Placed at the Special Me
of the Academic Co
held on 25.06.

APPENDIX – BM

MADURAI KAMARAJ UNIVERSITY

(University with Potential for Excellence)

M. Sc. (Branch IV(a)) Chemistry

(For those who join in July 2008 and afterwards)

Objectives

1. To gain knowledge on the basic and advanced level aspects in the different disciplines of chemistry.
2. To get an exposure to the basics in nanochemistry and Biochemistry.
3. To gain knowledge on the basic and advanced level experimental techniques.
4. To get an exposure on some current trends in chemistry.

Qualification for admission to M. Sc. Chemistry.

B. Sc. as the major subject with physics as one ancillary; The other ancillary subject may be any one of the following: Mathematics, Botany, Zoolo

Duration of the course: Two years duration with four semesters.

Medium of instruction : English

Scheme of Examination

Year	Semester	Paper	Credit	Internal	External	Total
I	I	Introduction to Organic Reactions	5	25	75	100
		Structure and Bonding	4	25	75	100
		Thermodynamics, Chemical Equilibrium and Electrochemistry	4	25	75	100
		Major Elective: 1. Medicinal and Pharmaceutical Chemistry. 2. Biochemistry	5	25	75	100
		Inorganic Qualitative and quantitative analyses and Preparations	5	25	75	100
I	II	Stereochemistry and Organic Reactions	4	25	75	100
		Coordination and Organometallic Chemistry	5	25	75	100
		Group Theory and Spectroscopy	4	25	75	100
		Major Elective: 1. Analytical Chemistry 2. Industrial Chemistry	5	40	60	100
		Organic preparation and Qualitative and Quantitative analyses	5	25	75	100
II	III	Organic Spectroscopy and Natural Products	4	25	75	100
		Inorganic Spectroscopy & Nanochemistry	4	25	75	100
		Quantum, Nano and Macromolecular Chemistry	5	25	75	100
		Non-Major Elective (any one): 1. Computer Applications 2. Environmental Science	5	40	60	100
		Conductometric and Potentiometric Titrations and, Kinetic, Adsorption and Spectral Measurements	5	40	60	100
II	IV	Biomolecules, Rearrangements and Synthetic methods	4	25	75	100

		Nuclear and Analytical Chemistry	4	25	75	
		Chemical Kinetics, Surface, Biophysical and Photochemistry	4	25	75	
		Major Elective: 1. Introduction to Nanoscience 2. Polymer Chemistry	5	25	75	
		Project/ Review of recent aspects of chemistry Project *Viva-Voce*	4	32	48 20	
		TOTAL	90			

Scheme of Examination (EXTERNAL)

Year	Semester	Paper	Duration	Total
I	I	Introduction to Organic Reactions	3 Hours	75
		Structure and Bonding	3 Hours	75
		Thermodynamics, Chemical Equilibrium and Electrochemistry	3 Hours	75
		Non-Major Elective: 1. Computer Applications 2. Environmental Science	3 Hours	75
		Inorganic Qualitative and quantitative analyses and Preparations	3 Hours	60
I	II	Stereochemistry and Organic Reactions	3 Hours	75
		Coordination and Organometallic Chemistry	3 Hours	75
		Group Theory and Spectroscopy	3 Hours	75
		Major Elective: 1. Analytical Chemistry 2. Industrial Chemistry	3 Hours	75
		Organic preparation and Qualitative and Quantitative analyses	3 Hours	60
II	III	Organic Spectroscopy and Natural Products	3 Hours	75
		Inorganic Spectroscopy & Nanochemistry	3 Hours	75
		Quantum, Nano and Macromolecular Chemistry	3 Hours	75
		Major Elective: 1. Medicinal and Pharmaceutical Chemistry. 2. Biochemistry	3 Hours	75
		Conductometric and Potentiometric Titrations and, Kinetic, Adsorption and	3 Hours	60

		Spectral Measurements		
II	IV	Biomolecules, Rearrangements and Synthetic methods	3 Hours	75
		Nuclear and Analytical Chemistry	3 Hours	75
		Chemical Kinetics, Surface, Biophysical and Photochemistry	3 Hours	75
		Major Elective: 1. Introduction to Nanoscience 2. Polymer Chemistry	3 Hours	75
		Project/ Review of recent aspects of chemistry Project *Viva-Voce*	3 Hours	48 20

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)

Scheme of Examination

Practicals

ar	Semester	Hrs. Per week	Name of the paper	Marks		
				Int	Ext	Total
	I	15	Inorganic qualitative and quantitative analyses and perparations	40	60	100
	II	15	Organic preparation, qualitative and quantitative analyses	40	60	100
	III	15	Coductometric and Potentiometric Titrations and Kinetic, Adsorption and Spectral Experiments	40	60	100
	IV	15	Project work/ review of recent aspects of chemistry	32	68	100

PROJECT WORK

1. Each learner can select for his/her research project in any one of the areas of chem
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
Department of chemistry one week prior to the commencement of the unive
examinations. If a candidate fails to submit his/her project report on the date prese
above, he/she may be permitted to submit the same four days prior to the date of viva-
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
appendices.

5. The project report shall be valued for a total of 150 marks out of which the exter
examiner and guide share 90 and 60 marks respectively. The sum of marks awarded
both the examiners shall be considered to be the final mark. For the pass in the project
learner shall secure a minimum of 75 marks. If the learner fails to get the minimum pa
mark in the project report he/she shall be permitted to resubmit his/her project report on
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
viva-voce examination of the above. The viva-voce carries a minimum of 50 marks and
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
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 I: 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 – Hyperconjugation – 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 Mechanism:
Reaction intermediates – free radicals, carbenes, nitrenes, carbanions, carbocations – 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 reversibility – Energy profile diagram – Hammond postulate.

Unit II: Aliphatic nucleophilic substitution:

Nucleophilicity and basicity – S_N1 and S_N2 mechanisms – effect of substrate structure – effect of the attacking nucleophile – effect of the leaving group – effect of the reaction medium – ambident nucleophiles – ambident substrates – neighbouring group participation of n, π and σ electrons – S_Ni 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 – S_E1, S_E2 and S_Ei mechanisms.

Unit III: Stereochemistry- I:
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 stereogenic 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 IV: Aromatic Character:

Aromatic character in benzene, six-membered rings, five, seven and e membered rings – other systems with aromatic sextets – Huckel's rule - Craig's rule concept of homoaromaticity and antiaromaticity – systems with 2, 4, 8 and 10 electron systems with more than 10 electron – Alternant and nonalternant hydrocarbons. Chemis of cyclopentadienyl anion – Fulvene, Azulene, Tropolones, Sydnones and Annulenes.

Novel ring systems: Nomenclature of bicyclic and tricyclic systems – chemistry adamantane, diamantane (congressane), cubane and catenanes.

Unit V: Oxidation and Reduction: Elimination of hydrogen and aromatization reaction – catalytic dehydrogenation – mechanism, applications and stereochemical aspects of the following oxidation-reduction reactions: Oxidation reactions involving CrO_3, SeO_2, OsO_4 lead tetraacetate, periodic acid, N-bromosuccinimide, H_2O_2 – Oppenauer oxidation.

Catalytic hydrogenation – reactions involving lithium aluminium hydride, trilisobutyl aluminohydride, DIBAL and sodium borohydride – Birch reduction – Meerwein-Ponndorf-Verley 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-dithiane, trimethylsilyl iodide, tri-n-butyltin hydride, Woodward and Prevost hydroxylation, DDQ, Merrifield resin, phase transfer catalysts, Peterson's synthesis, Baker 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. I and II, 5th edn., ELBS, 1975.
7. T.H.Lowry and K.S.Richardson, Mechanism and Theory in Organic Chemistry, Academic Press, 2002.
8. Reinhard Bruckner, Advanced Organic Chemistry, Reaction Mechanisms, Plenum Publishers, 2001.
9. F.A.Carey and R.J.Sundberg, Advanced Organic Chemistry, Part B, 4th edn.,
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.

Stereochemistry and Organic Reactions

Unit I: Stereochemistry II: Prochirality and prosterioisomerism, enantiotopic and diasteriotopic ligands and faces and their nomenclature-pro-R and pro-S and Re and Si faces. Stereospecific and stereoselective reactions. Asymmetric synthesis: Cram and Prelog rules. Optical isomerism due to axial chriality – biphenyls, allenes and spiranes. Molecules with planar chirality- paracyclophanes, trans cyclooctene , ansa compounds.

Unit II: Conformational analysis:

Configuration and conformation – 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 cyclohexanones – conformational analysis of aldohexopyranoses.

Unit III: Addition to multiple bonds:

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

Addition to carbonyl groups – mechanism – Aldol condensation – Perkin reaction – Knoevenagel reaction – Mannich reaction – Cannizaro reaction – Benzoin condensation – Claisen ester condensation – Darzen's reaction – Reformatsky reaction – Wittig 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 carbenoids to double and triple bonds.

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

Elimination: α-elimination – β-elimination – E1, E2 and E1cB mechanisms – stereochemistry of elimination – 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* eliminations – Brédt's rule.

Unit IV: Terpenes: Classification of terpenoids – structure, stereochemistry and synthesis of α-pinene, camphor, zingiberene, cadinene, α-santonin, abietic acid and squalene.

Vitamins: Structure and synthesis of Vitamins A, B_1, B_2, B_6, B_{12} (structural features only), C, E, H and K.

Unit V: Aromatic electrophilic substitution – orientation – reactivity – mechanism of nitration, halogenation, Friedel-Craft's reaction and sulphonation – partial rate factors – ortho/para ratio – Quantitative treatment of reactivity of the electrophile (the selectivity relationship) – Aromatic nucleophilic substitution reactions – S_NAr, S_N1 and benzyne mechanisms.

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

Suggested readings:

1. E.L.Eliel, S.H.Wilen & L.N.Mander, Stereochemistry of Carbon Compounds, John Wiley & Sons, 2003.
2. V.M.Potapov, Stereochemistry, MIR Publishers, Moscow, 1979.
3. I.L.Finar, Organic Chemistry, 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., Plenum Publishers, 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.

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 spectrometry: 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 II: Spectroscopy II:

^{1}H NMR spectroscopy: Origin of NMR spectra – chemical shift – spin-spin coupling – coupling constant – first and second order spectra - spin-spin splitting – influence of stereochemical factors on chemical shift of protons – simplification of complex spectra – deuterium substitution – spin decoupling – double resonance – shift reagents – Nuclear Overhauser Effect - CIDNP–NMR 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}C correlation COSY, HETCOR, ROESY, NOESY and TOCSY - Inadequate.

Unit III: 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 IV: Steroids: Classification – configurational 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 PGE1 and PGF1α.

Unit V: Alkaloids 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 acid.

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

Suggested readings:

1. John R.Dyer, Application of absorption Spectroscopy, Prentice – 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, Stereochemistry of Carbon Compounds, McGraw Hill, 1962.
9. P.Crabbe, ORD and CD in Chemistry and Biochemistry, Academic Press, 1972.
10. A.Braithwaite and F.J.Smith, Chromatographic Methods, Chapman and Hall, 4th edn., 1985.
11. K. W. Bently, Alkaloids, Vol I &II, Interscience, 1957.

Semester IV
Biomolecules, Rearrangements and Synthetic Methods

Unit I: Carbohydrates, Amino acids, proteins and Nucleic acids:

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

Pyranose and furanose, forms of aldohexoses and keto hexoses- methods used for determination of ring size- conformations of aldohexopyranoses- structure and synthesis of maltose, lactose, sucrose and cellobiose. A brief study of starch and cellulose.

Unit II: Photochemistry & Free radicals:

Conservation of orbital symmetry – electrocyclic reactions – cyclo addition reactions and sigmatropic rearrangements – applications of correlation diagram approach, 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 II type reactions – Paterno-Buchi reaction – photooxidation – photoreduction – photochemistry of arenes.

Free radicals: Formation, detection and stability of free radicals – free radical reactions – halogenation, addition, oxidation, reduction and rearrangement reactions – Barton, 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, Benzil-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 – dipolar 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 acid, trans-9-methyl-1-decalone and isonootkatone.

Suggested readings:

1. A.L.Lehninger, 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, McMilan India Ltd., 1978.
4. R.B.woodward and R.Hoffmann, The conservation of Orbital Symmetry, Verlog Chemie 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), Narosa 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

Qualitative 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 (five) 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 diatomic molecules like $BeCl_2$ BeH_2 and H_2O – concept of multicentered bond as applied to electron deficient molecules like diborane and metal alkyls – VSEPR theory – Walsch diagram.

Unit II: Bond properties and ionic bonding:

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

Unit III: Solid State Chemistry: Crystal defects - point, line and plane defects-Colour centers - Non-stoichiometry on physical properties - Electronic structure of solids - Free electron and band theories - Types of solids - Electrical conductivity and superconductivity - High temperature superconductors - Types of semiconductors - Thermo-electric power and Hall effect -Photovoltaic effect - Semiconductors in solar 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, Pa , U and platinum metals.

Suggested Readings

1. F.A.Cotton and G.Wilkinson, "Advanced 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.Langford, 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 constant- Factors affecting stability constant in solution- Determination of- stability constant spectrophotometry, polarographic and potentiometric methods.

Theories of bonding- VB - CFT - MO theories- Splitting of d-orbitals in Oh,Td, square planar and trigonal bipyramidal geometries- CFSE calculation in terms of Dq-Factors affecting crystal field splitting- Spectrochemical series- Magnetic properties of transition metal complexes- calculation of spin-only magnetic moments- quenching of orbital magnetic- moments.

Unit II: Reaction mechanism of coordination compounds: Substitution reactions of octahedral complexes- labile- inert complexes-mechanism of acid hydrolysis- base hydrolysis and anation reactions. Substitution reactions of square planar complexes- Factors affecting reactivity of square planar complexes- its applications- Electron transfer reactions-complementary and non complementary reactions- outer sphere and inner sphere electron transfer mechanisms - Synthesis of coordination compounds using electron transfer and 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

Carboxypeptidase A: structure, function – carbonic anhydrase – inhibition and poisoning – corin ring system – vitamin B_{12} and B_{13} 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 metal carbonyls, nitrosyls, dioxygen complexes and dinitrogen complexes- Application of EAN rule.

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

Catalysis using organometallic compounds: Oxidative addition- reductive elimination-insertion reaction- Catalytic mechanism in the following reactions: hydrogenation of olefins (Wilkinson catalyst)-Tolman catalytic loops- hydroformylation(exo process)- acetic acid from ethanol-oxidation of alkenes to aldehydes and ketones(Wacker process)-catalysis in the formation of synthesis of gas-olefin polymerisation (Ziegler-Natta)- Cyclooligomerisation of acetylenes (Reppe's or 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, Structural Inorganic chemistry, 4th edition, Oxford, New York, 1975.
3. F.A.Cotton and G.Wilkinson, Advanced Inorganic Chemistry, 5th Edn., John Wiley & sons, 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 Delhi, 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^1, 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 metal carbonyls.

Mossbauer 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 from 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 - hyperfine splitting – evaluation of g- and A tensors - factors affecting the magnitude of g-values-zero field splitting- Kramer's degeneracy- ESR of d^1 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 – measurements – examples – potential uses – zero dimensional, one dimensional and two dimensional arrangements.

Nanotubes: structure and characterisation of single walled carbon nanotubes – nanotubes properties – application of nanotubes.

Nanowires: vapour phase – Oxide assisted – carbothermal growth of nanowires – properties.

Nanorods: Seed mediated growth of inorganic nanotubes and nanorods.

Nanostructured polymers: conducting polymers – block-co-polymers – nanocages

Unit V : Molecular rearrangements and reactions of coordinated ligands

Molecular rearrangement of four coordinated complexes- six coordinated complexes- reaction at coordinated ligands- reaction due to metal ion polarization of coordinated ligands-hydrolysis of amino acid esters and amides and of peptides-Aldol condensation-imine formation, hydrolysis and substituent exchange-the template effect and macrocyclic ligands.

Suggested Readings

1. F.Basalo and R.G.Pearson, Mechanism of Inorganic reaction, 2nd Edn., Wiley, New York, 1967.
2. Adamson, Concept of Inoeganic Photochemistry, Wiley, New York, 1975.
3. S.F.A.Kettle, Coordination Chemistry-An Approach, Spectrum Academic Publishers, Oxford, 1996.
4. R.S.Drago, Physical Methods in Chemistry, Saunders Golden Sunburst Series, W.B.Saunders Company, London, 1977.
5. I.Bertini et al. Bioinorganic Chemistry, Viva Books Private Ltd, Chennai, 1998.
6. Chatwal Bhagi and Agarwal, Bioinorganic Chemistry, Sultan Chand Co., New Delhi, 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, Wiley-Interscience,
   A.John Wiley & Sons, Publications, Canada, 2003.
9. C.N.R.Rao, A.Muller and A.K.Cheetham, The Chemistry of Nanomaterials-Synthesis, Properties and Applications, Volumes 1 and 2, Wiley-VCH-Verlag Gmoh & Co., Wilhelm, 2004.
10. K.F.Purcell and J.C.Koltz, An Introduction to Inorganic Chemistry, W.B.Saunders Company, Philadelphia, 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, positron 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 reactions in stars –classification of reactors – power nuclear reactor – breeder reactor – nuclear reactors in India.

Applications of radioactive isotopes: characteristics of tracer isotopes – chemical investigations – age determination – medical field – agriculture – industry – analytical applications – 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- chronopotentiometry.' Amperometry: Amperometric titrations.

Thermoanalytical methods: Instrumentation and applications of thermogravimetry-Differential Thermal Analysis and Differential Scanning calorimetry.

Spectroanalytical Methods : Spectroanalytical methods: Laws of absorption and quantitative law of luminescence- principles and applications of colorimetry and spectrophotometry, fluorimetry, nepheleometry and turbidimetry- emission spectroscopy and flame spectroscopy-atomic absorption, atomic emission and atomic fluorescence spectroscopy. Optical rotatory dispersion and circular dichroism

Unit V: Computers in Chemistry. History and development of computers, Mainframe, micro and Super computer systems - CPU and other peripheral devices - Evolution of programming languages: Machine language, assembly language and higher level language. Syntax and structure of C language.

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

E-mail: Introduction – working way – mailing basics – e-mail ethics – advantages 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 Reinhold Company, New York, 1967.
2. G.Friedlander, J.W.Kennedy, E.S.Macias and J.M.Miller, Nuclear and Radiochemistry, John Wiley & Sons Inc., New York, 1981.
3. H.I.Arnikar, Essentials 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, Longman, 5th Edn., ELBS, Essex, 1989.
6. H.H.Willard, LL.Merritt and J.A.Dean, Instrumental Methods of Analysis, East-West Press, New Delhi, 1988.
7. D.A.Skoog and D.M.West, Fundamentals of Analytical Chemistry, Saunders College Publishing Co., Philadelphia, 1982.
8. J.G.Dick, Analytical Chemistry, Tata-McGraw Hill, 1973.
9. Alexis Leon and Mathews Leon, "Fundamentals of Information Technology", Leon Vikas, Chennai (1999).
10. Barbara Kraser, "Using the Internet", 4th edn., EE Edition, New Delhi, 1998.
11. Sathyaprakash, Advanced Chemistry of Rar Elements, S.Chand & Co. 4th Edn, 1986.
12. T.Moeller, 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.Chand & Company, New Delhi, 1986.

Semester I – Inorganic Qualitative and Quantitative analyses and preparations

1. **Semi-micro qualitative analysis:** Analysis of mixtures containing one familiar and one less familiar cations from the 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.
   (Insoluble and interfering anions may be avoided).

2. **Estimation** of one metal in the presence of another by EDTA (demonstration).
3. **Inorganic Preparations:** Preparation of atleast 6 (Six) inorganic complexes
4. **Quantative analysis:** Separation and estimation of mixture by volumetric and gravimetric methods.

   Cu, Ni; Cu, Zn; Ba, Ca; Fe, Ni ; Fe, Cu.

5. Preparation of one Ni(II) octahedral complex – its UV-Visible spectrum – evaluation of 10 Dq, B' and β (Demonstration only).

Physical Chemistry

Semester I

THERMODYNAMICS, CHEMICAL EQUILIBRIUM AND ELECTROCHEMISTRY

Unit I: Chemical Thermodynamics: Second law of thermodynamics- concept of entropy- Gibbs function- Gibbs- Helmholtz equation- Maxwell relations- Thermodynamic equation of state – Thermodynamics of systems 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 component systems- Formation of one pair, two pairs and three pairs of partially miscible liquids - Systems composed of two solids and a liquid.

Unit III: Statistical Thermodynamics : Aims of statistical thermodynamics- definition of state of a system- ensembles (micro, macro and grand canonical)- Boltzmann distribution law and its derivation- Boltzmann-Planck equation- partition functions- thermodynamic properties from partition functions- partition function and equilibrium constant- Quantum statistics- Fermi-Dirac and Bose-Einstein statistics- photon gas and electron gas according to such statistics- population inversion- Einstein's and Debye's theories of heat capacities of solids. Nuclear spin statistics- statistical basis of entropy of H_2 gas- ortho and para nuclear states- calculation of residual entropy of H_2 at 0 K in terms of ortho-para ratio.

Unit IV: Electrochemistry I : Theory of electrolytic conductance- inter-ionic attraction- ionic atmosphere- thickness of ionic atmosphere- The Debye-Huckel-Onsager conductance equation- its derivation and experimental verification- deviations and modifications- Debye Falkenhagan and Wein effects – mean ionic activity and activity coefficients of strong electrolytes.

The role of electrodes- the electrochemical potential- Types of electrodes- the gas/inert metal electrode- ion/insoluble salt/ metal electrode- oxidation-reduction electrode- liquid junction potential and membrane potential – Electro chemical cells- kinds of cells- notation- electrochemical cell reactions – EMF of 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, Gouy – Chapmen and Stern models- polarisable and non-polarisable interfaces- electrokinetic phenomena- dynamic electrochemistry- electrode processes and non-equilibrium electrode potential- over potential- Butler Volmer equation- Tafel equation- Current – potential curves- hydrogen over voltage.

Application of electrochemical processes- power generation and storage- Fuel cells- storage batteries and dry cells- principles of inhibition of corrosion- cyclic voltammetry- Photo electrochemistry and electrochemiluminescence

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 (25th 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. Atkins, Physical Chemistry- VI Edn., ELPS and Oxford University Press (1996).
7) S.H. Maron and J.B. Lando, Fundamentals of Physical Chemistry, Macmillan 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, 5th 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_{3h}- Direct product concept.

Unit II: Application of Group Theory to spectroscopy and Molecular Problems : Symmetry of normal modes of vibrations, 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 orbitals and symmetry selection rule for electronic transitions in simple molecules like ethylene, formaldehyde and benzene. Group theory and quantum mechanics- Wavefunctions as the basis of irreducible representation- group theory applied to hybridization- HMO theory- HMO calculations and delocalization energy for cyclopropenyl, butadiene and benzene systems.

Unit III: Molecular Spectroscopy I: Electromagnetic spectrum- Types of molecular energies- Absorption and emission of radiation- Einstein's coefficient- induced emission and absorption- Rotational spectra of rigid diatomic molecules- isotope effect in rotational spectra- Microwave spectrometer- Informations derived from rotational spectra.

Infrared spectroscopy- vibrational energy of a diatomic molecule- infrared selection rules- diatomic vibrating 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 parabola- Dissociation and predissociation spectra.

NQR - principles and applications - quadrupole moment and electrical field, nuclear quadrupole resonance, nuclear quadrupole coupling in atoms and molecules - identification of ionic character and hybridisation.

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 - double resonance 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 solution- Anisotropic systems- systems in triplet state- Zerofield 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 Publications, 1991.
4) K.V.Raman, Group Theory and its Application to Chemistry, Tata McGraw-Hill (1990).
5) A.Streitweiser, 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.Chang, Basic Principles of Spectroscopy, McGraw Hill, London (1976).
12) B.F. Straughan and S. Walker(eds.), 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. Carrington and A.D. McLachlan, 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- Introducing 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 in 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 wavefunctions - Slater determinants- Electronic configuration of many electron systems - Born - Oppenheimer approximation- VB and MO theories, MO treatment of hetero nuclear and homo-nuclear diatomic molecules.

Unit IV: Instrumentation in nanochemistry: Microscopic techniques for the characterisation of nanomaterials- UV-Visible 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, condensation and Zeigler-Natta polymerization processes. Emulsion 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 McGrawhill Publishing Co., New Delhi (1988)
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 Nanotehnology,(2004).
6. C.C. Koch Nano Structured Materials
7. R.Preidt,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. Gowarikee, N.V. Viswanathan and J. Sreedhar, Polymer Science, Wiley Eastern Ltd., New Delhi (1986).

Semester IV

CHEMICAL KINECTICS, SURFACE, BIOPHYSICAL AND PHOTOCHEMISTRY

Unit I: Chemical Kinetics I: Potential energy surfaces. Chain reactions - general characteristics- Steady state approximations- study of kinetics of chain reactions like H_2-Br_2 reaction- decomposition of acetaldehyde and N_2O_5- Study of H_2-O_2 explosive reactions.

Unimolecular reaction rate theories- the simple Lindemann treatment- Hisbelwood'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 microscopic 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 reactions on solid surfaces - kinetics, and mechanism of unimolecular and bimolecular -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 chemisorption- adsorption isotherms- Freundlich- Langmuir- BET – Temkin adsorption isotherms- Adsorption on liquid surface- surface tension- Gibbs adsopcion isotherms- 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- bimolecular 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 metabolites - 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 Mossbauer effect- NMR imaging- Applications of spin labeling in membrane research- Molecular recognition- An introduction to supra- molecular chemistry and photochemistry.

Unit V: Photo- and Radiation chemistry: Physical properties of the electronically excited molecules- excited state dipole moments, pKa and redox potentials- photo physical processes in electronically excited molecules- Fluorescence, phosphorescence and other deactivating processes. Stern-Volmer equation and its applications- electronic energy transfer mechanisms- photosensitisation and chemiluminescence. Experimental techniques in photchemistry - light sources- chemical actinometry- Elementary aspects of photosynthesis, photochemical conversion and storage of solar energy.

Radiation chemistry - Source of high energy- interaction of high energy radiation with matter- radiolysis of water- definition of G-value- mode of reactions 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, Theori es of Chemical Reaction Rates, McGraw Hill Book Co., London (1969).
3. F.Wilkinson, Chemical Kinetics and Reaction Mechanisms, Van Nostrand Reinhold Co., New York (1980).
4. C. Kalidas, Chemical Kinetic Methods, New Age International, 1996.
5. Margaret Robson Wright, Fundamental Chemical 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 (1968). (Radiation Chemistry).

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

I. Conductometric Experiments
   i. Double displacement & acid base titrations
      a) NH4Cl → NaOH→ Mixture of CH_3COOH & HCl.
      b) NH4Cl → NaOH→ Mixture of NH_4Cl & HCl.
   ii. Precipitation titration
      a) Na_2CO_3→ $Pb(NO_3)_2$ → Na_2CO_3
      b) K_2SO_4 → $BaCl_2$ → K_2SO_4
   iii. Determination of dissociation constant of weak acids

II. Adsorption Experiments
   Adsorption of oxalic acid/Acetic acid on charcoal

III Kinetic experiments
   i. Kinetics of alkaline hydrolysis of ester by potentiometric method
   ii. Perdisulphate and iodide ion reaction: Study of primary salt effect and determination of the concentration of given KNO_3

IV Potentiometric methods
   i. Precipitation titration: Ag+ vs halide mixture
   ii. Redox titrations: a) permanganate vs iodide ion
      b) ceric ammonium sulphate vs ferrous ion
   iii. Determination of dissociation constant of weak acids and pH of buffer solutions
   iv. Determination of solubility product of sparingly soluble salts.

V Titrations using pH meter
   Determination of first, second and third dissociation constants of phosphoric acid.

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

Semester I
Major Elective

Medicinal and Pharmaceutical Chemistry

Unit-I

Fundamentals of Medicinal Chemistry:

Definitions of Medicinal Chemistry, Pharmacology and molecular pharmacology- major process involved in drug action- pharmacokinetics phase- Quantitative structure Activity Relationship (QSAR)- Hansch approach – concept of bioisomerism- pharmacodynamics phase – receptors and classification of membrane bound receptors – enzyme inhibitors as drugs (illustrated with one example).

Unit-II

Medicinally useful antibiotics and steroids:

Structural features and mode of action of the following antibiotics- penicillin G, cephalosporin and their semisynthetic analogsw (β-lactum), streptomycin (aminoglycoside), terramycin (tetracylin), erythromycin (macrolide) and chloromphenicol.

Physiologically active steroids – their structural features and therapeutic use. Oral contraceptives, anabolic steroids, anti-inflammatory steroids.

Unit-III

Chemotherapeutic agents:

Antineoplastic agents: Classification, synthesis, Assay e.g., Cyclophosphamide, Ifosfamide, Chlorambucil, Busulfan, Decarbazine, Methotrexate, Azathioprine, 6-Mercaptopurine, 5-fluorouracil, Cisplatin, Carnplatin; **Antitubercular drugs**: Classification, Synthesis, Assay, e.g., Isoniazid, Rifampicin, Pyrazinamine, Ethambutol, Thiacetazone, Parnamino salicylic acid and Ethionamide.

Antimalarial drugs: Classification, synthesis, assay, e.g., Chloroquin, Primaquine, Amaodiaquine, Mefloquine, Proguanil Pyrimethamine, Diuretics : Classification, Synthesis, Assay eq., Furesemide, Acetazolamide, Chlorothiazide.

Unit - IV

Synthesis and Therapeutic action and SAR of certain drugs:

Antihypertensive drugs : Nifedipine, Captopril, Hydralazine, sodium nitropeuside, clonidine, methyldopa and guanothidine

Antihistamines : H1 – Antagonists : Pheniramine, Chlorpheniramine, Diphenylhydramine, Mepyramine, Promethazine, H2-Antagonists : Cimetidine, Ranitidine and Fomcridine

Unit – V

Anti – inflammatory drugs: Antipyretics & Non-narcotic analgestics : Aspirin, sodium salicylate, paracetamol, phenylbuttazone, oxyphenylbutaxone, Ibupcofen, Mepbenamic acid, Diclofenac sodium.

CNS Stimulant Drugs: Amphetamine, caffeine, Theobromine, Theophylline, Bemegride, Nikethamide, Methyl phenidate and pemoetrum.

CNS Depresent Drugs: Phenelazine, Isocarboxazide, Imipramine, Nortiptyline, Amitripcyline, Desipramine.

Suggested reading :

1. G.L.Patrick, An introduction to Medicinal Chemistry, II edn., Oxford University Press, 2001.
2. T.Nagradi, Medicinal Chemistry – A Biochemical Approach, Oxford University Press – 2004
3. J.B. Taylor and P.D. Kennewell, Introductory Medicinal Chemistry, Ellisworth Publishers, 1985
4. C.Laxmi, Medicinal Chemistry
5. B.Jeyasree Ghosch, Pharmaceutical Chemistry
6. Antoeknour, Medicinal Chemistry

Bio-Chemistry

Unit-I

Enzymes :

Classification, nomenclature, properties of enzymes, some features of active sites of enzymes , enzyme kinetics – Michaelis – Menton model – significance of K_M and V_{Max} values. Enzyme 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 phosphorylation – 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 – Encaryotic 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 – interactions of metal ions with nucleic acid – 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 photosystem II – Role of carotenoids in photosynthesis-The primary electron donor of photosystem II, P680- The stable primary electron acceptor Q_A and the secondary electron acceptor Q_B – The transient intermediate electron acceptor of photosystem II, pheophytin-Oxygen evolution-The role of manganese- The electron donor to $P680^+$- Charge recombination in photosystem II- Photosystem I-Light-harvesting chlorophyll-protein complexes of photosystem I-The primary electron donor of photosystem I, P700- The primary electron acceptor A_0 of photosystem I-The intermediate electron acceptor A_1 of photosystem I – Mobile electron carriers plastocyanin and ferredoxin and $NADP^+$ - reductase

Suggested Readings:

Unit I-III

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, Nath Publishers

Unit IV

1. I. Bertini, H. B. Gray, S. J. Leppard and J. S. Valentine, Bioinorganic Chemistry, Viva Books Pvt. Ltd., 1998
2. G.R. Chatwal and A. K. Bhagi, Bioinorganic Chemistry, Himalaya Publishing House.

Unit V

1. B. Ke, Advances in Photosynthesis, Vol.10 Photosynthesis- Photobiochemistry and photobiophysics, 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-minimisation 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 limit – comparison of results – Student's t-test – F test – comparison of the means of two samples – correlation and regression: linear regression (least square analysis).

Unit-III Electroanalytical 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-chronopotentiometry. Amperometry: Amperometric titrations

Unit-IV Thermoanalytical Methods

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

Unit-V Spectroanalytical Methods

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

Nephelometry and turbidimetry : principle – 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 – interferences – 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 Edition, Harcourt College Publishers, 1996
2. H. H.Willard , L. L. Merritt and J. A. Dean , Instrumental Methods of Analysis, East-West Press, New Delhi, 1988
3. J. Basset et al., Vogel's Text book of Qualitative Inorganic Analysis, Longman, 3rd Edition, ELBS, Essex, 1989.
4. J. G. Dick, Analytical Chemistry, Tata-McGraw Hill, 1973.

Industrial Chemistry

Unit I PRINCIPLES OF CHEMICAL TECHNOLOGY

Introduction – basic principles of chemical technology – importance of chemical technology – classification of technological processes – designing and modeling of chemical plants – unit process and unit operations.

Basic requirements of industrial reactors – choice and selectivity of reactor basic principles of homogeneous and heterogeneous processes and reactors with examples.

Unit II RAW MATERIALS AND ENERGY FOR CHEMICAL INDUSTRY

Raw materials - Characteristics of raw materials and their resources – methods of raw material concentration – integral utilization of raw materials.

Energy for chemical industry – power and fuels – classification of fuels – coal – fuel gases and liquid fuels – petroleum – cracking – chemical corrosion – types of corrosion and preventive measures

Unit III WATER POLLUTION AND ITS CONTROL

Water in chemical industry – soft and hard water – softening of water – basic principles of water pollution – water pollutants – pollution parameters – industrial pollution control – waste water treatment methods – pollution control act – water prevention act.

Unit IV SMALL SCALE CHEMICAL INDUSTRIES

Electro-thermal and electro-chemical industries: electroplating – surface coating industries – oils, fats and waxes – soaps and detergents – cosmetics.

Match industries and fire works: manufacture of some industrially important chemicals like potassium chlorate, potassium nitrate, barium nitrate and red phosphorus – metal powders.

Unit V LARGE SCALE CHEMICAL INDUSTRIES

Manufacturing process – raw materials – composition and uses of products in Portland cement – ceramics – plastics synthetic fibres – rubber – fertilizers – insecticides and pesticides – photo film industries – commercial aspects of starting an industry.

Reference Books

1. Mukhlyonov (ed.), Chemical Technology, Vol.1, Mir publication, Moscow, III edn., 1979.
2. A.K. De, Environmental Chemistry, Wiley Eastern Ltd., II edn., Meerut 1989. Chs. 5 – 7.
3. R.K. Goel, Process know – how and material of construction for Chemical Industries, S.B. Publ., Delhi,1977.
4. B.N. Chakrabarthy, Industrial Chemistry, Oxford and IBH Publ., New Delhi,1984.
5. R. Norris Shreve and J.A. Brink, Jr. Chemical Process Industries, IV edn., McGraw Hill, Tokyo, 1977.

Semester III
Non-Major Elective
Computer Applications

Unit I: BASIC CONCEPTS OF VB

Introduction to Visual Basic - the integrated development environment - the menu bar, the tool bar, the project explorer, the tool box, the properties of window, the form designer, the form lay out, the immediate window, the elements of the interface – programming an application common properties, common methods and common events – customising the environment.

Working with Forms : The appearance of form – the start up form – loading, showing and hiding forms – elementary concepts of drag and drop operations.

Basic active X controls : Elementary concepts of the Text Box control, the List Box and ComboBox controls.

Variables – declaring variables – variable types – strings, numeric and data variables – scope and life forms of variables – constants.

Unit II: THE LANGUAGE FORMS AND BASIC ACTIVE CONTROLS

Control flow statements: If ... Then and If... Then... Else.

Loop statements: DO...Loop, For...Next and While–Wend-nested control statement - the Exit statement.

Arrays: Declaring arrays – specifying arrays – multi dimensional arrays.

Procedures : Subroutines, functions, calling procedures – arguments – arguments passing mechanism – using optional arguments – functions returning arrays.

Unit III APPLICATIONS OF VB IN CHEMISTRY

Writing Simple programs in Chemistry:

i. Calculation of molecular weight of organic compound,
ii. Ionic strength of an electrolyte,
iii. Different velocities of a gas,
iv. NMR frequency values of nuclei,
v. Average rate constant,
vi. Unit cell dimensions,

vii. Thermodynamic parameters,
viii. Reduced mass.
ix. Empirical formula of an organic compound containing C,H and O,
x. Normality, molality and molarity of a solution,
xi. Half life period of a radioactive material,
xii. Surface tension and
xiii. Temperature in Kelvin scale into Celsius scale and *vice-versa*.

Practical : (Class work only)

Construction of programs in VB language, compiling, debugging and making executive files, printing the output.

Running Simple VB programs in Chemistry to calculate / determine the above problems.

Unit IV BASIC CONCEPTS OF COMMUNICATIONS SYSTEMS

Communication systems: Satellites – RADAR – optical fibers – advantages and disadvantages – ISDN – distributed systems – advantages and disadvantages.

Telecommunications: analog and digital signals – types and needs of modulations – MODEMS – Telecommunication software.

Computer networks: An overview – communication processors – protocols – network architecture.

Practicals (Class work only)

Salient features of Windows and MS Word for typing texts and equations in Chemistry – tabular columns – advanced concepts.
2. Basic concept of creating and accessing databases using MS Access.
3. Significance of Chemdraw - drawing chemical structures and pasting them in the text.

Unit – V BASIC CONCEPTS OF INTERNET AND APPLICATIONS IN CHEMISTRY

Internet : History of internet – the working way of internet - getting connected to internet – Internet protocols – Internet addressing – domain names – Internet services.

WWW : Web pages – home pages – web browsers – search engines – internet chat – chatting on web.

E-mail: Introduction – working way – mailing basics – e-mail ethics – advantages and disadvantages - creating e-mail – receiving and sending e-mails.

Intranet: Characterisation – advantages – drawbacks – need for intranet – extranet.

Applications of internet in Chemistry: Websites in Literature survey in chemistry – popular websites in chemistry – data bases in chemistry – URLS – WAIS – downloading the attachment / PDF files – opening, browsing and searching a website – literature searching online.

Practicals (Class work only):

1. Creating e-mail id, sending and receiving e-mails, attachment files, PDF files. Opening, browsing and searching a website – down loading – literature survey in chemistry – online searching.

Reference Books

1. Evangelos Petroutsos, Mastering "Visual Basic 6", BPB Publication, First Indian Edition, New Delhi, 1998, pp 1-51, 99-174, 177-180, 209-211, 227-262.
2. David Jung, Pierre Boutquin, John D. Conley III, Loren Eidahl, Lowell Mauer and Jack Pudum, "Visual Basic 6 Super Bible", First Indian Edition, Techmedia, New Delhi,1999.
3. Gary Cornell, "Visual Basic 6", Tata-McGraw Hill, New Delhi, 1998.
4. Barbara Kasser, "Using the Internet", Fourth Edition, EE Edition, New Delhi, 1998.
5. K.V. Raman, "Computers in Chemistry", Tata-McGraw Hill Publishing Company, New Delhi, 1993.
6. Alexis Leon and Mathews Leon, "Fundamentals of Information Technology", (Chapters 17 – 19 & 21 – 23), Leon Vikas, Chennai (1999).

Semester I

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-photochemical smog- effects and control-fly ash- effects and control-green house effect-global warming-effects and control-ozone layer-ozone depletion-cholorofluoro carbons- effects and control.

Unit : III Water Pollution

Introduction- types of water- water pollution-sources of water pollution- water pollutants-classification-physical, chemical and biological-inorganic pollutants and toxic metals-organic pollutants-radioactive pollutants in water-pesticides and fertilizers-suspended particles-water quality-water quality index- ill effects of water pollutants-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-treatment of solid wastes-thermal methods-land filling-composing-land protection-remedial measures for soil pollution.

Unit : V Analysis of Pollutants

Introduction-analysis of air pollutants-units- sampling-devices and methods for sampling-measurement: UV-Visible spectrometry-IR spectrometry-emission spectrometry-turbidimetry-nephelometry -gas chromatography-HPLC-chemiluminescence 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 pesticides, carcinogens and industrial pollutants.

Suggested Readings:

1. B. K. Sharma and H. Kaur, Environmental Chemistry, Krishna Prakashan, Meerut,1997.
2. A. K. De, Environmental 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, Physico-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 – Bioinmetic nanostructures – Worm micelles and Vesicles from block copolymers.

Reference:

1. C. P. Poole Jr., F.K. Owens, Introduction to Nanotechnology, John Wiley & Sons, 2003.
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. Müller, 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), Nanostructured Materials: Selected Synthesis Methods,Properties and Applications, KLUWER ACADEMIC, 2002.
6. G. Schmid, Nanoparticle: From Theory to Applications, Wiley-VCH Verlag GmbH & Co. KGaA, 2004
7. P. Dutta, S. Gupta (Ed), Understanding of Nanoscience and Technology, Global Vision Publishing House, 2006.
8. C.C. Koch, Nanostructured Materials: Processing, Properties and Applications, Jaico Publishing House, 2006.
9. Challa S.S.R. Kumar (Ed) Biological and Pharmaceutical Nanomaterials, John Wiley Verlag Cmbh & Co., KgaA, 2006.

Semester IV
Major Elective
Polymer Chemistry

Unit I CLASSIFICATION OF POLYMERS AND CHEMISTRY OF POLYMERISATION

Classification of polymers: linear polymers, non-linear or branched polymers, cross-linked polymers, homo chain hetero chain, homopolymers co-polymers block polymers and graft polymers.

Chemistry of polymerisation: Types of polymerization - mechanism - chain, growth, free radical, ionic, co-ordination, ring opening, metathetical, group transfer, polyaddition and polycondensation polymerisations.

Unit II INDIVIDUAL POLYMERS

Individual polymers: Monomers required general methods of preparation, repeat units and uses of the following polymers and resins – polyethylene, polystyrene, polyacrylonitrile, polymethylmethacrylate, PVC, polytetrafluoroethylene, polyisoprenes, polybutadienes and polychloroprene, polyesters, polycarbonates, polyimides, polyamides (Kevlar), polyurethanes, polyethylene glycols, phenol-formaldehyde, urea-formaldehyde, melamine-formaldehyde and epoxy resins - silicone polymers.

Unit III PROPERTIES OF POLYMERS

Intrinsic properties – processing properties – article properties – basic idea of isomerism of polymers – configuration of polymer chain – geometrical structure – syndiotatic, isotatic and atatic polymers.

Glass transition temperature: Definition - factors affecting glass transition temperature – relationships between glass transition temperature and (a) molecular weight, (b) melting point and (c) plasticiser – importance of glass transition temperature – heat distortion temperature.

Molecular weight and size of polymers: Number average, weight average, sedimentation and viscosity average molecular weights – molecular weights and degree of polymerisation – poly dispersity – molecular weight distribution in polymers – size of polymer molecules – kinetics of polymerisation.

Unit IV POLYMERISATION TECHNIQUES, DEGRADATION AND USES OF POLYMERS

Polymerisation Techniques: Bulk, solution, suspension, emulsion, melt condensation and interfacial polycondensation polymerisations.

Degradation: Types of degradation – thermal, mechanical, ultrasonic and photodegradation – photo stabilisers – oxidative degradation – antioxidants – hydrolytic degradation

Uses of polymers in electronics and biomedicine.

UnitV POLYMER PROCESSING

Polymer processing: plastics (thermo and thermosetting), elastomers, fibres, compounding, plasticisers, colorants, flame retardants.

Compression and injection mouldings – film extrusion and calendering – die casting and rotational casting – thermofoaming – reinforcing.

Reference Books

1. V.R.Gowariker, N.V.Viswanathan and Jayadev Sreedher, "Polymer Science", Wiely Eastern Ltd., New Delhi 1986.
2. G. Odian, "Principles of Polymerization", 2nd edn., John Wiley and Sons, New York, 1981.
3. D.W.van Krevelen and P.J.Hoftyrager, "Properties of Polymers", Elsevier, New York, 1976.
4. B.K. Sharma, "Polymer Chemistry", Goel Publishing House, Meerut, 1989.
5. P. J. Flory, "Principles of Polymer Chemistry", Cornell Univ. Press, Ithaca, 1953.
6. F.W.Billmeyer, "Text Book of Polymer Science", 3rd edn., John Wiley and Sons, New York, 1984.
7. Harry R. Allcock, F.W. Lampe and J.E. Mark, "Contemporary Polymer Chemistry", 3rd Edition, Pearson, Prentice Hall, Delhi 2005.