penicillin , chloramphenicol.

Suggested readings

1. John R. Dyer, Application of absorption Spectroscopy, Pretice – Hall.
2. William Kemp Organic Spectroscopy, ELBS 3rd edn.,
3. Robert M.Silverstein , Francis X.Webster Spectrometric Identification of Organic Compounds , 6th edn., John Wiley ,& Sons Inc, 2004.
4. I.L. Finar, Organic Chemistry , Vol. II, ELBS, 1975.
5. Paul de Mayo, Chemistry of Terpenoids Vol, I & II, academic Press.
6. L.Fieser and Mary Fieser , Steroids, Reinhold, 1953.
7. W.Klyne , The Chemistry of Steroids , Methuen & Co., New York , 1965.

8. E.L. Eliel , Sterochemistry of Carbon Compounds, Mo Graw Hill, 1962.
9. P. Crabbe, ORD and CD in Chemistry and Biochemistry , Academic 1972.
10. A.Braithwaite and F.J.Smith , Chromatographic Methods, Chapman and 4th edn., 1985.
11. Bently , Alkaloids , Vol I & II , Interscience, 1957.

SEMESTER IV
BIOMOLECULES, REARRANGEMENTS AND SYNTHETIC MEHODS

Unit 1: Carbohydrates, Amino acids and Nucleic acids

Classification of proteins- peptides- structure of peptides – synthesis of pept – chemistry of glutathione and oxytocin – an elementary treatment of enzymes, coenzy and nucleic acids – biosynthesis of amino acids – RNA and protein synthesis – Gen code – DNA and determining the base sequence of DNA.

Pyronose and furanose, forms of aldohexoses and keto hexoses – methods used determination of ring size – conformations of aldohexopyronoses – structure and synth of maltose, lactose, sucrose and cellobiose. A brief study of starch and cellulose.

Unit II: Photochemistry & Free radicals

Conservation of orbital symmetry – electrocyclic reaction – cyclo addition reaction and sigmatropic rearrangements – applications of correlation diagram apporch.. Frontier molecular orbital approach, Huckel- Mobius approach and Perturbation molecular orbital approach to the above reactions.

Photochemical reactions of ketones – photosensitization – Norrish I and Norrish type reactions- Paterno Buchi reaction – photooxidation – photoreduction photochemistry of arenes.
Free radicals: Formation, deterction and stability of free radicals – free radicals reaction halogenations, addition, oxidation, reduction, and rearrangement reactions – Bar sandmeyer, Gomberg, Bachmann, Ullmann, Pschorr and Hundsdiecker reactions.

Unit III: Molecular rearrangements

Mechanism of the following rearrangement reactions: Wagner – Meerwein, Pinacol, Demzanov, Beckmann, Hofmann, Curtius, Wolff, Baeyer- Villeger, Stevens, Sommelet- Hauser, Favorskii, Banzil-benzilic acid, Claisen, cope Fries, Dienone-phenol, di-pi methane, hydroxioamino – p- aminophenol and Benzidine rearrangement – Photochemical rearrangements.

Unit IV: Green Chemistry I

Principles of green chemistry – planning a green synthesis in a laboratory – general interest for solvent free processes – solvent free techniques – Microwave synthesis: Introduction and Characteristics of microwave heating – interaction of microwave radiation with the material – difference between conventional heating and microwave heating. Dielectric polarization – diapolar polarization – applications and advantages of microwave heating over conventional heating.

Unit V: Synthetic methods

Planning a synthesis – Relay approach and convergent approach to total synthesis – Retrosynthetic analysis of simple organic compounds – functional group interconversions – use of activating and blocking groups in synthesis – stereoselective problems of geometrical and optical isomerism – steric crowding – Transition metal complexes in organic chemistry – Homogeneous hydrogenation – Regioselectivity- Diastereoselectivity – Enantioselectivity – Umpolung synthesis – Robinson annelation – A schematic analysis of the total synthesis of the following compounds: 2,4 –dimethyl- 1,2 –hydroxypentanoic acids, trans- 9-metyl -1-decalone and isonootkatone.

Suggested readings

1. A.L. Lehniger, Biochemistry, nath Publishers.
2. C.H Depuy and O.L. Chapman, Molecular Reactions and Photochemistry, Prentice Hall,1972
3. S.M. Mukherji and S.P.Singh, Reaction Mechanism in Organic Chemistry, Mc.Milan India Ltd., 1978.
4. R,B,Woodward and R.Hoffmann, The conservation of Orbital Symmetry, Verlog Chemic GMBH and Academic Press, 1971.
5. Hung, The Chemistry of Free Radicals.
6. I.L.Finar, Organic Chemistry, Vol. II, ELBS, 1975.
7. P.De.Mayo, Molecular Rearrangements.
8. Jerry March, Advanced Organic Chemistry, John Wiley & Sons, 4th edn., 2000.
9. K.R.Desai , Green Chemistry (Microwave Synthesis), Himalaya Publishing House, Mumbai, 2005.
10. R.Sanghi and M.M.Srivastava, Green Chemistry (Environmental Friendly Alternatives), Narose Publishing House, New Delhi, 2003.
11. A.K. Ahluwalia, Green Chemistry (Environmentally Benign Reactions), Aru Books India, New Delhi,2006.
12. R.E.Ireland, Organic Synthesis, Prentice- Hall of India Pvt. Ltd., 1975.
13. R.T.Morrison and R.N.Boyd, Organic Chemistry, Prentice-Hall, 6th edn., 2001.

Semester II – Organic Preparation, Qualitative and Quantitative Analysis

Separation and analysis of two component mixtures. Identification of the components and preparation of solid derivative.

1. Quantitative analysis

a) Estimation of glucose by Lane and Eynon method and Bertrand method.
b) Estimation of glycine.
c) Estimation of formalin.
d) Estimation of methyl ketone.

2. Organic Preparations (only for class work)

About 5 two – stage preparations:

a) p-Nitroaniline from acetanilide benzophenone
b) p-Bromoaniline from acetanilide aniline.
c) m-Nitrobenzoic acid from methyl benzoate.
d) Benzanilide from
e) sym- Tribromobenzene from.

INORGANIC CHEMISTRY

Semester I
Structure and Bonding

Unit I: Nature of chemical bonds

Covalent bond: Hybridisation-Calculation of s and p characters- Bent's rule M.O theory; LCAO approximation-application of MOT to heteronuclear diatom molecules like $BeCl_2$, BeH_2,abd H_2O- Concept of multi centered bond as applied electron deficient molecules like diborane and metal alkyls –SEPR theory-Walst diagram.

Unit II: Bond properties and ionic bonding

Ionic radii-covalent radii-van der Waals radius-bond length, bond order, bio energy, bond polarity-partial ionic character of covalent bonds-electro negativity electron affinity-lattice energy- Born Haber cycle - Covalent character in Iron compounds - Different types of electrostatic interactions - Hydrogen bond.

Unit III: Solid State Chemistry

Crystal defects point, line and plane defects Colo centers-Non stoichiometry on physical properties- Electronic structure of solids electron and band theories- Types of solids- Electrical Conductivity superconductivity-High temperature superconductors Types of semiconductor-Thermo electric power and Hall effect – Photovoltaic effect Semiconductors in solid energy Conversion.

Unit IV: Inorganic Chains – Rings and Cages:

Silicates: Various silicate structures – Structure, property, correlation – Silicones.

Poly acids: Classification – isopoly acids like polymolybdate, polyvanadate and polytungstate – their structures – heteropolyacids: 12A, 12B, 9 and 6. Heteropolyacids-preparation and structures.

Phosphazenes and its polymer – Phosphonitrilic comounds- S_4N_4- Polymeric sulphur nitride (polythiazyl) Cage compounds: Nomenclature of Boranes and carboranes – Wade's rule – Styx number- preparation and structures of B_4H_{10}, $C_2B_{10}H_{12}$, $(B_{12}H_{12})^{2-}$-borazine.

Unit V: Metallurgy

Occurrence, isolation, purification, properties and uses of the following metals as well as their important compounds: Be, Ge, Ti, Zr, Th, V, Pu, U and platinum metals.

Suggested Readings

1. F.A.Cotton and G.Wilkinson, "Advances Inorganic Chemistry" 5th edn, John Wiley & Sons, Singapore, 1998.
2. K.M.Mackay and R.A.Mackay, Introduction to Modern Inorganic Chemistry, 4th edn., Prentice Hall, New Jersy, 1989.
3. James E.Huheey, Ellen A.Keitler and Richard L.Keitler, Inorganic Chemistry, 4th edn, Harper Collins College Publishers, New York, 1993.
4. P.W.Atkins, D.K.Shriver and C.H.Langfood, Inorganic Chemistry, Oxford- ELBS, U.K 1990.

5. K.F.Purcell and J.C.Koltz, An Introduction to Inorganic Chemistry, W.B.Saunders Company, Philadelphia, 1980.
6. N.B.Hanny, Solid State Chemistry

Semester II
Coordination and Organometallic Chemistry

Unit I: Coordination Compounds:

IUPAC Nomenclature of coordination compounds – isomerism in coordination compounds- Types of ligands – monodendate, ambidentate and macro cyclic ligands- Stability constsnt- Factors aftecting stability constant in solution- Determination of stability constant spectrophotometry, polarographic and potentiometric methods.

Theories of Bonding – VB – CFT – MO theories – Splittion of d-orbitals in Oh, Td, square planar and trigonal bipyramidal geometries – CFSE calculation in terms of Dq. Factors affection crystal field splitting – Spectrochemcal series Magnetic moments – quenching of orbital magnetic – moments.

Unit II: Reaction mechanism of coordination compounds:

Substitution reaction octahedral complexes – labile - inert complexes – mechanism of acid hydrolysis , hydrolysis and anation reactions. Substitution reactions of square planner complexes-. Factors affecting reactivity of square planar complexes – The trans – effect its applications – Electron transfer reactions - complementary and complementary reactions – outer sphere and inner sphere electron trans – mechanisms – Synthesis of coordination compounds using electron transfer substitution reactions.

Unit III: Bio – Inorganic chemistry – I

Porphyrin ring system – metalloporphyrins – hemoglobin and myoglobin – structures and work functions – synthetic oxygen carriers – cytochromes – structure and work functions in respiration chlorophyll – structure – photosynthetic sequence – Iron – sulphur proteins (non – heme iron protein) – Copper containing proteins – classification – blue copper proteins – structure of blue copper electron transferases - copper proteins as oxidases – cytochrome C oxidase – mechanistic studies of C oxidase – Hemocyanin.

Unit IV: Bio – Inorganic Chemistry – II

Carbosypeptidase A: Structure , function – carbonic anhydrase – inhibition and poisoning – corin ring system – vitamin B_{12} and B_{12} coenzymes – in – vivo and in – vitro nitrogen fixation – essential and trace elements in biological systems – metal ion toxicity and detoxification – molecular mechanism of ion transport across the membrane – sodium and potassium ions pumps – chelate therapy cis-platin.

Unit V: Complexes of π acceptor ligands:

Synthesis, structure and bonding in carbonyls nitrosyls, dioxygen complexes and dinitrogen complexes – Application of EAN rule.

Synthesis, properties, structure and bonding in Ferrocene, Arene and acetylene and allyl complexes.

Catalysis using organometallic compounds:

Oxidative addition – reduction elimination – insertion reaction – Catalytic mechanism in the following reaction – hydrogenation of olefins (Wilkinson catalyst) – Tolman catalytic low hydroformylation oxo process acetic acid from ethanol – oxidation of alkenes to aldo and ketones (wacker process) – catalysis in the formation of synthesis of gas – polymerization (Ziegler – Natta) – Cyclooligomerisation of acetylenes (Reppe wilke's catalysts) – olefin isomerisation using Ni catalyst.

Suggested Readings

1. W.E.Addison, structural Principles of Inorganic Chemistry Wiley 1961.
2. A.F.Wells, Structursl Inorganic chemisty , 4th edi., Oxford , New York ,1975.
3. F.A.Cotton and G.Wilkinson, Advanced Inorganic Chemistry, 5th edn., John Wilkinson , Singapore, 1988.
4. K.F.Purcell and J.C.Koltz, An Introduction to Inorganic Chemistry, W.B.Saunders Company, Philadelphia, 1980.
5. James E.Huheey, Ellen A.Keitler and Richard L.Keitler , Inorganic Chemistry, 4th edn., Harper Collins College Publishers, New York, 1993.
6. Y.Mido, Chemistry in Aqueous and Non – aqueous Solvents, Discovery Publishers House, New Dehli, 1969.

Semester III
Inorganic Spectroscopy and Nanochemistry

Unit I:

Electronic spectra of transition metal complexes and Photochemistry – d- d transition – charge transfer transition – selection rules – mechanism of break down of selection rules – bandwidths and shapes – Jahn Teller effect – Tanabe – Sugano diagram – evaluation of 10Dq and β for octahedral and tetrahedral complexes of d^3,d^6,d^7 and d^8 configurations - photochemistry – photo redox and substitution reaction occurring in Co(III) and Cr (III) complexes – photochemistry of ruthenium polypyridyls.

Unit II: Application of spectroscopy to the study of Inorganic compounds I

Application of IR and Raman spectra in the study of coordination compounds – application to metal carbonyls and nitrosyls – geometrical and linkage isomerism – detection of inter and intramolecular hydrogen bonding – stretching mode analysis of meta carbonyls.

Mossbaier and Photoelectron spectroscopy (PES):

Mossbauer effect resonance absorption – Doppler effect – Doppler velocity – Experimental technique of measuring resonance absorption – isomer shift – magnetic hyperfine splittings – application of Mossbauer spectroscopy in the study of iron and tin complexes.

Photoelectron spectroscopy:

Theory – XPS. UV-PES – instrumentation evaluation of Ionisation potential – Chemical identification of elements – Koopmann's theorem – chemical shift – UPS – XPES of N_2, O_2 and HCL- evaluation of vibrational constants froms UPS – spin orbit coupling – Auger spectroscopy – Principle and its application.

Unit III: Application of spectroscopy to the study of inorganic compounds II:

NMR Spectroscopy: ^{31}P,^{19}F, and ^{15}N – NMR – introduction - applications in structural problem – evaluation of rate constants – monitoring the course of reaction – NMR of fluxional molecules – NMR of paramagnetic molecules – contact shifts and shift reagents.

ESR Spectroscopy:

Principles – presentation of the spectrum – hperfine splitting – evaluation of g- and Atinsors – factors affecting the magnitude of g- values –zero field splitting – Kramer's degeneracy – ESR of d^3 octahedral – complexes – anisotropy and hyperfine splitting constant – Application of ESR in the study of transition metal complexes – Jahn- Teller distortion studies in Cu(II) complexes evaluation of spin – orbit coupling.

Unit IV: Nanochemistry

Basic idea of nanochemistry – defining nanoassemblies – measurement examples – potential uses – zero dimensional , one dimensional and two dimensional arrangements.

Nanotubes: Structure and characterization of single walled carbon nanocarbon and nanotubea properties – application of nanotubes.

Nanowires : vapour phase – Oxide assisted – Carbothermal growth of nanowire properties.

Nanorods: Seed mediated growth of inorganic nanotubes and nanorods.

Nanostructures polymers : conducting polymers – block-co-polymers – nanocage.

Unit V: Molecular rearrangements and reactions of coordinated ligands:

Molecular rearrangement of four coordinate complexes – six coordinated complexes – reaction – Coordination ligands – reaction due to metal ion polarization of coordinatinated ligands – hydrolysis of acid esters and amides and of peptides – Aldol condensation – imine formation, hydrolysis and sub exchange – the template effect and macrocylic ligands.

Suggested Readings:

1. F.Basalo and R.G.Pearson, Mechanism of Inorganic reaction, 2nd edn.,Wiley, New York, 1967.
2. Adamson , Concept of Inorganic Photochemistry , Wiley , New York, 1975.
3. S.F.A.Kettle , Coordination Chemistry – An Approach , Spectrum Academic Publish Oxford, 1996.
4. R.S.Drago, Physical Methods in Chemistry, Saunders Golden Sunburst W.B.Saunders Company , London, 1977.
5. I.Bertini et al . Bioinoganic Chemistry , Viva Books Private Ltd, Chennai, 1998.
6. Chatwal Bhagi and Agarwal, Bioinorganic Chemistry , Sultan chand Co., New York 2001.
7. M.A.O. Hill and P. Day (Eds.) Physical Methods in Advanced Inorganic chemistry Interscience, New York, 1968.
8. Charles P.Poole Jr, and Franck Owens, Introduction to Nanotechnology , Interscience, A.John Wiley & Sons , Publications, Canada,2003.
9. C.N.R.Rao, A.Muller and A.K.Cheetham, The Chemistry of Nanomaterials- system – Properties 1980.

Semester IV
Nuclear and Analytical Chemistry

Unit I: STRUCTURE OF NUCLEUS AND RADIOACTIVE DECAY

Composition of the nucleus – nuclear size, shape and density – principal, radial and magnetic quantum numbers – magnetic and electric properties of nucleus – elementary treatment of shell (independent particle) model – nuclear configuration – parity and its conservation – mass defect and binding energy – nuclear forces theory.

Radioactive decay: Group displacement law – decay series – rate of disintegration - - half life – average life – units of radioactivity – secular and transient equilibria – theories of alpha decay, beta decay, gamma emission, position decay, nuclear isomerism, internal conversion and electron capture – Auger effect.

Unit II: NUCLEAR FISSION AND FUSION AND APPLICATION OF RADIOACTIVE ISOTOPES.

Bethe's notation of nuclear process - nuclear reaction energies (Q value) – fission – energy release in nuclear fission – mass distribution of fission products – theory of nuclear fission fissile and fertile isotopes – energy from nuclear fusion – thermonuclear reaction in stars – classification of reactors – power nuclear reactor – brecder reactor – nuclear reactions in India.

Application of radioactive isotopes: characteristics of tracer isotopes – chemical investigation – age determination medical field – agriculture - industry – analytical application – isotope dilution analysis – neutron activation analysis – biological effects of radiation – waste disposal management.

Unit III: ACTINIDES AND LANTHANIDES:

Chemistry of Lanthanides and Actinides: Lanthanides – Occurrence, extraction from ores – Separation procedure – ion exchange method – solvent extraction method. Physical and chemical properties – Electronic configuration – common oxidation state – lanthanide contraction and its consequences – colour of lanthanide ions – magnetic properties of lanthanides – separation of actinide elements – separation of Pu from fission products – electronic configuration – oxidation state – Comparison of lanthanides and actinides – Position in the periodic table.

Unit IV: ELECTROANALYTICAL & THERMOANALYTICAL METHODS:

Electroanalytical Techniques :

Electrogravimetry: Theory of electrogravimetric analysis – electrolytic separation and determination of metal ions. Coulometry: Electrolytic cell-working electrodes – auxiliary electrode and reference electrode-coulometric titrations. Voltammetry: Cyclic voltammetry – stripping voltammetry – chrnopotentiometry. Amperometry: Amperometric titrations.

Thermoanalytical methods: Instrunmentation and applications of thermogravimetry – Differential Thermal Analysis and Differential Scanning calorimetry.

Spectroanalytical Methods: Spectranalytical methods: Laws of absorption quantitative law of luminescence – principles and applications of colorimetric spectrophotometry, fluorimetry , mepheleometry and turbidimetry – entio spectroscopy and flame spectroscopy – atomic absorption, atomic emission atomic fluorescence spectroscopy. Optical rotator dispersion and circular dichrome.

Unit V: COMPUTERS IN CHEMISTRY:

History and development of computer – Mainframe, micro and super computer systems – CPU and other peripare devices – Evolution of programming languages: Machine language, assist language and higher level language. Syntax and structure of C language.

Internet- History of internet – the working of internet and internet service applications of internet in Chemistry- websites in Literature Survey in Chemistry popular websites in Chemistry – data bases in Chemistry – downloading the attach PDF files – opening, browsing and searching a websites – literature searching online.

E-mail : Introduction – working way – mailing basica – e-mail ethics – advantage and disadvantages – creating e-mail id – receiving and sending e-mails.

Suggested Readings

1. S.Glasstone Source Book on Atomic energy 3rd edn., Van Nostrand Reld Company, New York, 1967.
2. G.Friedlander, J.W. Kannedy, E.S.Macias and J.M.Miller, Nuclear and Radiochemistry , John Wiley & Sons Inc., New York 1981.
3. H.I.Arnidar, Essintials of Nuclear Chemistry, 3rd edn., Wiley Eastern Ltd., New Delhi, 1987.
4. U.N.Dash, Nuclear Chemistry, Sultan Chand and Sons, New Delhi, 1991.
5. J.Basset et al Vogel's Text book of Quantitative Inorganic Analysis, Longmann edn., ELBS, Essex, 1989.
6. H.H Willard, LL.Merritt and J.A.Dean, Instrumental Mithods of Analysis, East press, New Delhi 1988.
7. D.A.Skoog and D.M.West, Fundamentals of Analytical Chemistry, Saunders Co- Publishing Co., Philadelphia, 1982.
8. J.G.Dick, Analytical Chemistry, Tata- McGraw Hill1973.
9. Alexis Leon and Mathews Leon, "Fundamentals of Information Technology", Vikas Chennai 1999.
10. Barbara Kasser, "Using the Internet", 4th edn, New Delhi, 1998.
11. Sathyaprakash, Advanced Chemistry of Rare Elements, S.Chand & Co. 4th edn.,
12. T.Moellar, The Chemistry of the Lanthanides, Chapman and Hall, London, 1963.
13. H.D.Mathur and O.P.Tandon Chemistry of rare elements 3rd edn., S.Chapman company New Delhi,1986.

Semester I

Inorganic Qualitative and Quantitative analyses and Preparations

Semi-Micro Qualitative Analysis: Analysis of mixtures containing one familiar and one less familiar cations from following.

W, Pb, Tl, Se, Te, Mo, Cu, Bi, Cd, Ce, Th, Zr, Ti, V, Cr, Mn, Al, U, Ni, Co, Zn, Ca, Ba, Sr, Li, and Mg

1. Estimation of one metal in the presence of another by EDTA (demonstration).
2. Inorganic Preparation: Preparation of atleast 6 Inorganic complexes.
3. Quantitative analysis: Separation and estimation of mixture by volumetric and gravimetric methods.

   Cu, Ni; Cu, Zn; Ba, Ca; Fe, Ni; Fe Cu.
4. Preparation of one Ni (II) octahedral complex – its UV – Visible spectrum – evaluation of 10 Dq,B' and β (Dimonstration only).

PHYSICAL CHEMISTRY

Semester I
Thermodynamics, Chemical Equilibrium and Electro Chemistry

Unit I: Chemical Thermodynamics:

Second law of thermodynamics – concept of entropy- Gibbs – Helmholtz equation – Maxwell relations – Thermodynamic equation of state – Thermodynamics of system of variable composition – Partial molar quantities , partial molar volume – Chemical potential, Gibbs – Duhem equation – Experimental determinations of fugasity of real gases and its determination – Third law of thermodynamics – Absolute entropies – Determination of absolute entropies – Exception to third law – Unattainability of absolute zero.

Unit II: Chemical and Phase Equilibria:

Reaction free energy / Reaction potential – Reaction isotherm and direction of spontaneity – Standard reaction free energy – its calculation from thermochemical, electrochemical and equilibrium data – Temperature coefficient of reaction free energy and equilibrium constant.

Gibbs phase rule – its thermodynamic derivation – Application of phase rule to three – compounds systems – Formations of one pair, two pairs and three pairs of partially miscible liquids – Systems composed of two solids and a liquid.

Unit III: Statistical Thermodynamics:

Aim of statistical thermodynamics – define of state of a system – ensembles (micro , macro and grand canonical)- Boltzmann distribution law and its derivation – Boltzmann – Planck equation – partition function thermodynamic properties from partition functions – partition function and equilibrium constant – Quantum statistics – Fermi – Dirac and Bose – Einstein statistics – photon gas electron gas according to such statistics – population invertion – Einstein's and Determination theories of heat capacities of solids. Nuclear spin statistics basis of entropy H_2 at 0K in temperature of ortho-para ratio.

Unit IV: Electro Chemistry I:

Theroy of electrolytic conductance – inter – ionic attraction – ionic atmosphere – thickness of ionic atmosphere - The Debye –Huckel – Onsager conductance equation – its derivation and experimental verification – deviations modifications – Debye Falkenhagan and Wein effects – means ionic activity and active coefficients of strong electrolytes.

The role of electrodes – the electrochemical potential- Types of electrodes – gas/ inert metal electrode – ion / insoluble salt / metal electrode – oxidation – reduction electrode – liquid junction potential and membrane potential – Electro chemical cells - Nernst equation – Application of EMF measurements – determination of equilibrium constant, dissociation constant solubility product and potentiometric titrations.

Unit V: Electrochemistry II:

The electrical double layer and Zeta potential- Perrin, G – Chapmen and Stern models – polarisable and non – polarisable interfaces – electrokin phenomena – dynamic electrochemistry

– electrode processes and non equilibrium electron potential – over potential – Butler Volmer equation – Tafel equation – Current – potentio curves – hydrogen over voltage.

Application of electrochemical processes – power generation and storage Fuel cells – storage batteries and dry cells – principles of inhibition of corrosion – voltammetry – photo electerochemistry and electro chemi lumunescence.

Suggested Readings:

1. S.Glasston, Thermodynamics for Chemists, East – West Press Private Ltd., New Delhi.
2. J.Rajaram and J.C.Kuriakose, Thermodynamics (III Edn.,) Shoban Lal Nagin, Chand & Co., Ltd., New Delhi 1999.
3. B.R.Puri, L.R.Sharma and M.S.Pathania, Principles of Physical Chemistry (Millennium Edn.,) Vishal Publishing Co., 2003.
4. Gurdeep Raj, Advanced Physical Chemistry 25ht edn., Goel Publishing Co., 2001.
5. D.A.McQuarrie and J.D.Simon , Physical Chemistry – A Molecular Approach Viva Books (P) Ltd., New Delhi 1998.
6. P.W. Alkins, Physical Chemistry . VI edn., ELPS and Oxford University Press 1996.
7. S.H.Maron and J.B. Lando Fundamentals of Physical Chemistry Maomillan Publishing Co., New York 1974.
8. D.N.Bajpai, Advanced Physical Chemistry S.Chand & Company Ltd., New Delhi 1998.
9. A. Findlay, The Phase Rule and its Applications, Campbell and Smith.
10. A.W.Adamson. Physical Chemistry of Surfaces , 5^{th} edn., John wiley & Sons New York 1990.
11. D.Attwood and A.T.Florence , Surfactant Systems – Their Chemistry , Pharmacy and Biology, Chapman and Hall, New-York 1983.

Semester II
Group Theory and Spectroscopy

Unit I: Group Theory:

Molecular symmetry elements and symmetry operations – vector and matrix algebra – symmetry operations and transformation matrices – Group – definition and properties of a group – symmetry point groups- representation of a group – reducible and irreducible representations- Great orthogonality theorem- characters – construction of character tables- C_{2v}, C_{3v}, C_{4v}, C_{2h} and D_{2d} – Direct product concept.

Unit II: Application of Group Theory to Spectroscopy and Molecular Problems:

Symmetry of normal modes of vibration, application of group theory to normal modes of vibrations and to normal ,mode analysis – symmetry properties of integrals – application for spectral selection rules of vibration spectra – IR and Raman active fundamentals. Symmetry of molecular orbital and symmetry selection rule for electronic transitions in simple molecules like ethylene, formaldehyde and benzene. Group theory and quantum, mechanics – Wave functions as the basis of irreducible and delocalization energy for cyclopropenyl, butadiene and benzene system.

Unit II: Molecular Spectroscopy I:

Electromagnetic spectrum – Types of molecular energies – Absorption and emission of radiation – Einstein's coefficient – induces emission and absorption – Rotational spectra of rigid diatomic molecules – isotope effect in rotational spectra – Microwave spectrometer – Informations derives from rotational spectra.

Infrared spectroscopy – vibrational energy of a diatomic molecule – infrared selection rules – diatomic vibration rotator – vibrations of polyatomic molecules – overtone, combination and difference bands – concept of group frequencies – coupling interaction- Fermi resonance Fourier transform infrared spectroscopy.

Unit IV: Molecular Spectroscopy II:

Raman spectroscopy – Theories of Raman scattering – Rotational Raman spectra – Vibrational Raman spectra. Mutual exclusion principle – Laser Raman spectra – Electronic spectra of diatomic and polyatomic molecules-intensity of vibrational electronic spectra – Franck – Condon principle rotation fine structure of electronic vibrational spectra- the Fortrat prapbola – Dissociation and predissociation spectra.

NQR – puinciples and applications – quadrupole moment and electrical field nuclear quadrupole resonace , nuclear quadrupole coupling in atoms and molecules – identification of ionic character and hybridization.

Unit V: Spin Resonance Spectroscopy:

Magnetic properties of nuclei – Resonance condition – NMR instrumentation – Relaxation processes – Bloch equations – chemical shift – spin – spin splitting , relaxation times , line shape and line width experimental technique- ENDOR, Overhauser effect , FT-NMR spectroscopy , Lanthanide shift reagents – NMR imaging.

ESR – principles of ESR – total Hamiltonian – hyperfine structure – ESR spectra of free radicals in solutions – Anisotropic systems – systems in triplet state Zero field splitting in ESR and Krammers degeneracy.

Recommended Books

1. F.A.Cotton, Chemical Applications of Group Theory 3rd edn, John Wiley & Sons, New York 1999.
2. G.Davidson Introduction to Group Theory for Chemist, Applied Science Publishers Ltd, London 1971.
3. V.Ramakrishnan and Gopinath Group Theory in Chemistry 2nd edn. Vishal Publication, 1991.
4. K.V.Raman, Group Theory and its Application to Chemistry Tat McGraw – Hill 1990.
5. A.Streetweiser Molecular Orbital Theory for Organic Chemistry, John Wiley & Sons.
6. C.N.Banwell and E.M.McCash. Molecular Spectroscopy, Tata McGraw Hill 4th edn., 1995.
7. G.Aruldhas, "Molecular Structure and Spectroscopy", Prentice Hall of India Pvt., Ltd New Delhi 2001.
8. R.S.Drago Physical methods in Chemistry, W.B Saunders Co., London 1977.
9. D.C.Harris and M.D Bertolucci, symmetry and spectroscopy – An Introduction to Vibrational and Electronic spectroscopy, Oxford University Press New York 1978.
10. G.H.Barrow Introduction to molecular spectroscopy, McGraw Hill.
11. R.Change , Basic Principles of spectroscopy McGraw Hill London 1976
12. B.F.Straughan and S.Walker Spectroscopy Vol ,1,2 and 3, Chapman & Hall , London 1976

13. P.W. Atkins, Physical Chemistry 6th edn., Oxford University Press Tokyo 1998
14. E.B.Becker, High Resolution NMR 2nd edn., Academic Press 1990
15. A. Carrignton and A.D.McLachian, Introduction to Magnetic Resonance, Harper and Row.
16. D.Shaw , Fourier Transform NMR Spectroscopy, Elsevier.

Semester III
Quantum, Nano and Macromolecular Chemistry

Unit I: The Birth of Quantum Mechanics:

Planck's explanation about black-body radiation – de – Broglie's concept of matter waves, Compton Effect. Heisenberg's uncertainty principle and complementarity. Operators – Linear operators – Method of getting the following quantum mechanical operators – Position, momentum, kinetic energy , potential energy, total energy, angular momentum, raising and lowering and spin angular momentum.

Postulates of quantum mechanics – Hermicity and proving the quantum mechanical operators are Hermitian – Commutator algebra – evaluation of commutators – vanishing and non-vanishing commutators – Eigen function and Eigen value – Introduction Dirac notation – Expansion theorem. Orthogonality and normalisation of wave functions.

Unit II: Application of Quantum Mechanics to Simple systems:

Derivation of Schrodinger wave equation – Application of SWE to simple systems – Free particle moving in one dimensional box – Physical interpretation of the one dimensional problem- characteristics of wave function – average momentum of a particle in a box is zero – Particle moving 3-D box – Degeneracy – distortion – Particle moving in a ring – Rigid rotator – Spherical harmonics – Simple harmonic oscillator – Hermite polynomials –Hydrogen atom problem –Radial wave function – Radial probability distribution – Shapes of various atomic orbitals – Term symbols – L-S coupling scheme –Spectroscopic states.

Unit III: Approximation methods in Quantum mechanics:

Need for approximation methods – Schrodinger equation for He atom and other many electron system – the time independent Perturbation theory (First order only) – Application to hydrogen atom – Variation theorem – Application to hydrogen and He atom – Hartee – Fock Self Consistent Field (HFSCF) method of many electron system and its application to He atom – Electron spin and Pauli principle – Anti symmetric nature of the wave functions – Slater determinants approximation – VB and MO treatment of hetero nuclear and homo nuclear diatomic molecules.

Unit IV: Instrumentation in Nanochemistry:

Microscopic techniques for the characterization of nanomaterials – UV and fluorescence spectroscopy AFM, SEM, TEM, X-ray diffraction and microanalysis.

Unit V: Macromolecules Overview of Polymers:

Types and properties of polymers Kinetics and mechanism of free radical, ionic comdinsation and Zeigler- Natta polymerization processes. Emulation and suspension polymerization techniques – Polymer molecular weight and its distribution – Molecular weight

determination – osmatic pressure method – light scattering method – ultracentrifuge method and viscosity method.

New polymers in material science – conducting polymers and polymer electrodes.

Recommended Books

1. A.K.Chandra , Introductory Quantum Chemistry , 3rd edn., Tata McGraw Hill Publishing Co., New Delhi 1998.
2. M.W.Hanna, Quantum Mechanics in Chemistry 2nd edn., The Benjamin/ Cummings Publishing Co., London 1969.
3. D.A.McQuarrie Quantum Chemistry 1st Indian edn., Viva Books(P) Ltd., New Delhi 2003.
4. P.W.Atkins, molecular Quantum Mechanics, 2nd edn., Oxford University Press, 1986.
5. C.P.Poole and F.J.Owens Introduction to Nanotechnology,2004.
6. C.C.Koch Nono Structured Materials
7. R.Predit , L.Costlow and A.Peter Introductory Nanotechnology
8. F.W.Billmeyer, Text Book of Polymer Science 3rd edn., Wiley – Interscience Publishers, New York 1984
9. V.R.Gowariker , N. V. Viswanathan and J.Sreedhar, Polymer Science, Wiley Eastern Ltd., New Delhi 1986

Semester IV
Chemical Kinetics, Surface, Biophysical and Photo chemistry

Unit I: Chemical Kinetics I:

Potential energy surface. Chain reactions – general characteristics Steady state approximations – study of kinetics of chain reactions like H_2-B_{r2} reaction – decomposition of acetaldehyde and N_2O_5 – study of H_2-O_2 explosive reactions.

Unimolecular reaction rate theories – the simple Lindermann treatment – Hishelwood's theory – Rice, Ramsperer and Kassel (RRK) theory – Advanced unimolecular theory - Marcus theory or Rice, Ramsperger, Kassel and Marcus (RRKM) theory – Slater's theory. Principle of mictroscopic reversibility and detailed balancing – Kinetic isotope effect – Reactions in solution – influence of solvent dielectric constant, ionic strength (Bronsted- Bjerrum – equation – primary and secondary salt effects) and pressure on reaction rates in solution – significance of volume of activation.

Unit II: Chemical Kinetics II and Catalysis:

Fast reactions techniques – chemical relaxation methods, temperature and pressure jump methods, ultrasonic absorption technique, reactions in flow system, continuous and stopped flow, shock wave tube methods; chemical kinetics in crossed molecular beams – Flash photolysis – Spin resonance technique in the study of reaction kinetics.

Catalysis in biological systems – Enzyme catalysis – Michaelis – Menten kinetics – Lineweaver and Burk plot – Eadie's plot – influence of pH on the enzyme catalysis. Heterogeneous catalysis – chemical reaction on solid surfaces – kinetics, and mechanism of unimolecular and biomolecular – reactions – Langmuir – Heinshelwood and Langmuir – Rideal – mechanism – ARRT of surface reactions – NH_3 synthesis , hydrogenation of C_2H_4 and cracking of hydrocarbons.

Unit III: Surface Chemistry:

Introduction – Adsorption of gases on solids – physisorption and chemisorptions isotherms – Freundlish – Langmuir – BET – Temkin adsorption isotherms. Adorption on liquid surface – surface tension – Gibbs adsorption isotherm – Surface area determination – Electrokinetic phenomena at interfaces- including electro-osmosis and electrophoresis – Spreading of a liquid on another surfactant – monolayers – preparation of LB films – Micelles – Critical micellar concentration (CMC) – structure – biomolecular reaction occurring in a micellar solution – reverse micelles – micro emulsion – Application of photoelectron spectroscopy – ESCA and Auger spectroscopy to the study of surfaces.

Unit IV: Biophysical Chemistry:

Basic concept of non – equilibrium thermodynamics – Onsager reciprocal relationship – Its application to biological systems – High energy metabolies – ATP and its role in bioenergetics- transfer of potential and coupled reaction – Biological energy conversion in catabolism and anabolism – Role of singlet oxygen in biology – Biophysical applications of Mosshauer recongnition – An introduction to super – molecular chemistry and photochemistry.

Unit V: Photo – and Radiation chemistry:

Physical properties of the electronically excited molecules – excited sate dipole moments, pKa and redox potentials – photo physical processes in electronically excited molecules – Fluorescence phosphoiescence and other deactivating processes. Stern – Volmer equation and its applications – electronic energy transfer mechanisms – photosensitiation and chemiluminescence. Experimental techniques in photochemistry – light sources – chemical actinometry – Elementary aspects of photosynthesis, photochemical conversion and storage of solar energy.

Radiation chemistry – source energy – interaction of high energy radiation with matter – radiolysis of water – definition of G-value – mode of reaction of hydrated electrons OH and H Experimental techniques of radiation chemistry – Dosimetry - Elementary aspects of radiation chemistry in biology and industry.

Recommended Books

1. K.J.Laidler, Chemical Kinetics 3rd edn., Harper International edn., London 1987
2. K.J.Laidler Theories of Chemical Reaction Rates, McGraw Hill Book Co., London 1969.
3. F.Wilkinson, chemical Kinetics and Reaction Mechanisms, Van Nostrand Relnhold Co., New York 1980.
4. C.Kalidas, Chemical Kinetics Methods New Age International,1996
5. Margaret Robson Wright, Fundamental Chemistry Kinetics – An Explanatory Introduction to the Concepts, Horwood Publishing Ltd., West Sussex 1999
6. A.W.Adamson. Physical Chemistry of surfaces 5th edn John wiley & sons New York 1990
7. D.Attwood and A.T.Florence surfactant systems- Their Chemistry Pharmacy and biology, chapman and hall , New York 1983
8. K.K.Rohatgi Mukherjee , Fundamentals of Photochemistry wiley eastern
9. N.J.Turro, Modern Molecular Photochemistry, Benjamin Cummings.
10. Hamil Williams and Mackay, Principles of Physical Chemistry II edn Prentice Hall of India Pvt., Ltd., New Delhi 1986.

Semester III
Physical Chemistry
Practical Conductometric and Potentiometric Titrations and Kinetic Adsorption and Spectral Experiments

1. Conductometric Experiments

i. Double displacement & acid base titration

a) NH_4Cl—NaOH – Mixture of CH_3 COOH & HCl

b) NH_4Cl—NaOh --- Mixture of NH_4Cl & HCl.

ii. Prepciptation titration

a) Na_2CO_3—$Pb(NO_3)_2$—Na_2CO_3

b) K_2SO_4—$BaCl_2$—K_2SO

iii. Determination of dissociation constant of weak acids.

2. Adsorption Experiments

Adsorption of oxalic acid/Acetic acid on Charcoal

3. Kinetic Experiments:

i. Kinetics of alkaline hydrolysis of ester by potentiometric method

ii. Perdisulphate and iodine ion reactions, Study of primary salt effect and determination of the concentration of given KNO_3

4. Potentiometric Methods

i. Precipitations titration Ag+ vs Halide mixture

ii. Redox titrations

a) permagnate vs iodide ion

b) ceric ammonium sulphate vs ferrous ion

iii) Determination of dissociation constant of weak acids and pH of buffer solution

iv) Determination of solubility product of sparingly soluble salts.

5. Titrations Using pH Meter:

Determination of first, second and third dissociation of phosphoric acids.

6. Experiments based on UV- Visible and Infrared Spectrophotometers.

MAJOR ELECTIVE

Semester I
BIO – CHEMISTRY

Unit I Enzymes:

Classification , nomenclature properties of enzymes some feature of active sites of enzymes, enzymes kinetics- Michaelis – Menton model –significance of K_M and V_{Max} values. Enzymes inhibition – Competitive and non-competitive. Allosteric interaction- Mechanism of enzyme action. Lysozyme and carboxypeptidase.

Unit II Generation and storage of Metabolic Energy

Metabolism – basic concepts and design: Glycolysis – citric acid cycle – oxidative phosphoryiation – pentose pathway and gluoneogenesis.

Glycogen and disaccharide metabolism, fatty acid metabolism – amino acid degration and urea cycle – photosynthesis.

Unit III Information, Storage transmission Expression of Genetic information

DNA – Genetic role structure and replication; messenger RNA and transcription genetic code and gene protein relationship – protein synthesis control of gene expression – Eucaryotic chromosomes, Recombinant DNA technology and viruses.

Unit IV Bio – inorganic chemistry

Metalloproteins and enzymes – Blue copper proteins – copper proteins as oxidases/ reductases – Nickel containing enzymes – structure of DNA- types of nucleic acid interactions – coordination – intercalation and hydrogen bonding- ineractions of metal ions with nucleic acids – redox chemistry , hydrolytic chemistry – monitoring the DNA binding by UV , IR, NMR and CV spectral techniques.

Unit V Biophysical aspects

Electron transport and oxidative phosphorylation – Thermodynamic and kinetic aspects – Photosynthesis – An overview – Photosystem II – The light harvesting chlorophyll-protein complexes of photo system II Role of carotenoids in photo synthesis – The primary electron donor of photo system II, P680- The stable primary electron acceptor Q_A and the secondary electron acceptor Q_B – The transient intermediate electron acceptor of photo system II, pheophytin – Oxygen evolution – The role of manganese – The electron donor to $P680^+$ - Charge recombination in photo system II- Photosystem I Light – harvesting chlorophyll protein complexes of photo system I- The primary electron donor of photo system I, P700 - The primary electron acceptor A_0 of photo system I The intermediate electron acceptor A1 of photo system I – Mobile electron carriers plastocyanin and ferredoxin and $NADP^+$- reductase.

Suggested Readings:

1. B.D.Hames and N.M. Hooper Biochemistry, Viva Books Pvt., Ltd., 2003.
2. J.M.Berg, J.L.Tymoczko and L.Stryer, Biochemistry 5th edn. W.H.Freeman and Company, New York, 2002.
3. A.L.Lehninger , Biochemistry , North Publishers.
4. I.Bertini H.B.Gray, S.J.Leppard and J.S. Valentine , Bioinorganic Chemistry Viva Books Pvt., Ltd., 1998.
5. G.R.Chatwal and A.K.Bhagi, Bioinorganic Chemistry Himalaya Publishing House.
6. B.Ke, Advances in Photosynthesis Vol., 10 Photosynthesis – Photo biochemistry and photo biophysics, kluwer Academic Publishers Dordrecht, 2001.

Semester II
Major Elective

Analytical Chemistry

Unit I: Precipitation Techniques:

Introduction – Properties of precipitates and precipitating reagents – Colloidal precipitates Co-precipitation – Post – precipitation- precipitates from homogeneous solution – surface adsorption – Drying and ignition of precipitates – Application of gravimetric methods.

Unit II: Error Analysis

Error analysis Classification of errors – accuracy and precision – minimization of errors significant figures – significant figures in computation – statistical treatment of data; mean median , standard deviations variance relative standard deviation – spread , errors – standard deviation of computed results- reliability of results – Q test, Tn test – Confidence lime comparsion of results – Student's t-test – F test comparsion of the means of two samples – correlation and regression; linear regression (least square analysis)

Unit III: Electro Analytical Methods

Electro analytical Techniques: Electro gravimetry Theory of electrogravimetric analysis electro analytical separation and determination of metal ions. Coulormetry Electrolytic cell-working electrodes – auxiliary electrode and reference electrode coulometric titrations.

Voltammetry: Cyclic voltammetry-stripping voltammetry chronopotentiometry, Amperometry; Amperometric titrations.

Unit IV: Thermo Analytical Methods

Thermal analysis: Theory and principles of DTA and TGA – factors affecting the position of DT and TG traces – applications of DTA and TGA to the thermal behavior of the following compounds – crystalline copper sulphate calcium oxalate monohydrate calcium acetate mono hydrate , ammonium nitrate, potassium chlorate with and without catalyst, ammonium Metavanadate zinc hexafluosilicates- complementary nature of DTA and TGA – principle and application of DSC – derermination of degree of conversion of high alumina cement – purity determination – phase transition study – in forensic laboratory.

Unit V Spectro Analytical Methods

Colorimetry: Beer and Lambert's law – terminology – condition for a satisfactory colorimetric analysis – methods of colour measurement of comparison – principles of colorimetric determination of NH_3, Cr ,Cu, Fe, Mn- simultaneous spectro photometric determination of Cr and Mn.

Nephelometry and turbidimetry: Pinciple – determination of sulphate and phosphate fluorimetry: principle – application of fluorimetry in the determination of Cd, Ca and Zn and determination of codeine and morphine in a mixture, flame spectrometry: theory – interference – AAS – applications in the determination of Mg^{+2} and Ca^{+2} in tap water V in lubricating oil, trace lead in a Ferrous alloy and trace elements in contaminated soil.

Suggested Readings:

1. D.A.Skoog, D.M.West and F.J.Hollar, Fundamentals of Analytical Chemistry 7th edn., Harcourt College Publishers, 1996
2. H.H.Willard, L.L.Merritt and J.A.Dean, Instrumental Methods of Analysis of East – West Press, New Delhi 1988
3. J.Basset et al., Vogel's Text book of Qualitative Inorganic Analysis Longman, 5th edn., ELBS Essex, 1989
4. J.G.Dick Analytical Chemistry, Tata – McGraw Hill, 1973.

Semester III
Non-Major Elective

Environmental Science

Unit I: Introduction and Classification

Introduction – Environmental science – Environmental chemistry – Ecology - Definition- Eco – System – Cycling of mineral elements and gases – Phosphate cycle-carbon cycle Hydrogen cycle – Nitrogen cycle – Hydrological cycle Environmental segments – pollution and its types: Air pollution –water pollution – soil pollution – radioactive pollution thermal pollution – noise pollution – marine pollution other types of pollution – and its effects and control – remedial measures.

Unit II: Air Pollution

`Introduction- sources of air pollution – air pollutants – classification and effects of air pollutants – Oxides of nitrogen, sulphur and carbon – acid rain –effects and control – hydrogen sulphide – effects and control – carbon mono oxide effects and control- photo chemical smog-effects and control fly ash- effects and control – green house effect – global warming- effects and control – ozone layer – ozone depletion – choloroflurоro carbons – effects and control.

Unit III: Water Pollution

Introduction – types of water – water pollution – water pollutants – classification – physical , chemical and biological inorganic pollutants and toxic metals – organic pollutants – radioactive polluntants in water – pesticides and fertilizers – suspended particles – water , quality – water quality index – ill effects of water polluntants fluorosis – water pollution control –water treatment – primary , secondary and tertiary treatment – desalination – reverse osmosis – sewage and industrial waste water treatment.

Unit IV: Soil Pollution

Introduction- types of soil- soil pollution – types – indicators of soil pollution – plants as indicators of pollution – sources of soil pollution – fertilizers and pesticides – radio active pollutants – solid wastes – soil sediments as pollutant – soil erosion – treatment of soil pollutants –solid wastes – thermal methods – land filling composting – land protection – remedial measure for soil pollution.

Unit V: Analysis of Polluntants

Introduction analysis of air pollutants – units – sampling –devices and methods for sampling – measurements: UV –visible spectrometry IR spectrometry – emission spectrometry – turbidimetry nephelometry – gas chromatography – HPLC – chemi-luminescence of nitrogen oxides –IR photometry – conductometry – analysis of water pollutants units sampling – devices and methods for sampling measurement : UV –Visible spectrometry titration – analysis of different water quality parameters – BOD-COD – analysis and monitoring of pesticids caroiongens and industrial pollutants.

Suggested Readings:

1. B.K. Sharma and H.Kaur , Environmental Chemistry Krishna Prakashan, Meerut, 1997
2. A.K. De, Enviroonmental Chemistry , Wiley Eastern Ltd.,Meerut,1994
3. A.K.Mukherjee , Environmental pollution and health hazards – Causes and Control Galgotia Press , New Delhi,1986

4. N.Manivasakam, physic chemical examination of water sewage and Industrial effluents, Pragati Prakashan Publ., Meerut, 1985.

Semester IV
Major Elective

Introduction to Nanoscience

Unit I: General Introduction

Forms of Matter – Crystal structures – Electronic properties of atoms and solids Surface energy and surface tension – Defining nanodimensional materials 0D,1D and 2D nanostructures – size dependence of properties – special properties resulting from nanodimensionality - Potential uses of nanomaterials.

Unit II: Synthesis of Nanomaterials

General approaches – Nucleation process – size of the crystal – Influence of nucleation rate on the size of the crystal – Chemical methods – Sol- gel techniques – Control of grain size – Co-precipitation – Hydrolysis – Sonochemical method – colloidal precipitation- Bottom up and top down approaches – Kinetically confined synthesis of nanoparticles.

Unit III: Principle and Instrumentation

Spectrophotometry, XRD, EXAFS, XPS, SEM, TEM, AFM – Application to nanomaterials characterization.

Unit IV: Optical Properties of Nanomaterials:

UV-Vis IR absorption – Photoluminescence and stimulated emission – Nonlinear optical mixing – photoconductivity.

Magnetic properties: Concepts of dia-, para-, and ferro-magnetism – Exchange correlation – Exchange interaction

Electrical properties: Electrical conductivity –Hall Effect – Charge carrier density – Activation energy; Electronic properties – Field emission properties.

Unit V: Biological nanomaterials:

Sizes of building blocks – Proteins – DNA double nanowire Enzymes – Protein synthesis – Micelles and Vesicles – Biomimetic nanostructures – Worm micelles and Vesicles from block copolymers.

Reference:

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2. M.D. Ventra, S. Evoy, J.R. Heflin, Jr., (Eds), Introduction to Nanoscale Science and Technology, Kluwer Academic, 2004.
3. G. Cao., Nanostructures & nanomaterials synthesis, properties and applications, Imperial College Press.
4. C.N.R. Rao, A. Mu¨ller, A.K. Cheetham (Eds.) The Chemistry of Nanomaterials: synthesis, Properties and Applications, WILEY-VCH Verlag, GmbH & Co. KGaA, Weinheim, 2004.

5. P. Knauth, J. Schoonman (Eds), Nanostrucred Materials: Selected SynthesismMethods, Propterties and Applications, KLUWER ACADEMIC, 2002.
6. G. Schmid, Nanoparticle: From Theory to Applications, Wiley – VCH Verlag GmbH & Co. KGaA, 2004.
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