SEMESTER I

CORE COURSE I – INORGANIC CHEMISTRY– I

UNIT – I **(18 hours)**

Acids And Bases : Brownsted and Lewis acids and bases, pH, pKa, acid – base concept in non – aqueous media, buffer solution, Protonic Acids – Proton Affinities – Differentiating and leveling Solvents – Acidic behaviour of the Binary hydrides – Strength of oxyacids – Hydrolysis – Amphoteric oxides – Non protonic concepts of Acid – base Reactions – Lux concept. Classification of Acids and Bases as Hard or Soft – Acid – Base Strength and Hardness and softness – Symbiosis – Theoretical basis of Hardness and softness – Electronegativity and hardness and Softness. Non aqueous solvent – Liquid Ammonia, Acetic acid, bromine trifluoride, dinitrogen tetroxide, liquid hydrogen fluoride as solvents.

UNIT II **(18 hours)**

Ionic Bond Crystal structure and Advances Covalent Bonding :

Ionic bonding – definitions and example.

Lattice energy – Born Lande equation derivation – important points arising from Born Lande equation. Application of lattice energy – Radius Ratio rules – calculation of some limiting radius ratio values for CN.3 (planar triangle), CN.4 (tetrahedral), CN.6 (octahedral).

Classification of Ionic Structure :

AX, AX_2, AX_3, types AX type (ZnS, NaCl, and CaCl) structure only. AX_2 type fluoride, rutile, beta crystobalite (structure only). Layer structure – CdI_2, Nickel arsenide structures. Schottky defect and Frenkel defect – metal excess defect – F Centers and interstitial ions – Metal deficiency defect – positive ions absent – extra interstitial negative ions – Band theory of solids – insulators, semiconductors, and superconductors.

UNIT III **(18 hours)**

Nuclear Chemistry :

Radioactive decay – Theories of decay processes – Laws of radioactivity – Detection and Measurements of radiations – Nuclear structure – Composition of nuclei – properties of nuclei – nuclear radii – nuclear spin etc – nuclear forces – its characteristics – Meson Field theory – nuclear stability – nuclear models – liquid drop, shell and collective models.

Artificial Radioacivity

Nuclear reactions – transmutation – Stripping and pick up, Fission product and fission yields, fusion, spallation and fragmentation reactions scattering reactions – nuclear cross section – Q – value nuclear reactors – charged particle accelerators.

Radioactive techniques – tracer technique neutron activation and isotopic dilution analysis, counting techniques such as G.M. ionization and proportional counter.

Applications of nuclear science in agriculture and biology.

Radiation risks and medical benefits – Natural and manmade isotopes.

UNIT IV **(18 hours)**

Polyacids anions :

Basic building, units of vanadate, molybdate and tungstate ions – apex sharing structure only Hetero poly anions – structure only.

Inorganic polymers :

Rings, Phosphazenes – structure – Craig and paddock model – Dewar model Cages of phosphorus – Boron hydrides and carboranes.

Clusters :

Metal clusters, dinuclear clusters – structure of Re_2Cl_8 – Qualitative M.O. diagrams for dinuclear rhenium and molybdenum complexes to explain the strength of quadrapole bond.

UNIT V **(18 hours)**

Chemistry of metals and Rare gases :

General properties of metals, occurrence, principles of isolation and complex formation of s,p and d block metals. Chemistry of lanthanides and actinides – Spectral and Magnetic properties, lanthanide contraction.

Rare gas : Isolation Chemistry and structure of rare gas compounds (Xenon Compounds)

References

1. Badie E. Duglas and Danl H.M. Daniel. Concepts and Models in Inorganic chemistry, Indian Edition, 1970, Oxford and IBH Publishing co., New Delhi.
2. J.D.Lee, A New concise Inorganic chemistry 4th Edition, ELBS, 1995 (UNIT – II)
3. G. Friedlander, J.W.Kennady and J.M.Miller, Nuclear and Radiochemistry (UNIT – III)
4. Keith F. Purchell and John, C.Ktz Inorganic chemistry, Saunders Golden Sunburst series W.B. Saunders Company Philadelphia.
5. Cotton and Wilkinson, Advances Inorganic Chemistry 5th edition, john Wiley and sons Newyork (UNIT IV)
6. W. Kain and B.Schwederski, bioinorganic chemistry, Inorganic elements in the Chemistry of life, John Wiley and Sons, Newyork (UNIT V)
7. James E. Huheey, Ellen A, Keiter and Richard L. Keiter, Inorganic Chenistry; principles of structure and reactivity, 4th Edition, Addison – Wesley Newyork, (UNIT I)
8. Shriver and Atkins, Inorganic chemistry, III Edition Oxford, 1999. India Gopssons PVT Ltd A – 14 Sector Noida.
9. Nuclear Physics by Arumugam
10. Inorganic chemistry by Sathya Prakash

CORE COURSE II – PHYSICAL CHEMISTRY – I

UNIT I **(18 hours)**

Quantum Chemistry – I : Schrodinger wave equation – elementary ideas on time dependent SWE – postulates of quantum mechanics – operator algebra – linear, non – linear, ladder, Hermitian operators (definition and theorems) – eigenfunctions and eigenvalues, normalization orthogonality – principle of superposition.

Application of SWE to model systems – particles in one and three dimenstional boxes – quantum numbers – distortion of the box, zero point energy and uncertainity principles – finite potential energy barriers and tunneling (definition only)

UNIT II **(18 hours)**

Molecular Spectroscopy I : Introduction aspects – interaction of radition with molecules – Einstein coefficient of absorption and transtition probabilities – basics of selection rules representation of spectra – the width and intensity of spectral transition – oscillator strength.

Electronic Spectra : Electronic spectra of molecules - Born Oppenheimer approximation vibrational course structure - Franck - Condon principle – dissociation energy - rotational fine structure of electronic vibrational transtitions – Fortrat diagram. Pre – dissociation – symmetry selection rules – polarization of bonds – various types of transtition – solvent effect on spectra.

Photoelectron spectroscopy: Basic principles – UPES, XPES and AES – Valence and Core binding analysis, koopman's theorem – ESCA and auger spectroscopy to the study of surfaces.

UNIT III **(18 hours)**

Classical Thermodynamics : Thermodynamics of systems of variable composition – partial molar quantities and additivity rules – chemical potential – relationship between partial molar quantities – Gibbs – Duhem equation – calculation of partial molar quantities from experimental data – Thermodynamics properties of real gases – fugacity – definition, calculation (real) and variation of fugacity temperature, pressure and composition (Duhem – Margules equation) – activity and activity co-efficient, definition – standard states – colligative properties and the activity of the solute – experimental determination of activity and activity coefficients of non electrolytes – activity in electrolytic solutions – determination of activity coefficient of electrolytes by freezing points.

UNIT IV **(18 hours)**

Chemical Kinetics : Theories of reaction rates (bimolecular collision theory, absolute reaction rate theory (ARRT) – significance of reaction co – ordinate – molecular dynamics – potential energy surfaces – kinetic isotopic effect – Lindemann's theory for unimolecular gaseous reactions.

Principles of microscopic reversibility – steady – state approximation chain reactions – thermal and photochemical reactions between hydrogen and halogen – gas phase auto oxidation, explosions and hydrogen – oxygen reactions. Factors influencing reaction rates in solutions – application of ARRT to solution kinetics – effect of solvents – double sphere and single sphere model and effect of ionic strength – influence of pressure on rates in solution – significance of volume of activation.

Homogeneous catalysis – acid base catalysis - Bronsted relation – Enzyme catalysis – mechanism of single substrate reactions – Michaelis Menton law – influence of pH and temperature.

UNIT V

Fast reaction techniques **(18 hours)**

Flow methods (continuous and stopped flow methods) – Relaxation method (T and P jump methods) – Pulse techniques (pulse radiolysis, flash photolysis, shock tube method) – molecular beam method – lifetime method.

Photochemistry : Photophysical processes in electronically excited molecules Jablonski diagram – Stern – Volmer equation and its applications – experimental techniques in photochemistry – chemical actinometers – laser and their applications.

Radiation chemistry : Differences between radiation chemistry and photochemistry – sources of high energy radiation and interaction with matter – radiolysis of water, solvated electrons – definition of G value – Curie – Linear energy transfer LET and Rad Scanvenging techniques – use of dosimetry and dosimeters in radiation chemistry – applications of radiation chemistry.

References:

1. A.K. Chandra, Introductory Quantum Chemistry, 4th edition, Tata – MeGraw Hill, 1994.
2. R.K. Prasad, Quantum Chemisatry, 2nd Ed., New Age International Publishers 2000
3. I.N. Lenine, Quantum Chemistry 4th Ed., Prentice Hall of India Pvt. Ltd.
4. D.A.MeQuarrie, Quantum Chemistry, University Science Books 1998
5. P.W.Atkins, Molecular Quantum Mechanics, clarendon 1973
6. S. Glasstone, therodynamics for Chemists East – West Affilited Pvt Ltd., New Delhi.
7. K.K. Rohatgi – Mukherjee, Fundamentals of Photochemistry, Wiley Eastern Ltd.
8. M.G.Arora Nuclear Chemistry.
9. Arnicker, Nuclear Chemistry.
10. Glasstone, Source book on atomic energy.

CORE COURSE – III INORGANIC CHEMISTRY PRACTICAL – I

Titrimetric and Gravimetric

I. Estimation of mixture solutions

1. Cu (V) and Ni (G)
2. Cu (V) and Zn (G)
3. Fe (V) and Ni (G)
4. Zn (V) and Cu (G)

II. Preparation of compounds

1. Tetrammine copper (II) sulphate
2. Potassium trioxalato aluminate (III)
3. Tris thiourea copper (I) chloride
4. Tris thiourea copper (I) sulphate

Reference

1. Vogel's text book for qualitative & quantitative analysis

CORE COURSE IV – ORGANIC CHEMISTRY PRACTICAL – I

I. **Qualitative analysis of an organic mixture containing two components**

Pilot separation, Bulk separation, Analysis, Derivatives.

II. **Preparation of Organic compounds (Single stage)**

1. Para-bromo acetanilide from acetanilide (bromination)
2. Para-nitroacetanilide from acetanilide (nitration)
3. 2,4,6-tribromo aniline from aniline (bromination)
4. Salicylic acid from methylsalicylate (Hydrolysis)

References:

1.Gnanapragasam & Ramamurthy

ELECTIVE COURSE I – ORGANIC CHEMISTRY I

UNIT I **(18 hours)**

Nomenclature of Organic compounds : - Naming of linear and branched alkanes, alkenes, polyenes and alkynes with and without functional groups by IUPAC nomenclature – aromatic and heteroaromatic system – nomenclature of heterocyclics having not more than two hetero atoms such as oxygen, nitrogen and sulphur – Nomenclature of alicyclic, bicyclic and tricyclic compounds.

Reactive intermediates : - Free radicals, carbenes, nitrenes, carbocation and carboanion – generation, stability, structure and reactivity – nonclassical carbocation.

Electronic effects : - Inductive effect – resonance effect – hyperconjugation (Baker Nathan effect) – hydrogen bonding – inter and intra molecular

UNIT II **(18 hours)**

Organic Stereochemistry – I : Optical Isomerism : Principles of symmetry concepts of chirality – optical purity elements of symmetry and chirality – Newmann, Sawhorse Fisher and flying wedge notations – Representation and interconversion – types of molecules exhibiting optical activity – Configurational nomenclature D and L & R and S nomenclature alicyclic and cyclic chiral compounds – stereo chemistry of allenes, spiranes (Atropisomerism) Stereochemistry of ansa compounds, cyclophanes and trans cyclic alkenes, Definition of terms like prochirality, enantiotrophic and diastereotopic groups faces asymmetric sysnthesis – Cram's rule.

UNIT III **(18 hours)**

Organic stereochemistry – II : Geometrical isomerism : E and Z nomenclature determination of configuration of the geometrical isomers.

Configuarion of cyclic and bicyclc ring systems : Cis and trans nomenclature of three, four, five and six membered substituted cyclic systems – configuration of cyclohexane mono and di substituted cyclohexanes, decalins.

Dynamic stereochemistry : Quantitative relations between conformation and reactivity. Winstein – Eliel equation,Curtin – Hammett principle – Conformation reactivity and mechanism of cyclic systems – saponification of an ester, esterification of an alcohol, chromic acid oxidation of cyclohexanol – neighbouring group participation, deammination of 2-amino cyclohexanol-Stereospecific and stereoselective reactions.

UNIT IV **(18 hours)**

Methods of dertermining reaction mechanisms : Thermodynamic and kinetic aspects of organic reactions – energy profile diagrams – intermediate versus transition states, isotope effect– kinetic and non-kinetic methods of determination of reaction mechanisms-Product analysis and its importance – crossover experiments – isotopic labeling studies.

Correlation analysis : Linear free energy relation – Hammett equation – significance of sigma and rho applications. Taft, Swan, Scott, Grunwald – Winstein equation and their applications. Classification of solvents.

UNIT V **(18 hours)**

Natural Products : Carbohydrates : Polysaccharides – structure of starch and cellulose configuration of carbohydrates – photosynthesis.

Peptides and proteins : Primary, secondary,tertiary and quaternary structures of proteins. Protection of ,N – terminal and C – terminal groups of proteins – synthesis of peptides. Merrifield solid state peptide synthesis.

Nucleic acids : chemistry of nucleic acids – structure of DNA properties ,biological implications of DNA, replication of DNA, Determining the base sequence of DNA. Structure of RNA –types of RNA and their functions

References:

1. J. March, " Advanced Organic Chemistry Reactions, Mechanisms and Structure", 4th edition, Wiley 1992.
2. R.K.Bansal "Organic reaction mechanisms" Tata McGraw Hill,1975.
3. P.S.Kalsi "Organic reaction mechanisms",New age international publishers.
4. E.L.Eliel "Stereochemistry of Organic compounds".
5. D.Nasipuri "Stereochemistry of Organic compounds".
6. I.L.Finar "Organic Chemistry" Vol. II, 5th edition ELBS, (1975)
7. O.P. Agarwal "Chemistryof Organic natural products" Vol. I&II
8. Chatwal "Chemistry of Organic natural products" Vol.

SEMESTER II

CORECOURSE – V INORGANIC CHEMISTRY – II

UNIT I **(18 hours)**

Co – ordination Chemistry : Nomenclature of mono and polynuclear complexes – Crystal field theory – shapes of d orbitals in octahedral symmetry – CFSE strong field and weak field splitting – Calculation of CFSE for d^{10} system. Splitting in tetrahedral symmetry-only weakfield splitting. Jahn-Teller distortion,splitting pattern in trigonal, square planar, tetragonal, trigonal bipyramidal, square pyramide and cubic symmetries. Factors affecting the magnitude of splitting (10 Dq) – Spectrochemical series. Jorgensens relation. Evidences for CFT. Magnetism and color of transition metal ions, LFT.

M.O. Theory – Octahedral, tetrahedral and square planar complexes, pi bonding and M.O. theory – ligand having empty and filled pi bonds – effect on 10Dq. Evidences for Pi bonding from X – Ray Crystallography, IR and Photoelectron spectroscopy. Nephelauxtic effect.

UNIT II **(18 hours)**

Kinetics and mechanisms of reaction in solutions:

Labile and inert complexes, ligand displacement reactions – hydrolysis equation in octahedral and square planar complexes – trans effect. Electron transfer reaction – Complementary and non complementary types – inner sphere and outer sphere processes – isomerization and racemization. Reaction of coordinated ligands, Template effect and synthesis of macrocyclic ligands.

Stability of co – ordination compounds :

Detection of complex formation in solution, Stability constants, stepwise and overall formation constants pH metric, polarographic and photometric methods of determining of formation of constants. Factors affecting stability – statistical and Chelate effects.

UNIT III **(18 hours)**

Inorganic photochemistry : Electronic transitions in metal complexes – metal centered and charged transfer reactions. Various photophysical and photochemical processes of coordination compounds – unimolecular charge – transfer photochemistry of Cobalt (III) complexes. Mechanism of CTTM photoreduction, ligand field photochemistry of Chromium (III) complexes. Adamson's rule. Photo active excited states, V-C model – photophysics and photochemistry of ruthenium – polypyridine complexes, emission and redox properties – photochemistry of

organo metallic compounds, metal carbonyl compounds, compounds with metal – metal bonding. Reinecke's salt – chemical actinometer.

UNIT IV **(18 hours)**

Complexes of pi-acceptors ligands : Carbonyls – 18 electron rule – isolobal – applications to structure of carbonyl compounds (simple and poly nuclear) carbonylate anions, carbonyl hydrides ,nitrosyl complexes – bridiging and terminal nitrosyl – bent and linear nitrosyl – dinitrogen complexes.

Metallocences – reactions – catalysis by organo metallic compounds. Hydrogenation and hydroformylation of olefins, aldehydes and ketones- polymerisation of alkenes cyclo-oligomerisation of acetylene- Fisher -Tropsch systhesis.

UNIT V **(18 hours)**

Medicinal Bio – Inorganic Chemistry

Bio – inorganic chemistry of toxic metals – lead, calcium, mercury, iron, plutonium. Detoxification by metal chelation – Drugs which act be binding the metal sites of metalloenzymes. Metalloporphyrins – Chlorophyll, haemoglobin, myoglobin, vitamin B12. Nitrogen cycle, nitrogen fixation and dinitrogen complexes. Anti cancer drugs and their mechanism of action.

Anticancer activity of Pt complexes: Different types of active Pt - complexes, toxic effects of anticancer Pt - complexes, mechanism of anticancer activity, non – activity of trans – Platin.

References:

1. James, E. Huheey, Ellen A. Keiter and Rechard L. Keitar Inorganic Chemistry. 4th Edition. Addison – Wesley (UNIT I, II, IV)
2. Shriver, Atkins and Longford Inorganic chemistry ELBS, 1994 (UNIT II)
3. Inorganic chemistry by J.D. Lee
4. Inorganic chemistry by Sathya Prakash
5. Inorganic chemistry by Cotton – Wilkinson
6. A.W. Adamson, Inorganic photochemistry (UNIT III)
7. Ajaykumar Bhagi, Inorganic and supra molecular chemistry.
8. Ivano,Bartini, Bioinorganic chemistry
9. Leninger, biochemistry
10. Asim K. Das, Bioinorganic chemistry,2008

CORE COURSES VI – ORGANIC CHEMISTRY – II

Unit I **(18 hours)**

Aliphatic nucleophilic substitution: S_N1, S_N2 and S_NI mechanisms – effects of substrate structure, leaving group, attacking nucleophile and solvent – neighbouring group participation – substitution at allylic carbons and reactivity, ambident nucleophiles.

Elimination reaction: E1, E2, E1CB and Ei mechanisms – stereo chemistry of Elimimations Hoffman and Saytzeff rules – competition between elimination and substitution reactions – Chugaev reacation, dehydration of alcohols – dehydrohalogenation – Hoffman degradation – cope elimination – bredt's rule.

Aliphatic electophilic substitution: S_E1, S_E2 and S_EI mechanisms – effect of substrate structure, leaving group, attacking electrophiles and solvent – stork – enamine reaction – decarboxylation halogenation of aldehydes and ketones.

Unit II **(18 hours)**

Aromatic compounds : Elements of aromaticity – Huckel's and Craig's rule effects of aromaticity on bond length – ring current, non benzenoid aromatic compounds – aromatic character of three, five, seven and eight membered rings – anti – aromaticity systems with 2, 4, 6, 10, 14 and 18 electron systems, annulene and syndones – alternant and non alternent hydrocarbons – chemicals consequences of aromaticity.

Aromatic electrophilic substitution : Aromatic ion mechanism – orientation and reactivity – nitration – halogenation, sulphonation, Friedal – Craft's reaction - Gattermann, Kolbe – Schmidt, Reimer – Teimen, Hauben – Housch reactions.

Aromatic nucleophillic substitution : Benzyne and intermediate mechanisms – effect of substrate structure, leaving groups, attacking nucleophiles and solvents. Selected reactions – Zeigler alkylation, Chichibabin reactions involving diazonium group as leaving group- Cine substitution – Von- Richter reaction.

Unit III **(18 hours)**

Addition reactions : Addition to carbon - carbon multiple bond $LiAlH_4$ – $NaBH_4$ – tri tertiary butyl aluminium hydrides – mechanistic and stereochemical aspects of electrophylic addition nucleophilic free radical addition, orientation and reactivity – Birch reduction –Diels alder reaction – Michael addition – Ozonolysis – carbenes and their addition to double bonds.

Addition to carbonyl group : Mannich, Crossed Cannizaro,Stobbe, Benzoin, formation of ketenes, Oppenauer oxidation, MPV reduction, Darzen's glycidic ester condensation, Wittig reaction.

Unit IV **(18 hours)**

Molecular rearrangements : Mechanism of the following Wagner Meerwin, dienone-phenol, Wolf, Lossen, Schmidt,Bayer Williger, Stevens, Wittig, Favorski rearrangements.

Reagents in organic synthesis : Complex metal hydride –$LiAlH_4$ – $NaBH_4$ – tri tertiary butoxy aluminium hydrides,Tri n-butyl tin hydride, Gilmann's reagents lithium dimethylCuprate, Lithium di isopropyl amide, dicyclohexyl carbo diimides 1-3 dithianes, tri methyl silyl iodide, DDQ, SeO_2,Phase transfer catalyst, Crown ethers, Merrifield resins.

Unit V **(18 hours)**

Natural products:

Terpenes : Structural elucidation and synthesis of alpha pinene, Camphor, and zingiberene.

Alkaloids: Structural elucidation and synthesis of quinine, reserpine,Morphine, and papavarine.

Vitamins : Physiological importance and structural elucidation ofVitamin B_6 and Vitamin-C.

References :

1. J.March "Advanced Organic Chemistry", Reaction mechanism and structure 4th edition Wiley,1999.
2. R.K. Bansal Organic Reaction Mechanism Tata Mcgraw Hill, 1975.
3. P.S. Kalsi, Organic Reaction and their Mechanisms, New Age International Publisher.
4. I.L.Finar, Organic Chemistry Vol II Vth Edition, ELBS – 1975.
5. O.P.Agarwal, Chemistry of Organic Natural Products, Vol I & II, Goel Publications.
6. T.H.Lowry and K.S.Richardson, Mechanism and Theorm in Organic Chemistry, Harper and Row, 1976.
7. Organic Reaction Mechanism by Gould.
8. Organic Reaction Mechanism by Liberlas.
9. Organic Reaction Mechanism by Chatwal.

CORE COURSE VII – INORGANIC CHEMISTRYPRACTICAL – II

1. Semi micro qualitative analysis of a mixture containing two common and two rare cations.
2. Colorimetric estimation of Copper, Iron and Nickel using photoelectric colorimeter.

Common cations

Lead, bismuth, copper, cadmium, antimony, Tin, Iron, Aluminium, Chromium, Manganese, Nickel, Cobalt, Zinc, Calcium, Barium, Strontium, Magnesium and Ammonium.

Less common cations

Tungsten, Thalium, Selenium, Tellurium, Molybdenum, Cerium, Zirconium, Beryllium and lithium.

References :

1. Vogel's text book for qualitative & quantitative analysis

CORE COURSE VIII – ORGANIC CHEMISTRY PRACTICAL II

I.Quantitative analysis of organic compounds

Estimation of Phenol, aniline, ketone, glucose, saponification value of an oil, iodine value of an oil.

II. Preparation of organic compounds : (Double stage)

1. Para – bromoaniline from acetanailide (bromination and hydrolysis)
2. Para – nitroaniline from acetanilide (Nitration and Hydrolysis)
3. Acetyl salicylic acid from methyl salicylate (hydrolysis and acetylation)
4. 1,3,5 – tribromo benzene from aniline (bromination and diazotisation)

References :

1.Gnanapragasam & Ramamurthy

ELECTIVE COURSE – II FOOD AND NUTRITION

Unit : I **(18 hours)**

Carbohydrates: Classification – available polysaccharides - unavailable carbohydrates or dietary fibres, carbohydrates in diets – digestion and absorption - regulation of blood glucose - insulin - adrenaline.

Unit II **(18 hours)**

Proteins : Sources and chemical nature – aminoacids – nitrogen balance – factors affecting nitrogen balance – physiological needs – dietary sources – biological tests – requirements – protein deficiency.

Unit III **(18 hours)**

Fats, Electrolytes and Minerals: Visible fats – phospholipids - digestion and absorption – essential fatty acids deficiency – dietary needs for fat salt – Na and K in the body. Water balance – Na excess – K deficiency – K excess,. Minerals – intake – absorption – substances – assisting absorption – recommended intake – trace elements – iodine – physiology – sources – prophylactic and therapeutic uses – fluorine – prevention of dentel carriers – fluorosis in man – fluoride and osteroporosis – opposition to fluoridation of water Pb – Hg – hazards.

Unit IV **(18 hours)**

Milk and Milk products: Composition of milk – flavour and aroma of milk – physical properties of milk – effect of heat on milk – pasteurisation – homgenisation – Milk Products – cream milk – icecream – milk powder.

Unit V **(18 hours)**

Food and Nutrients: Food – classification – cereals – wheat – distribution of nutrients in grain and flour – starches – invalid foods – sugars – syrups, nutritive properties of vegetables – fruits – nutrition properties of meat, fish and oil of sea foods – novel protein foods.

Food Quality: Food adulteration – determination of adulteration in food products by simple qualitative test.

References:

1. M.Swaminathan, Food and nutrition.
2. Sri lakshmi, Food and nutrition.
3. Vijaya D.Joshi, Hand book of Nutrition and Dietics.

SEMESTER III

CORE COURSE IX – INORGANIC CHEMISTRY – III

Unit I **(18 hours)**

Electronic Spectroscopy: Electronic configuration, Terms, States and Microstates, Derivation of term symbols(p^2, d^2) and arranging the various terms according to their energies. Spectroscopic terms – Effect of inter electronic repulsion and spin – orbit coupling – Racah parameters B and C, R-S coupling and jj coupling. Selection rules and the breakdown of selection rules – Group theoretical explanation. Ground states of free ions for d^n systems – Oh and Td systems and the corresponding energy level diagrams – mixing of orbits. Orgel diagram – characteristics – prediction and assignment of transitions for d^n weak field cases. Tenabe – Sugano diagrams – characteristics – prediction and assignment of transition for weak field and strong field. Calculation of B and 10dq for simple Octahedral complexes of Co and Ni – Change transfer spectra.

Unit II **(18 hours)**

IR and Raman spectroscopy:

Combined uses of IR and Raman spectroscopy in the structural elucidation of simple molecules like H_2O, ClF_3, NO_3, ClO_3. Effect of Co-ordination on ligand vibrations – uses of group vibrations in the structural elucidation metal complexes of urea, thiourea, cyanide, thiocyanate, nitrate, sulphate and dimethylsulphoxide. Effect of isotopic substitution on the vibtational spectra of molecules – Vibrational spectra of metal carbonyls with reference to the nature of bonding, geometry and number of CO stretching vibrations (Group theoretical treatment).

Mossbauer Spectroscopy: Mossbauer transition and Doppler effect – Isomer shift quardrupole effect of magnetic field on spectra – simple applications to iron and tin compounds.

Unit III **(18 hours)**

NMR Spectroscopy: Chemicals shift and coupling (spin – spin coupling involving different nuclei H^1, P^{31}, C^{13}) interpretation and applications to Inorganic compounds. Effects of quadrupolar nuclei on the H^1 NMR Spectrum. NMR paramagnetic molecules – isotopic shifts, contact and pseudocontact interactions – Lanthanide shift reagents. Applications of P^{31}, C^{13}, H^1NMR of inorganic molecules.

Unit IV **(18 hours)**

EPR Spectroscopy: Basic principles – characteristics of g – Hyperfine splitting on various structures – Bis (salicylaldimine copper(II) – factors affecting the magnitude of the g values of transition metal ions – Three conditions (i) Spin – Orbit coupling crystal field (ii) Strength of the crystal breaking the spin – orbit coupling (iii) very large crystal field Ni(II) octahedral complex – Cu^{2+} in a tetrahedral complex - Cu^{2+} in a tetragonal field – Zero field splitting – Line widths in solid state EPR Spin lattice – Spin relaxation – exchange processes.

Magnetic properties: Types of magnetism – Dia – Para – ferro and antiferro magnetism. Magnetic properties of free ions – Temperature independent paramagnetism. Anamalous magnetic moment – ferromagnetic and antiferromagnetic exchanges.

Unit V **(18 hours)**

X – Ray Crystallography:

Solid state : Difference between point group – screw axis – glide plane Crystal symmetry elements – crystal classes – crystal systems – unit cell – bravis lattices – asymmetric unit space group – equivalent positions – relationship between molecular symmetry and crystallographic symmetry – basic concepts, the concept of reciprocal lattice and its application – X – ray diffraction by single crystal – structure factor – systematic absences – determination of space group – heavy atom method.

Neutron diffraction – elementary treatment – comparison with X – ray diffraction Electron diffraction – basic principles.

References:

1. B.N.Figgis, Introduction to Ligand Fields, Willey Eastern, New Delhi, (Unit I,II,III & IV)
2. James E Huheey, Ellen A.Keither and Richard L.Keiter, In organic Chemistry, 4^{th} edition.
3. R.S.Drago, Physical Methods in Inorganic Chemistry.
4. A.F.A.Kettle, Co-ordination Compounds, ELBS (Unit I,II,III & IV).
5. D.F.Shriver, P.W.Atkins and C.H.Langford, Inorganic Chemistry, 2^{nd} Editions.
6. Silverstein, Advanced Spectroscopy.
7. William Kemp, Spectroscopy.
8. Y.R.Sharma,Spectroscopy.
9. Jagmohan, Spectroscopy.

CORE COURSE X – ORGANIC CHEMISTRY – III

Unit I **(18 hours)**

Organic photochemistry: Fundamental concept – Jablonski diagrams – energy transfer characteristics of photo reduction and photo oxidation – photoreaction of ketones and enols norrish type I and II – reactions – photo – chemistry of alkenes, dienes and aromatic compounds – photo sensitation photo additions – Barton reaction – Paterno Buchi reaction.

Pericyclic reactions: Concerted reactions – Stereochemistry – orbital symmetry and correlation diagram – Frontier molecular orbital approach – Woodward – Hoffmann rules – electrocyclicreactions – cycloaddition

Reactions – selection rules – sigmatropic rearrangements – selection rules with simple molecules – 1,and 1,5 hydrogen shifts – Cope and Claisen rearrangements.

Unit II **(18 hours)**

Ultra violet and visible spectroscopy: Basis principle of electronic transitions – correlation of energy change with electronic transitions – instrumentation and sample handling techniques – Application of UV- Visible spectroscopy – Woodward – Fieser – Scott rules – application to conjugated dienes, trienes and poleynes – unsaturated carbonyl compounds – conjugated cyclic ketones – acetophenones – benzene and its substituted derivatives.

Infrared spectroscopy: Instrumentation and sampling techniques – types of stretching and bending vibrations – characteristic group frequencies –(internal and external)- quatitative studies – organic structure determinations, finger print region – identification of functional groups – hydrogen bonding (intermolecular and intra molecular).

Unit III **(18 hours)**

NMR Spectroscopy: Chemical and magnetic non-equivalence, chemical shift – coupling constant – first and second order proton spin – spin splitting dependence of J on dihedral angles – vicinal and geminal coupling constants – karplus equation – long range coupling constants – influences of stereo chemical factors on chemical shift of protons simplification of complex spectra – double resonance techniques – shift reagents – chemical spin decoupling of rapidly exchangeable protons – OH, COOH, SH, NH, NH_2 – an elementary treatment of NOE phenomenon – to techniques – COSY – NOESY.

C^{13} NMR Spectroscopy : Basic principles – FT NMR Relaxation – broad band decoupling – off resonance decoupling – calculation of chemical shifts for simple aliphatic and aromatic compounds – conformation and chemical shift correlation – peak assignments – importance of NOE phenomenon in C^{13} spectroscopy.

Unit IV **(18 hours)**

Mass Spectrometry: Basic principles – resolutions – EI and CI methods – base peak – recognition of molecular ion peak – FAB fragmentation – general rules – nitrogen rule – McLafferty rearrangement – ortho effects – importance of metastable peaks.

Electron spin resonance spectroscopy: Basic principles – comparison between ESR and NMR spectra hyperfine splitting – factors affecting the magnitude of values applications to organic free radicals, Methyl and naphthyl radicals.

Optical rotatory dispersion and circular dichromism: Cotton effect – ORD curves – axial haloketone rule and its applications – octant rule – its applications – applications of ORD to determine absolute configuration of monocyclic ketones.

Unit V **(18 hours)**

Steroids: Classification – structural elucidation of cholesterol – (synthesis not required) – structural elucidation of vitamin D – estrone – progesterone, ergosterol, androsterone and cortisone – classification and functions of prostoglandins

Heterocyclics: Synthesis and reaction of azoles – pyrazole, imidazole, oxazole and thiazole.

References:

1. C.N. Banwell, Fundamentals of molecular Spectroscopy.
2. P.M.Silverstein, F.X.Wester, Spectroscopic Identification of Organic compounds.
3. P.S.Kalsi, Spectroscopic of Organic compounds.
4. W.Kemp, Organic Spectroscopy.
5. Y.R. Sharma Elementary Organic Spectroscopy.
6. J.D. Coyle, Organic Photochemistry, 1985.
7. G. R.Chatwall Organic Photochemistry,1998.
8. G,M. Barrow, Introduction to molecular Spectroscopy, 1964.
9. Jagmohan, Organic Spectroscopy.

CORE COURSE XI – PHYSICAL CHEMISTRY – II

UNIT I **(18 hours)**

Group Theory: Elements of Group Theory – properties of group and subgroup – classes – group multiplication tables – isomorphism, group - symmetry elements and symmetry operations – interrelations among symmetry operations – generators – point groups of molecules – Matrix representation theory – Consequences of great orthogonality theorem and construction of character tables – characters reducible and irreducible representation – Direct products and correlation tables.

Application of group theory to IR, Raman and electronic spectra – Projection operators – SALC procedure – evaluation of energies and MO's for system like ethylene – butadiene planar monocyclic aromatic Compounds – hybridisation schemes of orbitals.

Unit – II **(18 hours)**

Quantum Chemistry – II

Application of SWE to simple harmonic oscillator (Hermite Polynomial, eigen function, eigen values – rigid rotator with free Axis (SWE) in polar coordinates, separation of angular functions and their solution, Legendre and associated Legendre polynomials, degeneracy of rotational states – hydrogen and hydrogen like atoms (separation of angular and radial functions and solution to radial equation, Laguerre and associated Laguerre polynomials, quantum numbers, space quantization, electron spin) – the anti symmetry or Pauli exclusion principle and slater determinant – ground state helium atom).

Unit III **(18 hours)**

Molecular Spectroscopy

Infra red spectroscopy: Vibrational spectra selection rule – (fundamentals absorption, first and second overtones, hot bands etc.) vibrational spectra of diatomic molecules, selection rule for the rigid rotor – harmonic oscillator mode – relative intensities – coupling and rotation of vibration – linear molecules and symmetric top molecules(parallel and perpendicular bands).

Raman spectroscopy: Raman effect elastic and inelastic scattering – selection rule – pure rotational raman spectra (linear, spherical top, symmetric top and asymmetric top molecules – vibrational raman spectra – polarization of light and Raman effect – comparison of IR and Raman spectra – simplemolecule – mutual

exclusion principle – Fermi resonance – laser Raman spectroscopy – elementary treatment only.

Unit IV **(18 hours)**

Statistical Thermodynamics

Calculation of thermodynamic probability of a system – Difference between thermodynamic and statistical probability – Ensembles, phase space – ergodic hypothesis – definition of micro and macro states – different methods of counting macro states – distinguishable and indistinguishable particles – classical statistics – derivation of Maxwell – Boltzmann distribution law.

Partition Function: Translational, rotational, vibrational, Electronic – calculation of enthalphy, internal energy, Entropy and other thermodynamic functions – application of partition functions to mono atomic and diatomic molecules.

Unit V **18 hours)**

Surface phenomena: Adsorption and free energy reaction relation at inter – phase – physisorption and chemisorption – potential energy diagram – Lennard- Jones plot – Langmuir, BET isotherm – surface area determination – heats of adsorption, determination – adsorption from solution – Gibbs adsorption isotherm.

Role of surfaces in catalysis: Semiconductor catalysis – n and p type surfaces – kinetics of surface reactions involving adsorbed species – Langmuir – Hinshelwood, mechanism of bimolecular reaction – Langmuir – Rideal mechanism of bimolecular reaction – Rideal – Eler mechanism.

References:

1. F.A.Cottan, Chemical Application of Group Theory 2nd edition, Wiley – Baster(1971)
2. R.L.Flowry,Jr,Symmetry Groups – Prentice Hall, NewJersy(1980)
3. C.N.Banwell, Fundamentals of Molecular Spectroscopy, Tata Megraw Hill edition(1993)
4. R.K.Prasad, Quantum Chemistry, 2nd edition.
5. Gupta, Statistical Thermodynamics.
6. G.C.Bond, Heterogeneous Catalysis – Principles.
7. Mathematics for quantum chemistry, J.M.Anderson, Benjamin.
8. Introductory quantum chemistry, A.K.Chandra, Tata – MeGraw Hill edition.
9. Molecular quantum mechanics, P.W.Atkins, Clarenden.
10. Levine, Quantum Chemistry.
11. K.V.Raman, Group theory and its applications.

CORE COURSE XII – PHYSICAL CHEMISTRY PRACTICAL – I

1. Determination of molecular weight of substance by Transition Temperature method.
2. Determination of molecular weight of substance by Rast's method.
3. Determination of Critical Solution Temperature(CST) of phenol – water system and effect of impurity on CST.
4. Study of phase diagram of two components forming a simple eutectic.
5. Study of phase diagram of two components forming a compound.
6. Kinetics – Acid hydrolysis of an Ester – Comparison of strength of acids.
7. Kinetics – Acid hydrolysis of an Ester – Determination of Energy of Activation (Ea)
8. Kinetics – Persulphate – Iodine reaction – Determination of order, effective of ionic strength on rate constant.
9. Adsorption – Oxalic acid/Acetic acid on charcoal using Freundlich isotherm.

References:

1. Findlay's Practical Physical Chemistry Revised and edited by B.P.Levitt, 9th edition.
2. J.N.Gurtur and R.Kapoor, Advanced Experimental chemistry, Voli,Chand &co., Ltd, New Delhi.

ELECTIVE COURCE – III MEDICINAL CHEMISTRY

Unit I

Introduction – definition of allergy, intolerance and side, effects, drug induced side effects – tolerance, resistance and dependence.

First aid for accidents – rules of first aid – cuts, abrasions, bruises, bleeding, fractures, burns, fainting and poisonous bites – detection of hallucinogens and poisons – antidotes for poisoning.

Unit II

Analgesics : Classification – non narcotic and narcotic analgesics – antipyretic analgesics – paracetamol, phenacetin – synthesis and uses, Asprirn –synthesis, uses and toxic effects. Anti inflammatory analgesics – ibuprofen and indo methacin – synthesis,uses and toxic effects.

Unit III

Antibiotics : Introduction – classification pencillins, streptomycin and chloromphenicol – synthesis, toxic effects and uses. Antifungal antibiotics – hystatin.

Anti malarials: Quinine synthesis,uses and toxic effects.

Unit IV

Vitamins : Classification –source and deficiency. Vitamin A,D,E,K,B complexes(B_1, B_2, B_6, and B_{12},), folic acid and vitamin – C.

Hormones: Definition – classification – thyroxin, oxytocin, insulin, progesterone and andestrone and its importance and uses

Unit V

A general study of the following classes of compounds

1. Sedatives, hypnotics and transquilizers.
2. Antiseptics and disinfectants.
3. Anticancer drugs.
4. Diabetic & hypoglycemic drugs.

Reference :

1. Alfred Burger, “Medicinal Chemistry” part I & II, 3rd edn, Willey interscience.
2. Goodman and Gilman “Pharmacology and Pharmacothearputics” .
3. Ahsulosh Kar, “Medicinal chemistry” Wiley Eastern, Madras.
4. Harkrishan singh and V.K.Kapoor, “Organic pharmaceutical Chemistry”, Vallabh Prakashan, Delhi.
5. I.L.Finar, “Organic Chemistry” Vol I & II ELBS.
6. Jayashree ghosh, a text book of “Pharmaceutical Chemistry”.

SEMESTER IV

CORE COURSE XIII – PHYSICAL CHEMISTRY – III

UNIT I **(18 hours)**

Quantum chemistry – III – Need for approximation method – variation method (Statement, proof, secular equation, application to hydrogen and helium atom) – perturbation method for non-degenerate systems (first order correction to Eigen value and Eigen function to helium atom)-elementary idea of Hartree - Fock self-consistent field method. Hybridization, solving wave equation for sp,sp^2, and sp^3 hybrid orbitals- Huckel's molecular orbital theory and its application to ethylene and butadiene (charge density, n bond and free valence)

UNIT II **(18 hours)**

Quantum statistics : Bose- Einstein (BE) distribution function – Fermi Dirac (FD) distribution function – comparison of them with Maxwell-Boltzmann statistics – Application of BE statistics to photo gas, application of FD statistics to electron gas and thermionic emission.

Heat capacities of solids: Einstein and Debye's treatments - concept of negative Kelvin temperature.

UNIT III **(18 hours)**

Electrode – Electrolyte equilibrium: Nernst equation and its limitations – equilibrium electrode potentials – classification of electrodes – concentration cells liquid junction potentials –thermodynamic quantities from EMF data.

Electrochemical energy: Storage systems – primary and secondary batteries – fuel cells.

Ionics: Transport of ions in solution - Debye - Huckel theory – radius of ionic atmosphere and its calculation - Debye- Huckel - Onsagar equation modifications – asymmetry and electrophoretic effects – evidences for ionic atmosphere – Debye-Falkenhegen and Wien's effects – extension to Debye- Huckel - Onsagar theory.

UNIT IV **(18 hours)**

Electrokinetic phenomena: Theories of electrical double layer – Electrical double layer potential – theory of multiple layers at electrode electrolyte interface – double layer capacity - electrokinetic phenomena (zeta potential, electro osmosis, sedimentation potential)

Processes at the electrodes: The rate of charge transfer – current density – Butler – Volmer equation ,Tafel equation.

Principles of Electro deposition of metals: Electrochemical corrosion – construction and use of pourbaix and Evans diagram and prevention of corrosion – electrochemical oxidation and reduction.

UNIT V **(18 hours)**

Polarography and Cycilc Voltametry: Voltametry - Polarography –Principle – Instrumentation, current – voltage relationship, polarographic waves – half wave potential, reversible and irreversible waves – residual current –migration current – Polarographic cells - Dropping mercury electrode - advantages of DME – application of polarography.

Tensametry – chronopotentiometry – instrumentation , procedure and applications – cyclic and stripping voltametry – Principle and applications – amperometry – principles , indicators – instrumentation –amperometric titrations – titration with two indicator electrodes – Dead stop – endpoint method – potentiometric titrations - advantages, disadvantages and applications.

References:

1. A.K. Chandra, Introductory Quantum Chemistry .
2. R.K.Prasad, Quantum Chemistry.
3. Gupta, Statistical Thermodynamics.
4. S.Glasstone “Introduction to Electrochemistry”.
5. J.AIberty, “Electrokinetics”.
6. Bockris and Reddy, Electrochemistry.
7. Kaur, Instrumental methods of chemical analysis.
8. Skoog and West, Analytical Chemistry.
9. Vogel,A.I . Text book of quantitative Inorganic Analysis.
10. Chatval and Anand, Instrumental methods of chemical analysis.

SEMESTER IV

CORE COURSE XIV – PHYSICAL CHEMISTRY PRACTICAL – II

I. **Conductometric Titrations**

1. Acid – base titrations
2. Precipitation titration
3. Displacement titrations
4. Determination of dissociation constant of weak acids
5. Solubility product of sparingly soluble silver salts

II. **Potentiometric Titrations**

1.Acid – base titrations

2.Precipitation titration

3. Redox titrations

4. Determination of dissociation constant of weak acids

5. Determination of solubility of silver salts

III. Determination of pH of a Buffer solution (CH_3COONa + HOAc)

References

1. Findlay's Practical Physical Chemistry Revised and edited by B.P. Levitt,9th edition.

2. J.N.Gurtur and R.Kapoor, Advanced Experimental chemistry, Voli. Chand & Co., Ltd, New Delhi.

3. J.B.Yadhav, Practical Physical Chemistry.

SEMESTER IV

ELECTIVE COURSE IV – RECENT TRENDS IN CHEMISTRY

UNIT – I **(18 hours)**

Introduction to computing and networking:

Introduction to computers and computing – hardware – basic organization of a computer – CPU – main memory – secondary storage – i/o devices – software system and applications of software – high and low level languages compilers – algorithms and flow charts.

Introduction to networking –Computer networks – LAN, WAN, internet and internet – worldwide web – internet for chemists – online search of chemistry data bases – e-journals - search engines for chemistry.

UNIT – II **(18 hours)**

Nano chemistry

Introduction to nanotechnology – molecular nanotechnology – nanomanipulator, nanotweezers, atom manipulation – nanomaterials– preparation of nanomaterial - plasma arcing method, chemical vapor deposition method,electrodeposition method– applications of nanomaterials (batteries, medical implants, motor vehicles and aircraft – nanotubes – properties and uses of nanotubes, Nano medicines, environmental applications. Fullerenes - properties & uses.

UNIT –III **(18 hours)**

Research methodology

Introduction to primary sources (journals and patent), secondary sources (chemical abstract, Dictionary, Monographs and Review articles), Chemical abstracts – Subject index – author index and formula index and other indexes with examples – current contents – organization – methods of using the titles and index – preparation and presentation of research papers in journals and seminars.

UNIT – IV **(18 hours)**

Green chemistry:

Principles(12) - inception – scope – areas – green solvents – biocatalyst and biocatalysis – synthesis of safer product.

Green chemistry – photochemical principles – photo oxidation – photo degradation – removal of hazardous chemicals from water – cleaner production concept – implementation – Government role .

UNIT-V **(18 hours)**

Molecular modeling basics

Molecular modeling – coordinate systems – Cartesian and internal coordinate systems – bond lengths, bond angles and torsion angles, potential energy surfaces. Molecular mechanics – applications and parameterization – advantages and limitations of force fields.

References

1. E.Balaguruswamy, programming in ANSIC", Tata McGraw Hill. 2nd edition,
2. NewDelhi, 1999.
3. Robert Lafore, "Object Oriented Programming in Turbo C++",Galgotia, New Delhi, 1995.
4. K.V.Raman , Computers in chemistry, Tata McGraw Hill, New Delhi 1993.
5. M.M.Srivatsava, Rashmi saneni chemicals for green environment, Narosa publishing house, New Delhi.
6. T.Pradeep, "Nano the essentials – understanding nano science and nano technology" Tata McGraw Hill publishing Ltd, New Delhi.
7. A.R.Leach, Molecular Modeling Principles and applications, 2nd edition prentice Hall, 2001.
8. Green chemistry, Ahluwalia