PG & RESEARCH

DEPARTMENT OF CHEMISTRY

M.Sc., (Chemistry)-SYLLABUS

Effect from the Academic Year 2015-2016

NEHRU MEMORIA COLLEGE (AUTONOMOUS)
Puthanampatti, Trichy- 621 007

NEHRU MEMORIAL COLLEGE (AUTONOMOUS) PUTHANAMPATTI

PG COURSE STRUCTURE UNDER REVISED CBCS PATTERN (2015-2016 ONWARDS)

M.Sc., CHEMISTRY

SEM	Course	Subject Title	Subject Code	Hrs/ Week	Credit	Int	Ext	Total
I	CC-I	Inorganic Chemistry-I		6	5	40	60	100
	CC-II	Organic Chemistry-I		6	5	40	60	100
	CC-III	Inorganic Chemistry Practical-I		6	4	40	60	100
	CC-IV	Organic Chemistry Practical-I		6	4	40	60	100
	CEC-I	Physical Chemistry-I		6	4	40	60	100
		Total		**30**	**22**	**200**	**300**	**500**
II	CC-V	Inorganic Chemistry-II		6	5	40	60	100
	CC-VI	Organic Chemistry-II		6	5	40	60	100
	CC-VII	Inorganic Chemistry Practical-II		6	4	40	60	100
	OEC	Green & Industrial Chemistry/Food Chemistry		6	4	40	60	100
	CEC-II	Physical Chemistry-II		6	4	40	60	100
		Total		**30**	**22**	**200**	**300**	**500**
III	CC-VIII	Inorganic Chemistry-III		6	5	40	60	100
	CC-IX	Organic Chemistry-III		6	5	40	60	100
	CC-X	Organic chemistry Practical-II		6	4	40	60	100
	CC-XI	Physical Chemistry Practical-I		6	4	40	60	100
	CEC-III	Physical Chemistry-III		6	4	40	60	100
		Total		**30**	**22**	**200**	**300**	**500**
IV	CC-XII	Inorganic Chemistry-IV		6	5	40	60	100
	CC-XIII	Organic Chemistry-IV		6	5	40	60	100
	CC-XIV	Physical Chemistry Practical-II		6	5	40	60	100
	CEC-IV	Physical Chemistry-IV		6	4	40	60	100
	CC-XV	Project Work**		6	5	40	60	100
		Total		**30**	**24**	**200**	**300**	**500**
		Grand Total		**120**	**90**	**800**	**1200**	**2000**

****Dissertation:**

Two Reviews (20+20) = 40 Marks
Report Valuation = 40 Marks
External Viva-Voce = 20 Marks

- CC-Core Course; EC-Elective Course
- OEC-I* to be offered by the Chemistry Department (Green &Industrial Chemistry(or) Food chemistry.
- Except for Practical (6 hrs), End Semester Examination Hours for each course – 3 Hrs

CC-I- INORGANIC CHEMISTRY -I

Semester: I Hour/week: 6

Course Code: credits: 5

Objectives:

1. To enable the students to understand the basic concepts of Inorganic Chemistry including nomenclature, structure and bonding
2. To enable the students to understand the concepts of main group chemistry such as B, P, S and interhalogens.
3. To provide and introduce the concepts of solid state and crystal chemistry.

UNIT – I

Basic concepts of inorganic chemistry

Nomenclature of simple inorganic compounds and its salts – Oxy acids (hypo, ous, ic, per acids), Ortho, meta and pyro acids. The periodic properties of elements –Ionic radii, ionization potential, electron affinity, electronegativity.

Structure and bonding: Atomic orbitals, electronic configuration of atoms(L-S Coupling), concept of hybridization. Molecular orbitals and electronic configuration of homonuclear diatomic molecules. Shapes of poly atomic molecules – VSEPR theory – Bond lengths, bond angles, bond order and bond energies. Types of chemical bond, intermolecular forces(weak and strong), structure of simple ionic and covalent solids.

UNIT – II

Acids and Bases

Acid – base concepts - Bronsted and Lowry, Arrhenius, Luxflood, Usanovich, Lewis, solvent system and generalized acid base concepts- measure of acid base strength – steric effect and solvation effects – effect of substitutes on acidity of carboxylic acid. Hard and soft acids and bases – principles, theories of hardness and softness and application of HSAB. Non – aqueous solvents – liquid ammonia, liquid HF, liquid SO_2, liquid dinitrogen tetroxide.

Interhalogens (ICl,ClF_3, IF_5, IF_7), pseudo halides and noble gas compounds – synthesis, bonding and structure.

Unit III

Main group chemistry - I

Boranes- Classification, preparation of higher boranes by Stock's method and pyrolysis of diborane, reactions of diboranes with Lewis bases- symmetric and unsymmetric cleavage - types of bonds in higher boranes- the styx number, Wades rule as applied to boranes. Geometrical structures of B_4H_{10}, B_5H_9, B_5H_{11}, B_6H_{10} and $B_{10}H_{14}$. Carboranes- classification, nomenclature, structures of CB_5H_9, $C_2B_4H_8$, $C_3B_3H_7$ and $C_4B_2H_6$. Metallocarboranes – Preparation from 1,2-dicarba-closo-dodecaborane, sandwich structure. Borazines- Preparation, properties and structure. Difference in chemical properties between borazine and benzene. Preparation and structure of boron nitride.

Phosphazenes-Classification, Cyclophosphazenes-$(NPCl_2)_3$ and $(NPCl_2)_4$- preparation and structure, Linear polyphosphazenes- preparation and applications.
Sulphur-nitrogen compounds- Preparation and structures of S_4N_4 and S_2N_2, (SN)x.

Unit – IV

Main group chemistry - II

Oxy acids of nitrogen and their salts – Hyponitrous acids-nitrous acid – calcium ammonium nitrate (CAN) – Ammonium sulphate nitrate.

Oxyacids of Phosphorus and their salts –pyrophosphorus acid – orthophosphoric acid – Triphosphoric acid - Ammonium dihydrogen phosphate – Sodium ammonium hydrogen phosphate (or) micro cosmic salt

Oxyacids of sulphur and their salts — hyposulphurous acid – pyrosulphuric acid– Dithionic acid – Barium dithionate- polythionic acids – differences between dithionic acid and polythionic acids.

Oxyacids of halogens and their salts – hypochlorous acid –Bleaching powder – perchoric acid– potassium perchlorate – hypoiodous acid – Meta periodic acid – para periodic acid.

Unit - V

Solid state and crystal chemistry

Lattice energy – Born – Landeequation,Kapustinski equation – structures of one, two, three- dimensional silicates - molecular sieves –defects in solids – Schottky and Frenckel defects - band theory of solids - insulators and semiconductors

Radius ratio rule – shapes of ionic crystal – structures of metallic crystals – structures of Ionic crystals – TiO_2,CaF_2,ZnS

Text books:

1. Purcell and Kotz, “Inorganic Chemistry”, Saunders Golden Sunburst Series, W.B.Saunders Company, Philadelphia.
2. F.A. Cotton and G. Wilkinson, “Advanced Inorganic Chemistry “, 4^{th} ed., A Wiley – Interscience Publication, John – Wiley & Sons, USA.

References:

1. M.C. Day and J.Selbin , “theoretical Inorganic Chemistry “ , Affiliated East West Press Pvt. Ltd. 2^{nd} ed., 1985.
2. J.E.Huheey, Inorganic chemistry “, 3^{rd} ed., Harper & Row publisher, Singapore.
3. S.Glasstone, “Source Book on Atomic Enertgy “, D.VanNostrand , New York 1967(Affiliated East-West Press ,New Delhi 1969)
4. J.D.Lee,A New Concise Inorganic Chemistry, 4th ed., ELBS, 1995.

CC-II-ORGANIC CHEMISTRY -I

Semester: I Hour/week: 6

Course Code: credits: 5

Objectives:

To introduce the following concepts in Organic Chemistry to the students

- Nomenclature of Organic compounds, Structure and bonding
- Aromaticity
- Stereo Chemistry
- Carbohydrates & nucleic acids
- Aliphatic nucleophilic & electrophilic substitution.

UNIT – I

1.1 **Nomenclature of organic compounds :**

IUPAC system of nomenclature – Naming of linear and branched alkanes, alkenes, alkynes without and with functional groups by IUPAC method. Aromatic and hetero aromatic systems – nomenclature of hetero cycles having not more than two hetero atoms such as oxygen, nitrogen and sulphur. Nomenclature of alicyclic, bicyclic and tricyclic compounds.

1.2. **Structure and Bonding:**

Localized Chemical bonding – Electronic structure of molecules, Electronegativity, Dipole moment, Inductive and Field effects, Bond distances, Bond angles, Bond energies.

Delocalized chemical bonding – Bond energies and bond distances in compounds containing delocalized bonds, cross conjugation, resonance – steric inhibition of resonance, hyperconjugation, keto – enoltautomerism.

UNIT – II

Aromaticity:

Aromaticity – definition – Huckel's and Craig's rules – effects of aromaticity on bond lengths – ring currents – aromatic character in 3,4,5,6,7,8 member rings and non-benzenoid- rings with 2, 4, 8, 10, 14 and 18 π electron systems - Antiaromaticity – alternant and non-alternant hydrocarbons. Aromaticity of annulenes – 10, 12, 14, 16and 18 annulenes, heteroannulenes, sydnones and fullerenes.

Reactive intermediates:

Generation, stability, structure and reactivity of carbocations, non- classical carbocations, carbanions, free radicals, carbenes and nitrenes

UNIT -III

Stereochemistry- I:

Stereoisomerism – definition and classification. Molecular representations – Wedge, Fischer, Newmann and Saw-horse formulae – their representations and

interconvertibility. Optical activity and chirality – types of molecules exhibiting optical activity. Dissymmetric and asymmetric molecules – Fischer projection.

Configurational nomenclature:

D-L and R-S configuration, Cahn-Ingold- Prelog rules for simple acyclic and cyclic chiral molecules, stereochemistry of allenes, spiranes and biphenyls – Walden inversion – asymmetric synthesis based on Cram's rule – Enantiotopic behavior and prochiralcentres.

UNIT – IV

Aliphatic Nucleophilic substitution:

S_N1 , S_N2 &S_Ni - mechanisms - effect of substrate structure, leaving group, attacking nucleophile and solvent – neighboring group participation – substitutions at allylic carbons and reactivity – ambident nucleophiles.

Aliphatic Electrophilic substitution:

S_E1, S_E2&S_Ei– mechanisms – effect of substrate structure, leaving group, attacking electrophile and solvent – Stark –enamine reaction – decarboxylation of aliphatic acids – halogenations of aldehydes and ketones.

UNIT – V

5.1 **Methods of determining reaction mechanisms:**

Homolytic and heterolytic cleavages of bonds – types of reaction – thermodynamic and kinetic aspects of organic reactions – energy profile diagrams – intermediate versus transition state – Hammond's postulate – isotope effects – kinetic and non – kinetic methods of determining reaction mechanisms – kinetic isotopic effect (primary and secondary) – product analysis and its importance. Cross-over experiments – stereochemical studies – isotopic labeling studies.

V 5.2 **Correlation analysis:**

Linear free energy relationship – Hammett equation – significance of substituent and reaction constants (σ , σ^+ , σ^- and ρ) – applications and limitations of Hammett equation. Taft, Swain – Scott ,Grunwald – Winstein equation and their applications.

Text books:

1. R.T. Morrison and R.N.Boyd, Organic Chemistry 6th edition, Prentice – Hall of India, 2007.
2. E.L.Eliel and S.H.Wilen, Stereochemistry of Organic Compounds, John – Wiley, 2003.
3. D. Nasipuri, Stereochemistry of Organic Compounds, 2nd edition, new age international, 1994.
4. R.K.Bansal, Organic Reaction Mechanisms, 3rd edition, Tata McGraw Hill, 2005.
5. P.S.Kalsi, Organic Reactions and their mechanisms, 4th edition, new age international, 2006.

6. P.S. Kalsi , Stereochemistry conformation and mechanism, 5th edition, new age international , 2003.
7. J.March, Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 4th edition, Wiley, 1992.
8. O.P . Agarwal, Organic chemistry of Natural Products, volume I &II , 29th edition, Goelpublishing houses, 2005.

References:

1. R.Panico, WH. Powell, L.Jean ,C.Richer, A guide of IUPAC Nomenclature of organic compounds, 1993.
2. R.S.Cahn and O.C.Dermer, Introduction to chemical Nomenclature, 5th edition, Butterworths, 1997.
3. I.L.Finar, Organic Chemistry, Vol.II , 6th edition , pearson education, 2005.
4. F.A.Carey and R.J.Sunberg , Advanced Organic Chemistry , Parts A&B, Plenum,1984.
5. Stanley H Pine, Organic Chemistry, 5th edition, Tata McGraw –Hill, 2007.
6. Bernard Miller and Rajendra Prasad, Advanced Organic Chemistry, Reaction and Mechanisms, 2nd edition, pearson education, 2006.

CC – III -INORGANIC CHEMISTRY PRACTICAL-I

Semester: I Hour/week: 6

Course Code: credits: 4

Objectives:

To give practical training for

1. Separation and identification of a mixture containing two common and two rare cations.
2. Colorimetric estimation.

INORGANIC CHEMISTRY PRACTICAL – I

A. **Semimicro qualitative analysis** of a mixture containing two common and two rare cations.

B. **Colorimetric estimation** of Copper, Iron, Nickel and Chromium using Photoelectric colorimeter.

Text Books:

1. V.Venkateswaran, R. Veerasamy and A.R. Kulandaivelu, Basic Principles of Practical Chemistry, Sultan Chand & Sons, Second Edition, 1997.
2. K.K.Sharma and O.S.Sharma, An introduction to Practical Chemistry, Vani Educational Books, Second Edition, 1982.

References:

1. ARTHUR I.VOGEL, A Text Book of Macro and Semi-micro Qualitative Inorganic Analysis, Longman Group Ltd., First Indian Edition, 1975.
2. V.V. Ramanujam, Inorganic Semi-micro Qualitative Analysis, The National Publishing Co., Madras, Second Edition, 1970.

CC-IV- ORGANIC CHEMISTRY PRACTICAL-I

Semester: I Hour/week: 6

Course Code: credits: 4

Objectives:

- To teach and give practical training to the students
  - The techniques and separation of binary organic mixture using pilot and bulk separation.
  - Qualitative organic analysis for identification of various functional groups.

- To help students prepare organic compounds involving following processes
  - Bromination
  - Ozonisation.

A. Qualitative analysis of Binary organic mixture :

i) Pilot separation-
ii) Bulk separation-
iii) Analysis
iv) Derivatives

B. Single stage preparation of organic compounds :

a) Bromination : 2,4,6-tribromophenol from phenol
b) Osazonisation : Glucosazone from Glucose.
c) Acetylation : Resacetophenone from Resorcinol.
d) Oximation : Benzophenoneoxime from Benzophenone
e) Oxidation : p- benzoquinone from Hydroquinone
f) Diazotisation : Phenyl – azo – 2-naphthol from aniline.
g) Sandmeyer reaction : o- chlorobenzoic acid from Anthranillic acid.

Text Books:

1. V.Venkateswaran, R. Veerasamy and A.R.Kulandaivelu, Basic Principles of practicalcheamistry , Second edition , sultan chand& sons, (1997).
2. K.K.Sharma and O.S.Sharma , An introduction to practical chemistry, Vani Educational Books , 2nd edition (1982).

References :

1. ARTHUR I. VOGEL, Elementary pracatical organic chemistry qualitative organic analysis, CB Publishers and distributors, Delhi
2. B.S.Furniss, A.J.Hnnaford, V.Rogers, P.W.G. Smith and A.R.Tatchell, Vogel's Text Book of Practical Organic chemistry, Longman, London(1978).

EC – I - (Elective Course) - PHYSICAL CHEMISTRY -I

Semester: I Hour/week: 6

Course Code: credits: 4

Objectives:

1. To impart students an understanding of group theory.
2. Students will be able to grasp chemical kinetics.
3. Students will be able to know the third law of thermodynamics.

UNIT – I

Group Theory:

Elements of group theory – Group axioms, similarity transformations, conjugate elements and classes, group and subgroup, group multiplication tables, isomorphism groups.

Symmetry elements, symmetry operations and point groups, point group of molecules and their systematic identification.

Representation theory of finite groups – Matrix representation of symmetry operations – characters – reducible representations – Great orthogonality theorem – construction of character tables (C_2v& C_3v) – symmetry adapted linear combinations – projection operators.

UNIT –II

Group theory Applications:

Symmetry aspects of molecular orbital theory – planar pi systems – symmetry factors of Huckel determinants - solving for energy and molecular orbitals for ethylene,1,3-butadiene and benzene. Prediction of allowed electronic spectral transtitions – ethylene, formaldehyde. Molecular vibrational symmetry – types of normal modes – prediction of activity of fundamentals in IR and Raman.

Sigma bonding in AX_n molecules – hybridizations – tetrahedral, octahedral, square planar, linear – hybrid orbitals as Linear Combination of Atomic Orbitals.

UNIT – III

Chemical Kinetics – I:

Theories of reaction rates (collision theory, absolute reaction rate theory ARRT) – Potential energy surface – Kinetic isotopic effect – opposing, parallel, chain and consecutive reactions.

Hinshelwood's theory – Kassel Rice and Ramsperger Theory (KRRT) – KRRM method – slater treatment – principle of microscopic reversibility – steady state approximation – photo chemical reactions between Hydrogen and bromine – gas phase auto-oxidation – hydrogen – oxygen reactions.

UNIT – IV

CHEMICAL KINETICS – II:

Applications of ARRT to solution Kinetics - effect of solvent and ionic strength, Influence of pressure on reaction rates in solution – significance of pressure on rates in

solution – significance of volume of activation – enzyme catalysis mechanism of single substrate reactions – MichaelisMenton law.

Introduction, relaxation methods, T and P – jump methods, shockwave technique, continuous and stopped flow methods, flash photolysis reaction.

UNIT – V

THERMODYNAMICS – I:

Need for the third law – Nernst heat theorem and other forms of stating the third Law. Thermodynamics quantities at absolute zero – statistical meaning of third law – exceptions to the third law.

Gibb's free energy – Gibb's Helmholtz equation – thermodynamics of systems of variable composition – partial molar properties – chemical potential – relationship between partial 2olar quantities – Gibbs Duhem equation and its application (the experimental determination of partial molar properties not included).

Thermodynamic properties of real gases – fugacity concept – calculation of fugacity of real gas – activity and activity coefficient – concept – definition – standard states and experimental determinations of activity and activity coefficient of electrolytes by freezing points methods.

Text books:

1. F.Albert cotton,Chemical Applications of Group Theory, 3rd Edition John Wiley & Sons, Singapore, 2003.
2. K.J. Laidler,Chemical Kinetics, 2nd ed., Tata McGraw Hill, 1975.

References:

1. R.L. Flowry, Jr,symmetry Groups – Prentice Hall, New Jersy, 1980.
2. K.V. Raman, Group theory and its Applications in Chemistry, TMH, 1990.
3. A.A.Frost and R.G.Pearson, "Kinetics and Mechanisms", John Wiley & Sons, New York, 1953.
4. I.Amdur and G.G. Hammes,"Chemical Kinetics Principles and selected Topics", McGraw Hill, NewYork, 1966.
5. P.K. Bhattacharya,Group Theory and its Chemical Applications, 2nd Edition. Himalaya Publishing House, 2003.
6. V.Ramakrishnan& M.S. Gopinathan,Group Theory in Chemistry, 2nd Edition. Vishal Publications, 1995.
7. S.Glasstone, Thermodynamics for Chemistry, Affiliated East West Press, 1969.

CC-V- INORGANIC CHEMISTRY - II

Semester: II Hour/week: 6

Course Code: credits: 5

Objectives:

- Students will get in depth knowledge on co-ordination chemistry under the following headings.
  1. Reaction mechanism of co-ordination compounds
  2. Photo chemistry of co-ordination compounds
  3. Applications of co-ordination compounds and organometallic chemistry.

UNIT –I

Coordination chemistry:

Theories of Metal –Ligand bond - VB theory and its limitations – Crystal Field Theory – splitting of d orbitals under various geometries. Factors affecting splitting – CFSE and evidences for CFSE (Structural and thermodynamic effects) – spectro-chemical series – Jahn -Teller distortion – spectral and magnetic properties of complexes – site preferences – spinal and inverse spinal – limitations of CFT – Ligand Field theory – MO theory – sigma and pi bonding in complexes – nephelauxetic effect – the angular overlap model.

Studies of coordination compounds in solution – detection of complex formation in solution – Job's method – stability constants – stepwise and overall formation constants – simple methods (Potentiometric and Photometric methods) of determining the formation constants – factors affecting the stability - statistical and chelate effects – forced configurations.

UNIT II

Reaction Mechanism of Coordination compounds:

Reactions of metal complexes – labile and inert complexes –types of coordination reactions - ligand substitution reactions- S_N1,S_N2, S_N1CB – Electron transfer reactions - Inner sphere and outer sphere processes,complementary and non-complementary reactions.

Reactions of coordinated ligands - Isomerisations reaction – acid hydrolysis, base hydrolysis and anation reactions – Transeffect –theory and applications –template effect

UNIT III

Photochemistry of coordination compounds:

Photochemical reactions of coordination and organometallic compounds – photo oxidation, photo reduction, photo substitution and photo isomerisation reactions.

18 - electron rule,EAN rule applied to metal carbonyls –preparation and properties of metal carbonyls – $Ni(CO)_4$, $Fe_2(CO)_9$, $Cr(CO)_6$ and$Re_2(CO)_{10}$ –carbonylate anions - cabonyl hydrides – nitrosyl complexes - preparation – bridging and terminal nitrosyls.

UNIT – IV

Applications of coordination compounds:

Metal complexes in medicinal chemistry – complexation in food poisoning – metal complexes in therapy - Metal complexes in industrial processes – heavy metals – protein complexes in the raschig process – metal complexes in alkene conversions – complexation and electroplating – complexation in metallurgy – complexes in water softening.

Magnetic properties of metal complexes –types of magnetic character, Determination of magnetic susceptibility - magnetic properties of complex ions- magnetic criterion of bond type in complexes – orbital contribution to magnetic moment – Quenching of orbital contribution – spin- orbit coupling and magnetic moments –magnetic character of poly nuclear complexes**.**

UNIT – V

Organometallic chemistry of transition elements:

Synthesis, structure and bonding of ferrocene, organometallic reagents in organic synthesis and in homogeneous catalytic reactions, hydrogenation, hydroformylation, isomerisation and polymerization – pi-acid metal complexes – activation of small molecules by coordination.

Text books:

1. R.H.Crabtree, The organometallic chemistry of transition metals.
2. A.W.Adamson and P.D.Fleischaur, " Concepts of Inorganic Photochemistry ", Wiley,New York,1975.
3. Purcell and Kotz, "Inorganic Chemistry",Saunders Golden Sunburst Series, W.B.Saunders Company ,Philadelphia
4. J.D.Lee,A New Concise Inorganic Chemistry,4th ed., ELBS,1995.

References :

1. S.F.A.Kettle, Physical inorganic chemistry, A coordination chemistry Approach,spectrum Academic Publishers,Oxford,1996.
2. J.E.Huheey ,Inorganic chemistry ", 3rd ed., Harper & Row publisher,Singapore.
3. F.A. Cotton and G. Wilkinson , " Advanced Inorganic Chemistry " , 4th ed., A Wiley – Interscience Publication ,John – Wiley & Sons, USA.
4. S.Glasstone, "Source Book on Atomic Enertgy ", D.VanNostrand , New York 1967(Affiliated East-West Press ,New Delhi 1969)

CC-VI- ORGANIC CHEMISTRY - II

Semester: II Hour/week: 6

Course Code: credits: 5

Objectives:

1. To impart basic ideas about elimination reactions, electrophilic aromatic substitution and molecular rearrangements.
2. To enable the students to elucidate the structure of organic compounds using UV & IR spectroscopy techniques.
3. To help students understand the reaction kinetics and method of determining reaction mechanisms.

UNIT – I

Elimination Reactions:

E_1, E_2 and E_1CB mechanisms –Influence of structure, leaving group, base and solvent. Orientation of the double bond – Hoffmann and Saytzeff rules – Competition between elimination and substitution reactions – Typical eliminations to be studied – dehydration of alcohols, dehydro halogenation and Hoffmann degradation. Mechanisms of pyrolytic eliminations – examples - Chugaev and Cope eliminations.

Aromatic Electrophillic Substitution:

Arenium ion mechanism – Isotopic effect - orientation and reactivity – nitration, halogenation, sulphonation, Friedel - Crafts reaction – Gattermann, Kolbe-Schmitt, Reimer- Tiemann, Houben-Hoeschreactions, Aromatic nucleophilic substitution – benzyne mechanism and Chichibabinreaction.

UNIT – II

Reduction:

Catalytic Hydrogenation and dehydrogenation. Clemmensen, Wolff-Kishner, MPV and Birch reductions. Reduction with $LiAlH_4$, $NaBH_4$, tritertiarybutoxyaluminium hydride, sodium cyanoborohydride, trialkyltin hydride, Wilkinson's catalyst.

Oxidation:

Selectivity and synthetic uses of the following oxidants - chromyl chloride, periodic acid, selenium dioxide, lead tetraacetate, osmium tetroxide, Ruthenium complex, PCC (pyridiniumchloro chromate), DDQ, phase transfer catalysts(PTC),crown ethers, Baker's yeast, Swern, and Oppenauer Oxidation .

UNIT – III

Stereochemistry – II:

Configuration of cyclic and bicyclic ring systems:

Cis and Trans isomerism of three, four and five membered substituted cyclic systems- E and Z nomenclature – determination of configuration of the geometrical isomers.

Conformation analysis:conformation of methane, ethane and propane derivatives.Conformational equilibrium of cyclohexane and mono substituted

cyclohexanes. Conformation, optical activity and stability considerations of disubstitutedcyclohexanes.

Dynamic Stereochemistry: Quantitative correlation betweenconformation and reactivity - Winstein-Eliel equation - Curtin Hammet principle -saponification of an ester - esterification of an alcohol - chromic acid oxidation ofcyclohexanols - neighbouring group participation - deamination of 2-amino cyclohexanol - Stereoselective and stereospecific reactions.

UNIT –IV

Ultraviolet and visible Spectroscopy:

Basic principles of electronic transitions – correlation of energy change with electronic transitions – Instrumentation and sample handling techniques – Applications of UV – visible spectroscopy – Woodward Fisher Scott rules – applications to conjugated dienes, trienes and polyenes – unsaturated carbonyl compounds – conjugated cyclic ketones – acetophenones – benzene and its substituted derivatives – other aromatic hydrocarbons – heterocyclic systems – differentiation of position isomers – stereochemical factors affecting electronic spectra of biphenyl and binaphthyls – cis - trans isomers – angular distortion – cross conjugation.

Infrared Spectroscopy:

Instrumentation and sampling techniques – types of stretching and bending vibrations – characteristic group frequencies – both internal and external – quantitative studies – organic structure determination, finger print region – identification of functional groups – hydrogen bonding, intermolecular and intra molecular – conformational aspects in cyclic 1,2 diols and 1,3 diols – transannular interactions in UV and IR – determination of reaction rates and mechanisms of reactions involving IR and UV spectroscopy – (basic aspects).

UNIT –V

Carbohydrates:

Polysaccharides – structure of starch and cellulose (elucidation not required). Configurations of carbohydrates – photosynthesis.

Peptides and Proteins:

Synthesis of peptides – Primary, Secondary, tertiary and quaternary structure of proteins. Protection of N and C – terminal groups of proteins, biosynthesis of proteins.

Nucleic Acids:

Chemistry of nucleic acids – structure of DNA, properties, biological implications of DNA, Replication of DNA, structure of RNA - types of RNA and their functions.

Text Books:

1. R.T. Morrison and R.N.Boyd, “Organic Chemistry”, 6 th ed., PHI private limited,1990.
2. E.L.Eliel, “ Stereochemistry of Carbon Compounds” , McGraw Hill, 1962.

3. D. Nasipuri , Stereochemistry of Organic Compounds , 2nd edition, New Age International,1994.
4. P.S. Kalsi , Organic Reactions and their mechanisms, 4th edition, New age international Publisher , 2006.
5. R.K. Bansal, "Organic Reaction Mechanisms", Tata McGraw Hill,1975.
6. Y.R.Sharma, Elementary Organic Spectroscopy- Principles and Chemical Applications, S.Chand, 1992.
7. J.March, Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 4th edition, Wiley, 1992.
8. P.S. Kalsi, Spectroscopy of Organic Compounds, New Age International Publishers.

References:

1. R.M. Silverstein, F. X. Wester, " Spectroscopic Identification of Organic Compounds", 6 th ed., Wiley, 1998.
3. J.R.Dyer, "Applications of Absorption Spectroscopy of Organic Compounds", Prentice Hall, 1965.
4. W.Kemp, Organic Spectroscopy, ELBS, 1991.
5. I.L.Finar, Organic Chemistry Vol II, 5th Edn., ELBS, 1975.

CC-VII - INORGANIC CHEMISTRY PRACTICAL- II

Semester: II Hour/week: 6

Course Code: credits: 4

Objectives:

1. To make students estimate the metal ions present in the mixture using titrimetric and gravimetric methods.
2. To expose students to various preparation steps in synthesizing inorganic complexes.

A. Titrimetry and Gravimetry

Only mixture(s) of solutions should be given for estimation

(i) Cu(V) and Ni(G)
(ii) Cu(V) and Zn(G)
(iii) Fe(V) and Zn(G)
(iv) Fe(V) and Ni(G)

B. Preparation of the following complexes

1. Tetramminecopper(II) sulphate.
2. Potassium trioxalato chromate(III)
3. Hexammine cobalt(III) chloride
4. Potassium trioxalatoferrate(III)
5. Tristhiourea copper (I)chloride
6. TristhioureaPrussian blue

Text Books:

1. V.Venkateswaran, R.Veerasamy and A.R.Kulandaivelu, Basic Principles of Practical Chemistry, Sultan Chand & Sons, Second Edition, 1997.
2. K.K.Sharma and O.S.Sharma, An introduction to Practical Chemistry, Vani Educational Books, Second Edition, 1982.

References:

1. ATHUR I. VOGEL, A Text Book of Macro and Semi-micro Qualitative Inorganic Analysis, Longman Group Ltd., First Indian Edition, 1975.
2. V.V.Ramanujam, Inorganic Semicmicro Qualitative Analysis, The National Publishing Co., Madras, Second Edition, 1970.
3. J.Bassett, R.C.Denney, G.H.Jeffery and J.Mendhan, Vogel's Text Book of Inorganic Quatitative Analysis, ELBS-Longman, London, 4th Edition, 1978.

OEC – I*(OPEN ELECTIVE COURSE) GREEN AND INDUSTRIAL CHEMISTRY

Semester: II Hour/week: 6

Course Code: credits: 4

Objectives :

1. To give them understanding of selection of alternate methods for the synthesis of compounds and treatment of wastes.
2. To learn some of the industrial products and their manufacturing processers.
3. To become aware of the application of the industrial products.

UNIT – I

Environment and Eco system – origin – big-bang Nucleo synthesis – evolution of life on the earth – cosmic evolution – elements of life and biodistribution of elements – environment and its components.

Ecosystem – Ecology – ecological factors – classifications and components of ecosystems - productivity and energy flow in an ecosystem – food chain and food web- pollution of environment – concept and scope.

UNIT – II

Green Chemistry- Introduction – twelve principles – green chemistry in action – replacement of wood preservative – production of bio diesel, biopolymers and bioplastics.

Waste management – sources and types of waste –waste treatment – integrated waste management of plastics.

UNIT – III

Water in industry – pollution of water by fertilizers, detergents, pesticides and industries – BOD, COD – water treatment – ion exchange, reverse osmosis and softening of hard water.

Chemical explosives – origin of explosive, preparation and chemistry of lead azide,, nitroglycerine, nitro cellulose, TNT, dynamite, cordite, picric acid and gunpowder.

UNIT – IV

Rubber industries – natural rubber – synthetic rubber – polymerization – butadiene – styrene – neoprene – urethane rubber.

Plastics – manufacture – types – condensation polymerization – polyamides – nylon-66, polyester – terelene.

UNIT – V

Coal – varities of coal – composition – coal gasification – carbonization – coal – tar and coal - tar based chemicals– coal mines in India.

Petroleum – refining – cracking – knocking – octane number – LPG – synthetic petrol by Bergius process

Fuel gases – manufacture and uses of coal gas, water gas, producer gas and oil gas.

Text books :

1. RashmiSanghi , M.M. Srivaslava , Green chemistry environment friendly alternatives, S.Chand&Company Ltd, New Delhi, 1998.

2. J.L. Jain, Sunjay Jain, Nitin Jain, Fundamentals of Biochemistry, 6th Ed., S.Chand& Company Ltd, New Delhi, 2005.

3. B.N.Chakrabarathy, Industrial chemistry , Oxford and IBH publishing Co., New Delhi , 1981.

References :

1. Asim k. Das , Environmental chemistry with green chemistry,1st Ed., Books and allied (P) ltd., 2010.

2. V.K. Ahluwalia ,Rajender. S.Varma, Green solvents for Organic synthesis , 3rd Ed., S.Chand&Company Ltd, New Delhi, 2003.
3. B.K.Sharma , Industrial Chemistry, Goel publishing House, Meerut, 1996.

OEC-I*(OPEN ELECTIVE COURSE) FOOD CHEMISTRY

Semester: II Hour/week: 6

Course Code: credits: 4

Objectives :

1. To understand the nutrition present in our day to day food.
2. To learn the kinds of adulteration in the food products.
3. To enhances the awareness of biological activities in our body.

UNIT – I

Meaning of food – classification of food – functions of food and metabolism – digestion. Food preservation – refrigeration and freezing, canning, dehydration, freeze – drying - chemical preservation.

UNIT – II

Carbohydrates – classification – properties of glucose and fructose – functions of carbohydrates in body – digestion, adsorption, metabolism.

Proteins – classification – structure of proteins – functions of proteins in the body – physiological and metabolic roles – digestion, adsorption, metabolism.

UNIT – III

Vitamins – classification – water soluble and faqt soluble virtamins – vitamin A, D, E, K – physical and chemical characteristics, structure, biological functions and deficiency disorders.

Water soluble vitamins – vitamin C (ascorbic acid) – vitamin B complex – B_1, B_9 and B_{12}.

UNIT – IV

Water – nutrient – important of life – water balance – water sources – special needs – fluid replacement.

Minerals - types – metabolism of P, Ca, Fe, I – its functions, deficiency and sources. Estimation of Fe, P and water content.

UNIT – V

Introduction – common food adulterants – analysis of food adulterants in edible oils, ghee, coffee powder, chilly powder, turmeric powder, milk. Effects of adulterants.

Food additives – sweeteners, preservatives, flavors, colorants, toxicants and pesticide contaminants.

Text books :

1. Alex V Ramani, Food Chemistry ,MJP publishers, 2009.
2. KirpalSingh , " Chemistry in daily life" , 3rd edition, PHI learning private limited, New Delhi, 2012.
3. Harish Kumar Chopra," Food Chemistry" Parmjit Singh Panesar, Narosa Publishing House Pvt. Ltd, 2010

References :

1. Yadav Seema, "Food chemistry" ,anmol publications, 2002.
2. Atherton, " Chemistry and testing of dairy products", 4th Edition, CBS publishing, 2003.
3. Ion C. Baianu" physical chemistry of food processes: fundamental Aspects", CBS publishing, 1997.

EC-II – (ELECTIVE COURSE) PHYSICAL CHEMISTRY - II

Semester: II Hour/week: 6

Course Code: credits: 4

Objectives:

1. To impart in depth knowledge of group theory, quantum chemistry, thermodynamics, chemical kinetics and its applications.
2. To impart theoretical knowledge on physical aspects of Raman, NMR, ESR spectroscopy to students.
3. Introduce the need for 3rd law of thermodynamics & Gibb's free energy.

UNIT – I

Quantum Chemistry – I

Inadequacy of classical mechanics, black body radiation, Planck's quantum concept, photoelectric effect. Bohr's theory of hydrogen atom-Hydrogen spectra, wave particle dualism, uncertainty principle, Inadequacy of old quantum theory.

Schrodinger equation, postulatory basis of quantum mechanics. Operator algebra: operator, linear and Hermitian, Eigen functions and Eigen values, angular momentum operator, commutation relations, related theorems.

Applications of wave mechanics to simple systems – particle in a box, one and three dimensional, distortion of the box and Jahn-Teller effect, quantum numbers, zero point energy. Orthogonalisation and normality, finite potential barrier – tunneling.

UNIT – II

Quantum chemistry –II:

Applications of wave mechanics, the rigid rotator, harmonic oscillator – Hydrogen atom solution – shapes and nodal properties of orbitals – space quantization – electron spin – many electron atoms – one electron orbitals – Pauli principle – determinantal form of wave function , helium atom and effective nuclear charge.

Approximation methods – variation methods, application to Hydrogen and Helium atoms – perturbation method for nondegenerate systems.

Angular momentum in many electron systems – spin orbit interaction, L-S and J-J coupling schemes. Atomic structure calculation –Hartee and HarteefockSelf consistent Field method for atoms.

UNIT – III

Molecular Spectroscopy – I:

Introductory aspects – Interaction with molecules Einstein's transition probabilities – basics of electron rules – representation of spectra, the width and intensity of spectral transitions.

Microwave spectroscopy – rotational spectra of diatomic molecules, rigid and non-rigid rotors- intensity of spectral lines – effect of isotopic substitution – microwave spectra of polyatomic molecules – linear and symmetric top molecules.

Electronic spectra: Electronic spectra of molecules – Born- Oppenheimer approximation – vibrational coarse structure – Franck-Condon Principle, dissociation energy, predissociation – rotational fine structure of electronic vibrational transitions – Fortrat diagram. Various types of transitions.

2.4 Infrared spectroscopy: Vibrational spectra – selection rules – harmonic and Anharmonic oscillators – vibration and rotation – vibrational spectra of diatomic molecules – vibrational spectra of polyatomic molecules (CO_2, H_2O) – Fermi resonance – influence of rotation on the spectra of polyatomic molecules – parallel and perpendicular bands.

UNIT – IV

SPECTORSCOPY – II:

RAMAN SPECROSCOPY:

Raman effect – elastic and inelastic scattering – selection rules – rotational and vibrational Raman spectra – polarization of light and Raman effect - comparison of IR and Raman spectra – structure determination from Raman spectra(H_2O& CO_2) – exclusion principle - Fermi resonance – Laser Raman spectroscopy.

NMR SPECROSCOPY:

Spin and applied magnetic field – Larmor precession – Relaxation process – PMR chemical shift – spin interaction – FT - NMR – Multiple pulses NMR - C^{13} NMR spectroscopy – chemical exchange.

ESR SPECTROSCOPY:

Basic principles – presentation of spectrum – Hyperfine splitting, Factors affecting Hyperfine splitting.

UNIT – V

Photo Chemistry:

Photo physical process in electronically excited molecules – luminescence and energy transfer process – Jablonski diagram – Stern -Volmer equation– experimental techniques in photochemistry – chemical actinometers – lasers and their applications.

Radiation chemistry:

Differences between radiation chemistry and photochemistry – source of high energy radiation and interaction with matter – radiolysis of water , solvated electron. Definitions of G value, Curie, Linear energy transfer (LET)and Rad – scavenging techniques – use of dosimetry and dosimeters in radiation chemistry – applications of radiation chemistry.

Text Books:

1. A.K.Chandra,Intoductory Quantum Chemistry, 4th ed., Tata McGraw Hill,1994.
2. C.N.Banwell,Fundamentals of molecular Spectroscopy, 3rd ed., TMH,New Delhi, 1983.
3. J.Rajaram and J.C.Kuriacose,Thermodynamics for students of Chemistry : Classical, Statistical and Irreversible, shobanLalNagin, New Delhi, 1981.
4. L.K.Nash,Elements of Chemical Thermodynamics, Addision Wesley, 1962.
5. S.Glasstone,Thermodynamics for chemists, Affiliated East West Press, New Delhi, 1960.

References:

1. R.S.Drago,Physical Methods in Chemistry, W.B.Saunders Company, Philadelphia, London, 1976.
2. B.P. Straughan and S.Walker“Spectroscopy Vol.3, Chapman Hall London,1976.
3. G.M.Barrow,Introduction to Molecular Spectroscopu, McGraw Hill, New York,1964.
4. R.Chang,Basic Principles of Spectroscopy , McGraw Hill Pub., Ltd., 1971.
5. B.P.Strangham and S.Walker,Spectroscopy Vol 1, Chapman Hall, London,1976.
6. A.A.Frost and R.G.Person,kinetics and Mechanisms, John wiley& Sons, New York,1953.
7. I.Amdur and G.G.Hammes,Chemical Kinetics Principles and Selected Topics, McGraw Hill, New York, 1966.
8. R.K.Prasad,Quantum Chemistry, New Age International Ltd, 2006.
9. D.A.Mcquarrie,Quantum Chemistry, University Science Books,1998.
10. F.L.Pillar, Elementary Quantum Chemistry, McGraw Hill,1968.
11. J.P.Lowe,Quantum Chemistry, Academic Press, 1978.
12. I.N.Levine,Quantum Chemistry, Allyn and Bacon, 1983.
13. P.W.Atkins,Molecular Quantum Mechanics, Clarendon Press New York, 1973.
14. S.Glasstone,Thermodynamics for Chemist, Afiliated East West Press, 1969.

CC-VIII- INORGANIC CHEMISTRY - III

Semester: III Hour/week: 6

Course Code: credits: 5

bjectives:

1. Students get knowledge on EPR, electronic spectroscopy and magnetic properties of complexes.
2. Various analytical techniques and their applications in Quantitative estimation will enable student to get practical idea about the use of such equipments.
3. Special unit on bio chemistry give insight about metals in biology and also about medicinal bio inorganic chemistry.

UNIT –I

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.. R-S coupling and J-J coupling.

Selection rules and the breakdown of selection rules –splitting of orbitals in octahedral field. Ground states of free ions for d^n systems in Oh and Td systems and the corresponding energy level diagrams – mixing of orbitals.

Orgel diagram – characteristics – prediction and assignment of transitions for d^1, d^2, d^3 weak field cases.Tanbe – Sugano diagram - Racah parameters B and C (calculation not required).

UNIT –II

EPR spectroscopy:

Basic principles– characteristics of 'g' – Hyperfine splitting – selection rules – Hyperfine splitting in various structures – Bis(salicylaldiamine)copper(II) –factors affecting the magnitude of the 'g' values. 'g' values of transition metal ions – dependence on spin –orbit coupling and crystal field effects.

EPR of d^1 to d^9 systems of first transition series. Zero – field splitting – Effective spins mixing of states and zero field splitting. Line widths in solid state EPR – spin - lattice relaxation – spin-spin relaxation – exchange processes. Effect of distortion. Calculation of g(parallel),g(perpendicular),g(average) and information obtained from them.

UNIT –III

Supramolecular Reactivity and Catalysis

Catalysis by Reactive MacrocyclicCation Receptor Molecules. Catalysis by Reactive Anion Receptor Molecules. Catalysis with Cyclophane Type Receptors.SupramolecularMetallocatalysis. Cocatalysis: Catalysis of Synthetic reactions. Biomolecular and Abiotic catalysis

Supramolecular Chemistry in solution: Cyclodextrin, Micelles, Dendrimmers, Gelators. Classification and typical reactions- Applications.

UNIT –IV
Topics in analytical chemistry:

Application of atomic and molecular absorption and emission spectroscopy in quantitative analysis light scattering techniques including nephelometry and Raman spectroscopy.

Electron analytical techniques ,voltametry, cyclic voltametry,polarography, amperometry, coulometry, conductometry, ion-elective electrodes, anodic stripping voltammetry,TGA, DTA,DSC and online analyzers - SEM and TEM.

UNIT –V
Bio inorganic chemistry:

5.1**Heme and Non-hemeProteins:**Hemoglobin and Myoglobin – Oxygen transport and storage – Electron transfer and Oxygen activation.Cytochromes, Ferredoxins and Rubredoxins – Model systems, mononuclear non-heme iron enzymes.

Copper ContainingProteins: Classification and examples - Electron transfer – Oxygen transport - Oxygenation – oxidases and reductases – Cytochrome c oxidase – Superoxide dismutase (Cu, Zn).

Text Books:

1. E.A.V.Ebsworth,Structural Method's in inorganic chemistry , 3rd ed., ELBS,Great Britain,1987.
2. G.Friedlander, J.W. Kennady and J.Miller, "Nuclear and Radiochemistry,3rd ed., Wiley interscience Publications, John Wiley & sons New York.
3. S.J.Lippard and J.M.Berg,principles of bioinorganic chemistry ,Panima Publishing company,New Delhi,1997.
4. S.M.Khopkar, Basic concepts of analytical chemistry,New Age International (P) Ltd,New Delhi,1998.

References:

1. R.S.Drago, Physical Methods in inorganic chemistry ; 3rd ed., Wiley Eastern Company (units I,II,III &IV)
2. R.S.Drago, "physical methods in chemistry",W.B.Saunders Company, Philadelphia,London.
3. F.A. Cotton and G. Wilkinson, "Advanced Inorganic Chemistry "3rd ed., Wiley – Eastern company, New Delhi, 1990.
4. D.A.Skoog and D.M.West, Fundamentals of analytical chemistry,W.B.Saunders,New York,1982.
5. Lehn, J.M. Transition metals in supramolecularchemistry : John Wiley & sons: New York, 1999.

CC-IX - ORGANIC CHEMISTRY -

Semester: III | Hour/week: 6

Course

Objectives:

1. This paper gives exposure to retrosynthetic analysis, reagents involved in organic synthesis and how to protect functional groups.
2. They also highlight NMR spectroscopy (C^{13}, Proton NMR) techniques and their use in interpreting and arriving at the structure of organic compounds.
3. A unit on terpenes and alkaloids will help students to learn natural products.

UNIT – I

Addition and condensation reactions:

Addition to carbon –carbon multiple bonds:

Electrophilic, nucleophilic and free radical additions – orientation and reactivity. Stereochemical factors influencing the addition of bromine and hydrogen bromide, hydroxylation, 1,2- dihydroxylation (Woodward and Prevost hydroxylations) and hydroboration leading to formation of alcohols, oxidation and ozonolysis. Addition to conjugateddienes – Diels - Alder reaction.

Addition to carbon – hetero multiple bonds:

Addition mechanism and reactivity - Selected name reactions involving addition to carbonyl group – Aldol, Reformatsky, Perkin, Stobbe, Darzen'sglycidic ester, Knoevenagel , Dieckmann and Benzoin condensations. Michael reactions and Robinson ring annulations – Mannich reaction- wittig reaction and its stereo selectivity.

UNIT – II

Reagent and Protecting groups in Organic synthesis:

Lithium diisopropylamide (LDA),Dicyclohexylcarbodimide ,(DCC), Tri-n-butyl tinhydride,Peterson's olefination,Merrifield resin, Gilman's reagent, 1,3-dithiane (reactivityumpolung) and trimethylsilyl iodide

Protection of alcohol, amine, aldehydes , ketone and carboxylic acid.
Deprotection, Resistivity of protecting group.

UNIT – III

Reterosynthetic analysis:

Definition of reterosynthetic analysis. Simple definition of terms – synthon, refron, synthetic equivalence, transform , synthetic tree , umpolung. Different synthetic approaches (i) relay approach (ii) Convergent approach and (iii) Disconnection approach.

Disconnection approach:

Reterosynthetic analysis of monofunctional and 1,2 ; 1,3 ; 1,4 and 1,5 - difunctional compounds.Protection anddeprotection during synthesis – functional group strategy – retero – Diels – Alder Strategy. C-C disconnection – functional group addition, removal and modification.

Objectives:

- To provide a basic training in laboratory skills for physical chemistry.
- To relate the experimental work to the scientific theory behind the experiment and thus give a fuller understanding of the theory. After studying this unit the student should be able to
    - ❖ Use scientific apparatus with care and confidence
    - ❖ Make essential observations accurately and estimate the possible errors.
    - ❖ Produce a scientific report of their work.
    - ❖ Gain a critical appreciation of the purpose, significance and limitations of any experimental study.

1. Comparison of strength of acids by the study of kinetics of hydrolysis of an ester.
2. Determination of the velocity constant, catalytic coefficient, temperature coefficient, energy of activation and Arrhenius parameters for the acid hydrolysis of an ester.
3. Determination of Molecular weight of substances by Rast's method.
4. Determination of Molecular weight of substances by transition temperature method.
5. Study of phase diagram of two components forming simple eutectic.
6. Study of phase diagram of two components forming compound.
7. Conductometric titration of mixture of weak and strong acids.
8. Conductometric precipitation titration of $BaCl_2$ with $MgSO_4$ and K_2SO_4.
9. Conductometric determination of dissociation constant of weak acid.
10. Potentiometric titration of mixture of weak and strong acids.
11. Potentiometric titration – precipitation titration.
12. Potentiometric determination of dissociation constant of weak acid.
13. Determination of Onsagar parameters for a strong electrolyte by conductometry

Text Books:

1. Findlay's Practical Physical Chemistry, Revised and edited by B.P.Levitt 9th ed., Longman, London, 1985.
2. J.N. Gurtu and R. Kapoor, "Advanced Experimental Chemistry", Vol.1, S Chand & Co., Ltd., New Delhi.

References:

1. Findlay's Practical Physical Chemistry, Revised and edited by B.P.Levitt 9th ed., Longman, London, 1985.
2. J.N. Gurtu and R. Kapoor, "Advanced Experimental Chemistry", Vol.1, S Chand & Co., Ltd., New Delhi.
3. S.R. Palit and D.E. Sadhan Kumar, "Practical Physical Chemistry", 1st Ed., Science Book Agency, 1971.

EC – (ELECTIVE COURSE) III - PHYSICAL CHEMISTRY - III

Semester: III Hour/week: 6

Course Code: credits: 4

Objectives:

1. To introduce the basic principles and some applications of electro chemistry after studying the unit, students should be able to
   - Understand the electro chemical cell
   - To know about the electro analytical methods.
2. To provide an introduction to the physical chemistry of interfaces and to demonstrate its significance in catalysis, after studying this units, students should be able to explain the qualitative and quantitative basics of catalysis and physical adsorption.

UNIT – I

ELECTRO CHEMISTRY – I:

Cell terminology – electrode potential - Nernst equation – Types of electrode – electro chemical cells – chemical cells with and without transference – electrode, electrolyte concentration cells without transference – concentration cells with transference – liquid junction potentials.

Processes at the electrodes – the rate of electrode process & EMF – Butler-Volmer equation – Tafel equation – Theories of Electrical double layer - Helmholts, GouyChapmann and Stern's theory – Double layer capacity - Measurement of Zeta potential (electrophoresis and electro osmosis) – Fuel cells – Hydrogen-oxygen fuel cell – Commercial cells – Leclanche cell and Lead storage cell.

UNIT – II

ELECTRO CHEMISTRY – II:

Electro Analytical Methods :

Principles and applications of polarography – advantages and disadvantages of polarography – Advantages of dropping mercury electrode, interpretation of current-voltage curves, determination of 'n' values (usefulness of Illkovic equation), polarographic maxima-minima and current-time curves.

Modern developments – Working of polarographic cells - Types of polarography – oscillographic polarography, advantages over polarographic techniques – Chronopotentiometric titration – advantages and disadvantages – Colorimetric titration.

UNIT-III

ELECTRO CHEMISTRY-III

Debye Huckel theory-Radius of ionic atmosphere-Calculations of thickness of ionic atmosphere-Evidence of ionic atmosphere-Asymmetry effect-Electrophoretic effects-Falkenhagen effect-Wien effect-Debye-Huckel Onsager equation-Modification and verification of the equation-Debye Huckel limiting law.

Activity, activity coefficients-activity coefficient with concentration-Derivation of Debye Huckel limiting law- Modification and verification-Finite ion size model-Huckel-Bronsted equation-calculation of activity coefficient.

Determination of ion size parameter-Solubility product solubility of sparingly soluble salt-Common ion effect- Neutral salt effect and solubility-Determination of solubility and solubility product.

UNIT – IV

Surface Chemistry:

Surface phenomena – adsorption and free energy relation at interfaces – derivation of Gibb's adsorption isotherm – solid-liquid interfaces – contact angle and wetting – solid-gas interface – physisorption and chemisorption.

Derivation and applications of Langmuir and BET isotherms – soluble and insoluble film – surface area determination.

UNIT – V

Heterogeneous Catalysis:

Role of surfaces in catalysis – semiconductor catalysis – n- and p-type surfaces – kinetics of surface reactions involving adsorbed species – Langmuir – Hinshelwood mechanism – Langmuir – Rideal mechanism – Rideal – Eley mechanism – photo catalysis.

Mechanisms of a few specific catalysed reactions – Fischer – Tropsch type reaction and hydrogenation of ethylene.

Text Books:

1. Classical,Statistical and Irreversible, ShobanLalNagin, New Delhi,1981.
2. L.K.Nash, Elements of Chemical Thermodynamics, AdditionWesley,1962.
3. S.Glasstone, Thermodynamics for Chemists, Affiliated East West Press, New Delhi, 1960.
4. F.W.Billmayer, Jr., A text Book of Polymer Science, John Wiley and Sons, New York, 1971.
5. S.Glasstone, Introduction of Electrochemistry, Affiliated East West Press, 1968.
6. G.C.Bond, Heterogeneous Catalysis – Principles and applications, Clarendon, 1974.

References:

1. S.Glasstone, Introduction to Electrochemistry, Affiliated East West Press, 1968.
2. J.Albery, Electrode Kinetics, Clarendon Press, Oxford Chemical Series, 1979.
3. J.O.Bockris and A.K.N.Reddy, Modern Electrochemistry,Vol I & II, Plenum, 1970.
4. L.I.Anthrapov, Theoretical Electrochemistry, Mir Publishers, Moscow, 1972.
5. A.W.Adamson, Physical Chemistry of Surface, 4th ed., John Wiley and Sons, New York, 1982.

CC- XII - INORGANIC CHEMISTRY -IV

Semester: IV Hour/week: 6

Course Code: credits: 5

Objectives :

1. IR, Raman, NMR, X-ray studies to give overall structural determination of complexes possible for students.
2. Special focus on advanced materials, method of preparation, structure and applications are provided to keep abreast of current development in material chemistry.

UNIT –I

IR and Raman spectroscopy:

Combined uses of IR and Raman spectroscopy in the structural elucidation of simple molecules like H_2O, CF_3, NO_3^- and ClO_3^-. Effect of co-ordination on ligand vibrations – uses of group vibrations in the structural elucidation of metal complexes of urea, thiourea, cyanide, thiocyanate, nitrate, sulphate and dimethyl sulphoxide. Effect of isotopic substitution on the vibrational spectra of molecules – vibrational spectra of metal carbonyls with reference to the nature of bonding, geometry and number of C-O stretching vibrations (group theoretical treatment).

Moss Bauer Spectroscopy:

Moss Bauer transition and Doppler effect – isomer shift – quadrapole effect of magnetic field on spectra – simple applications to iron and tin compounds.

UNIT –II

NMR and NQR spectroscopy:

Chemical shift and coupling constants (spin-spin coupling involving different nuclei ^{1}H, ^{31}P, ^{13}C) interpretation and applications to inorganic compounds. NMR of paramagnetic molecules – isotopic shifts, contact and pseudo contact shift and their interactions – lanthanide shift reagents.

NQR – principle, effect of magnetic field on the spectra, Relationship between the electric field gradient and molecular structure, Halogen Quadrupole Resonance – applications.

UNIT –III

Crystal symmetry – combination of symmetry elements – crystal classes – screw axis and glide planes – space group – crystal axes – crystal systems, unit cell, Bravis lattices, asymmetric unit – space group,point group – equivalent positions – relationship between molecular symmetry and crystallographic symmetry - basic concepts and examples.

X-ray diffraction by single crystals – structure factor – determination of space group by systematic absences – phase problem in structure analysis – heavy atom method – Fourier synthesis – refinement of structure. Neutron diffraction – an elementary treatment -

applications and comparison with X-ray diffraction, Electron diffraction – basic principles and applications to simple molecules – Ferrocene.

UNIT –IV

Nuclear chemistry:

Radioactive decay and equilibrium – nuclear reactions - Q-value – significance of nuclear reaction - cross sections – types of reactions – chemical effects of nuclear transformations – fission and fusion – fission products and fission yields.

Radioactive techniques – tracer techniques – neutron activation analysis – isotopic dilution analysis –hot atom chemistry –counting techniques such as GM, ionization and proportional counters.

UNIT –V

Inorganic Materials:

Nanomaterials

Introduction – Methods of preparation – CVD,electrodeposition,Sol- gel techniques. Nanotubes – synthesis and purification – electronic structure – properties – applications. Self Assembled Monolayers –monolayers on gold – preparation – structure – applications. Nanosensors – nanobiosensors.

Dielectric Materials

Semiconductors – super conductors – type –I and type-II - superconductors – temperature and frequency effects – electric breakdown – ferroelectric materials.

Text books:

1. T.Pradeep , "Nano- The essentials " Tata – McGraw Hill,2007.
2. F.A. Cotton and G. Wilkinson, "Advanced Inorganic Chemistry "3rd ed., Wiley – Eastern company, New Delhi, 1990.

References:

1. R.S.Drago, "Physical Methods in inorganic chemistry", 3rd ed., Wiley Eastern Company (units I,II,III &IV)
2. E.A.V.Ebsworth, "Structural Method's in inorganic chemistry",3rded., ELBS,Great Britain,1987.
3. G.Friedlander, J.W. Kennedy and J.Miller, " Nuclear and Radiochemistry,3rd ed., Wiley interscience Publications, John Wiley & sons New York.
4. K.Ragavan,Materials Science and Engineering .

CC-XIII- ORGANIC CHEMISTRY -IV

Semester: IV Hour/week: 6

Course Code: credits: 5

Objectives:

1. Organic photochemistry, pericyclic reactions to give indepth knowledge to students on these topics
2. Mass spectroscopy, ORD, CD curves helps the students to understand organic compounds and its structures.
3. Synthesis, structure, classification of antibiotics, steroids will play a greater role in current trends of bio technology.

UNIT – I

Organic Photochemistry:

Fundamental concepts – Jablonski diagram – energy transfer characteristics of photo sensitization – characteristics of photo reactions of ketones - Norrish type I and II – reactions – photochemistry of alkenes, dienes and aromatic compounds – reactions of unactivatedcentres – photo additions – Patterno-Buchi reaction. Photo substitution Barton reaction – Hoffmann – Loffler - Freytag reaction. Photo rearrangement - Photo – Fries and di - π methane rearrangements.

UNIT – II

Pericyclic reactions:

Concerted reactions – stereochemistry – orbital symmetry and correlation diagram - Frontier molecular orbital approach – Woodward – Hoffmann rules – electrocyclic reactions – cycloaddition reactions – selection rules –and stereochemistry of electro cyclic, cycloaddition and sigmatropic shifts – 1,3 & 1,5 hydrogen shifts –Sommelet, Hauser, Cope and Claisen rearrangements – ene reactions.

UNIT - III

Heterocycles:

Synthesis and reactivity and applications of the following heterocycles- Furan , thiophenePyrrole, Pyridine, Indole, quinolines and isoquinolines.

Reduction:

Catalytic Hydrogenation and dehydrogenation. Clemmensen, Wolff-Kishner, MPV and Birch reductions. Reduction with $LiAlH_4$, $NaBH_4$, tritertiarybutoxyaluminium hydride, sodium cyanoborohydride, trialkyltin hydride, Wilkinson's catalyst.

UNIT – IV

Mass spectroscopy:

Basic principles – resolutions – EI and CI methods – base peak – isotopic peaks – metastable peaks – parent peaks – determination of molecular formula – recognition of

molecular ion peak – fragmentation – general rules – nitrogen rule – pattern of fragmentation of various classes of compounds – McLafferty rearrangement – importance of metastable peaks.

Optical Rotatory Dispersion (ORD) and circular dichroism (CD):

Introduction to theory and terminology – cotton effect – ORD curves – axial haloketone rule and its applications – octant rule – its applications – applications of ORD to determine absolute configuration of monocyclic ketones – comparison between ORD and CD – their inter relationships.

UNIT – V

Natural Products– III

Antibiotics:

Structure and synthesis of penicillin, Streptomycin – cephalosporin-C and chloramphenicol.

Steroids:

Classification – conformational representation - alpha and beta representation of substituents – structural elucidation of cholesterol and ergosterol(synthesis not required) – synthesis and properties of vitamin D – esterone, progesterone.

Text Books :

1. S.M.Mukherji and S.P.Singh, Reaction Mechanism in Organic Chemistry, 3rd edition, Macmillan, 1984.
2. R.T.Morrisonand R.N.Boyd, Organic Chemistry, 6th edition, Prentice- Hall of India, 2005.
3. R.K.Bansal, Organic Reaction Mechanisms, 3rd edition, Tata McGraw Hill, 2005
4. P.S.Kalsi, Organic Reactions and their mechanisms, 4th edition, New Age International, 2006.
5. Y.R.Sharma, Elementary Organic Spectroscopy - principles and chemical applications, S.chand,1992.
6. P.S.Kalsi, Spectroscopy of Organic comopounds, New Age International, 2003.
7. O.P.Agarwal, Organic Chemistry of Natural Products,Volume I and II, 29th edition, Goel Publishing House, 2005.

References:

1. C.H.Depuy and O.S.Chapman, Molecular Reactions and Photochemistry, Prentice Hall, 1975.
2. I.L.Finar, Organic Chemistry, Vol II, 6thed, Pearson Education, 2005.
3. F.A.Carey and R.J.Sunberg, Advanced Organic Chemistry, Part-A & Part-B, Pienum Press, 1990.

CC-XII- PHYSICAL CHEMISTRY PRACTICAL - II

Semester: IV Hour/week: 6

Course Code: credits: 4

Objectives:

- It is an exercise in various experiments in physical chemistry that will provide a deeper understanding of basic concepts in physical chemistry.

1. Determination of critical solution temperature (CST) of phenol – water system and effect of impurity on CST.
2. Distribution law – study of iodine – iodide equilibrium.
3. Construction of adsorption isotherm for the adsorption of oxalic acid on charcoal using Freundlich isotherm.
4. Study of phase diagram of three components system (Acetic acid, Benzene and Water)
5. Conductometric titration of mixture of alkali against HCl.
6. Conductometric titration of KCl and KI against $AgNO_3$.
7. Conductometry-Solubility product of sparingly soluble silver salts.
8. Potentiometric titrations- Redox titrations.
9. Potentiometric estimation of mixture of halides.
10. Potentiometry-Determination of Activity and activity coefficient of ions.
11. Polarimetric study of the kinetics of acid catalyst inversion of sucrose.
12. Determination of velocity constant between potassium persulphate and potassium iodide.

Text Books:

1. Findlay's Practical Physical Chemistry, Revised and edited by B.P.Levitt 9th ed., Longman, London, 1985.
2. J.N.Gurtu and R. Kapoor, "Advanced Experimental Chemistry", Vol1, S Chand & Co., Ltd., New Delhi.

References:

1. Findlay's Practical Physical Chemistry, Revised and edited by B.P.Levitt 9th ed., Longman,London, 1985.
2. J.N.Gurtu and R. Kapoor, "Advanced Experimental Chemistry", Vol1, S Chand & Co., Ltd., New Delhi.
3. S.R.Palit and D.E.Sadhan Kumar, "Practical Physical Chemistry", 1st Ed., Science Book Agency, 1971.

EC- IV – (ELECTIVE COURSE) - PHYSICAL CHEMISTRY -IV

Semester: IV Hour/week: 6

Course Code: credits: 4

Objectives:

- This course provides an introduction to Thermodynamics. Students will be able to demonstrate an understanding the statistical thermodynamic.
- Students should be able to understand the partition functions.
- To learn the basics of Nano chemistry and data analysis.

UNIT – I

Thermodynamics – III:

Calculation of thermodynamic probability of a system – derivation of the Maxwell – Boltzmann distribution equation (classical statistics) – derivation of S = Klnw – definition of Ergodic hypothesis – physical significance of partition function.

Quantum statistics – derivations of Bose – Einstein and Fermi – Dirac distribution equations – comparison of B.E and F.D statistics with Boltzmann statistics – concept of negative kelvin temperature.

UNIT – II

Partition functions – translational, rotational, vibrational and electronic partition function – Relation between partition function and thermodynamic properties like E, S, H, A, G – Calculation of the above thermodynamic properties from partition function – derivation of equilibrium constants.

Non – equilibrium Thermodynamics – postulates and methodologies, linear laws, Onsager reciprocal relation.

UNIT – III

Quantum Chemistry – III:

The Born-oppenheimer approximation – The MO method for H_2^+ MO and valence bond treatment of H_2molecule. Ionic-covalent bond resonance - polarity of bonds – comparison of MO and VB methods. Polyatomic molecules – localized bonds.

Hybridisation, solving wave functions for sp^1, sp^2 and sp^3 hybrid orbitals, delocalized systems. Huckel theory of conjugated systems like ethylene and butadiene.

Bond order and charge density calculations – extended Huckel theory and its simple chemical applications. Fundamentals of density functional theory.

UNIT – IV

NANO CHEMISTRY:

Definitions of nano, nanoscience and nano technology - Historical milestone in the saga of nano – size effects – Implications of nanoscience and nanotechnology on society – forecasting and nanofuture – Unique properties of nanoscience.

Elementary aspects of nanotechnology – some important recent discovery and history of nanoscience and technology – technological inventions of the 20^{th} Century in nano.

UNIT – V

DATA ANALYSIS:

Various types of errors, precision and accuracy, significant figures, mean value, variance and standard deviations – Student's – t- distribution and tests.

Comparison of mean with the expected value, comparison of results of two different methods. Comparisons of the precision of two methods of F-test – Linear regression, regression line, standard deviation, correlation coefficient.

Text Books:

1. F.W.Bilmayer, Jr., A Text Book of Polymer Science, John Wiley and Sons, New York, 1971.
2. A.Tager, Physical Chemistry of Polymers, Mir Publishers, Moscow, 1978.
3. R.Gopalan, P.S.Subramaniyan and K. Rengarajan, Elements of Analytical Chemistry, Sultan Chand & Sons, New Delhi, 1995.

References:

1. B.K.Sharma, Instrumental methods of Chemical analysis, Goel Publishing House,
2. T.Pradeep, 'Nano-The essentials' Tata-McGraw Hill, 2007.