Qualification: B.Sc., as the major subject with physics as one ancillary. The other ancillary subject may be Mathematics or Botany or Zoology.

Duration of the Course: M.Sc., Chemistry - 2 years (4 Semesters)

Medium of instruction: English

OBJECTIVES OF THE COURSE:

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

Question Paper: Three Parts A, B and C

Section – A - 10 x 1 = 10 marks (multiple choice, True or False)

Section - B - 5 x 7 = 35 marks (either A or B)

Section – C - 3 x 10 = 30 marks (3 out 5 questions)

Passing minimum for theory paper (External)-34 marks

Internal and external put together-50 marks

Mode of evaluation of Internal Assessment for the theory papers:

Seminar - 5 Marks assignment - 5 Marks

Test - 15 Marks (Three tests: Best of Two)
## Scheme of Examination

<table>
<thead>
<tr>
<th>Year</th>
<th>Semester</th>
<th>Code</th>
<th>Paper</th>
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<tr>
<td>I</td>
<td>I</td>
<td>14PCHC11</td>
<td>Introduction to organic Reactions</td>
<td>5</td>
<td>25</td>
<td>75</td>
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<td></td>
<td></td>
<td>14PCHC12</td>
<td>Structure and Bonding</td>
<td>4</td>
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<td>14PCHC13</td>
<td>Thermodynamics, Chemical Equilibrium and Electrochemistry</td>
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<td>Stereochemistry and Organic Reactions</td>
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Objectives:

- To create an idea about the minute studies of electron displacement
- To develop the synthetic aspect among the students
- Make the students to enter the gate way of mechanisms
- To learn how an organic reaction is takes place and how the rate
  Changes correspondingly

Unit I: Electron displacement:

Inductive and field effects-Bond distances- Bond energies-delocalized bonds-Cross
conjugation-rules of Resonance-Resonance energies-Resonance effects-Steric inhibition of
resonance-Hyper conjugation-Hydrogen bonding-Addition compounds-EDA Complexes-
Crown ether complexes-Inclusion compounds-Effect of Structure on the dissociation
constants of acids and bases-concepts of hard and soft acids and bases.

Introduction to reaction mechanism:

Reaction Intermediates-Free radicals, Carbenes, Nitrenes, carbanions, carbocations-
formation and stability of reaction intermediates-Methods of determination of reaction
mechanism – kinetic and thermodynamic control of Chemical reactions. Kinetic and non-
kinetic methods for determining organic reaction mechanism – principle of microscopic
reversibility-energy profile diagram-Hammond postulate.

Unit II: Aliphatic Nucleophilic substitutions:

Nucleophilicity and basicity-SN1 and SN2 Mechanisms-Effect of substrate structure-
Effect of the attacking Nucleophile-Effect of the leaving group - Effect of the reaction
medium-ambident nucleophiles-ambident substrate-Neighbouring group participation of n, π
and σ electrons-SNi mechanism-Nucleophilic substitution at an Aliphatic trigonal carbon-
Nucleophilic substitution at allylic carbon-Nucleophilic substitution at a Vinyl carbon.

Aliphatic electrophilic substitution: Electrophilic substitution at saturated carbon-SE1
mechanism, SE2 and SEi mechanism.

UNIT III: Stereochemistry – 1

Symmetry elements and point group classification-concept of chirality, necessary and
sufficient condition for chirality- relationship between substrate symmetry and chirality.
Projection formulae-Wedge, Fischer, Sawhorse and Newmann.Optical isomerism due to
centre of chirality.Molecules with one stereogenic center (Chiral centre) and molecules with
more than one chiral centre.Properties of enantiomers and disastereoisomers.Erythro and
Threeo nomenclature. Configuration - determination of configuration. Cahn, Ingold and Prelog system of designation of configuration.

Geometrical Isomerism: E-Z nomenclature-determination of configuration of geometrical isomers using physical and chemical methods- stereoisomerism in monocyclic compounds (upto six membered rings)

UNIT IV: Aromatic character

Aromatic character in Benzene, six membered rings, five, seven and eight membered rings- other systems with aromatic sextets-Huckel’s rule- Craig’s Rule- concept of Homoaromaticity and Antiaromaticity-Systems with 2, 4, 8 and 10 electrons-systems with more than 10 electron- Alternate and Non-alternate hydrocarbons. Chemistry of Cyclpentadienyl anion-Fulvene, Azulene, tropolone, sydnones, annulenes.

Novel ring systems: Nomenclature of Bicyclic and tricyclic systems-Chemistry adamantane, Diamantane, (congressane), cubane and catenanes.

UNIT V: Oxidation and Reduction:

Elimination of hydrogen and aromatization reactions – catalytic dehydrogenation-mechanism, applications and stereochemical aspects of the following oxidations- reduction reactions: Oxidation reactions involving CrO₃, SeO₂, OsO₄, Lead Tetraacetate, Periodic acid, N-Bromosuccinimide, H₂O₂-Oppenauer oxidation.

Catalytic hydrogenation-reactions involving lithium aluminum hydride, Triisobutylaluminio hydride, DIBAL and Sodium Borohydride-Birch reduction-Meerwin-pondoff-verley reduction-wolff-kishner reduction

Reagents in organic synthesis: Gilman’s reagents (Lithium dimethyl cuprate), lithium diisoproylamide (LDA), Dicyclohexylcarbodiimide, 1,3-dithane, Trimethylsilyl iodide, Tri-n-butyl tin hydride, Wood and Prevost hydroxylation, DDQ, Merrifield resin, Phase transfer catalyst, Peterson’s synthesis. Baker yeast.

Suggested Readings:

Semester I

<table>
<thead>
<tr>
<th>14PCHC12</th>
<th>Structure and Bonding</th>
<th>Hours-5 / Credits – 4</th>
</tr>
</thead>
</table>

Objectives
- To identify the geometry of the molecules.
- To know the properties of various bonds.
- To study the different types of solids and their electrical conductivity.
- To evaluate the chain, ring and cage structures in certain inorganic compounds.
- To study about metals in detail.

Unit I: Nature of chemical bonds

**Covalent bond:** Hybridization - calculation of s and p characters-Bent's rule-M.O. theory; LCAO approximation-application of MOT to heteronuclear diatomic molecules like BeCl₂, BeH₂ and H₂O-concept of multicentered bond as applied to electron deficient molecules like diborane and metal alkyls - VSPER theory - Walsch diagram.

UNIT II: Bond properties and ionic bonding:

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

UNIT III: Solid state chemistry:

Crystal defects-points, line and plane defects- Colour centers - Non-stoichiometry on physical properties-Electronic structure of solids- Free electron and band theories-TYPES of solids-Electrical conductivity and superconductivity-High temperature superconductors-Types of semiconductors-Thermo-electric power and Hall effect-Photovoltaic effect-Semiconductors in solar energy conversion.

UNIT IV: Inorganic chains - Rings and cages:

Silicates: Various silicate structures-structure, property, correlation-silicones.

Poly acids: Classification-isopolyacids like polymolybdate, polyvanadate and polytungstate-their structures - heteropolyacids: 12A, 12B, 9 and 6 heteropolyacids- preparation and structures.
Phosphazenes and its polymers -Phosphonitrile compounds-S₄N₄-Polymeric sulphur nitride (Polythiazyl) cage compounds: Nomenclature of Boranes and carboranes-Wades rule-STYX number- preparation and structure of B₄H₁₀, C₂H₁₀H₁₂, (B₁₂H₁₂)²⁻ - Boranzine.

UNIT V:

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

Suggested readings:
6. N.B. Hanny, SOlid State chemistry.

Semester I

<table>
<thead>
<tr>
<th>14PCHC13</th>
<th>Thermodynamics, Chemical Equilibrium and Electrochemistry</th>
<th>Hours-5 / Credits – 4</th>
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</thead>
</table>

Objectives

- To get an idea about the concepts of second law of thermodynamics, derivation of equations & absolute entropy.
- To enable the students to understand the effect of pressure and temperature on phase equilibrium.
- To study phase rule.
- To understand about statistical thermodynamics.
- To learn about Electro chemistry and its applications.

UNIT I: Thermodynamics:

UNIT II: Chemical and Phase Equilibria:

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

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

UNIT III: Statistical Thermodynamics:


UNIT IV: Electrochemistry I:

Theory of electrolytic conductance - inter-ionic attraction - ionic atmosphere - thickness of ionic atmosphere - The Debye-Huckel-Onsager conductance equation - its deviation and experimental verification - deviations and modifications - Debye Falkenhagand and Wein effects - mean ionic activity and activity coefficients of strong electrolytes.

The role of electrodes - the electrochemical potential - types of electrodes - the gas/inert metal electrode - ion/insoluble salt/metal electrode - oxidation-reduction electrode - liquid junction potential and membrane potential - Electrochemical cells - kinds of cells - notation - electrochemical cell reactions - EMF of cells - Nernst equation - Application of EMF measurements - determination of equilibrium constant, dissociation constant, solubility product and potentiometric titrations.

UNIT V: Electrochemistry II:

The electrical double layer and Zeta potential - Perrin, Gouy-Chappman and Stern models - polarisable and non-polarisable interfaces - electrokinetic phenomena - dynamic electrochemistry - electrode processes and non-equilibrium electrode potential - over potential - Butler Volmer equation - Tafel equation - Current-potential curves - hydrogen over voltage.

Application of electrochemical processes - power generation and storage - Fuel cells - storage batteries and dry cells - Principles of inhibition of corrosion - cyclic voltammetry - Photo electrochemistry and electrochemiluminescence.
Suggested Readings:


<table>
<thead>
<tr>
<th>Semester I</th>
<th>Major Elective</th>
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<tr>
<td>14PCHE11</td>
<td>Medicinal and Pharmaceutical Chemistry</td>
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</table>

Objectives:

- To study about the drugs and their interactions with various organs of humans.
- To learn the synthesis of new drug molecules and their biological activities.
- To ascertain the elucidations of drugs interactions with receptors viz., DNA and enzymes.
- To know the therapeutic uses of steroids, antibiotics, antihistamines, antihypertensive drugs, anti-inflammatory drugs and CNS stimulants etc.

UNIT I: Fundamentals of Medicinal Chemistry:

Definitions of Medicinal Chemistry, Pharmacology and Molecular Pharmacology - major process involved in drug action - pharmacokinetics phase – Quantitative structure – Activity relationship (QSAR) – Hansch approach – concept of bio-isotomer – receptors and classification of membrane bound receptors-enzyme inhibitors as drugs (illustrated with one example).
UNIT II: Medicinally useful antibiotics and steroids:

Structural features and mode of action of the following antibiotics – penicillin G, cephalosporin and their semi synthetic analogs (β-lactum), streptomycin (aminoglycoside), terramycin (tetracyclin), erythromycin (macrolide) and chloramphenicol. Physiologically active steroids - their structural features and therapeutic use. Oral contraceptives, anabolic steroids, anit-inflammatory steroids.

UNTI III: Chemotherapeutic agents:

Antineoplastic agents: Classification, synthesis e.g., Cyclophosphamide, Ifofamide, Chlorambucil, Busulfan, Decarbazine, Methotrexate, Azathioprine, 6-Mercaptopurine, 5-fluorouracil, Cisplatin, Carnplantin.

Anti-tubercular drugs: Classification, synthesis, e.g., Isoniazid, Pyrazinamine, Ethambutol, Thiacetazone, Paramino salicylic acid and Ethionamide.

Antimalarial drugs: Classification, synthesis, e.g., Chloroquin, Primaguine, Amoediaquine, Mefloquine, Proguanil, Pyrimethamine.

Diuretics: Classification, Synthesis, e.g., Furesemide, Acetazolamide, Chlorothiazide.

UNIT IV: Synthesis and Therapeutic action and SAR of certain drugs:

Antihypertensive drugs: Nifedipine, Captopril, Hydralazine, Sodium nitroprusside, clonidine, methyldopa and guanothidine.


UNIT V:

Anti-inflammatory drugs: Antipyretics & Non-narcotic analgesics; Aspirin, sodium salicylate, Paracetamol, phenylbutazone, Oxyphyelbutazone, Ibuprofen, Mefenamic acid, Dichlofenac sodium.

CNS stimulant Drugs: Amphetamine, Caffeine, Theobromine, Theophylline, Bemegride, Nikethamide, MethyPhenidate.

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

Suggested Reading:

SEMESTER II

| 14PCHC21 | Stereochemistry and Organic Reactions | Hours-5 / Credits – 4 |

Objectives:

- To study about the stereochemistry of organic compounds and their nomenclature.
- To assign the conformation and configuration of simple acyclic, monosubstitutated and disubstituted cyclohexanes.
- To understand the mechanism of electrophilic, nucleophilic and free radical addition reactions and also know about E1, E2 AND E1CB elimination reactions.
- To get knowledge about terpenoids and vitamins.

Unit I: Stereochemistry II

Prochirality and prostereoisomerism, enantiotopic and disatereotopic ligands and faces and their nomenclature – pro-R and pro-S and Re and Si faces. Stereospecific and stereoselective reactions. Asymmetric synthesis; Cram’s rule and Prolog rules. Optical isomerism due to axial chirality – biphenyl, allenes and spiranes. Molecules with planar chirality- paracyclophanes, transcyclooctene and ansa compounds.

Unit II – Conformational analysis:


Unit III: Addition to multiple bonds:

condensation – Claisen ester condensation – Darzen’s reaction – Reformatsky reaction – Wittig reaction – Grignard reactions.

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

Elimination: α-elimination - β-elimination – E1 and E2 and E1CB mechanisms - Stereochemistry of elimination – orientation of the double bond – effect of changes in the substrate, base, leaving group and medium on E1, E2 and E1CB reactions- elimination vs. substitution- pyrolyticcis elimination- Bredt’s rule.

Unit IV:

Terpenes: Classification of terpenoids-struture, stereochemistry and synthesis of α-pinene, camphor, zingeberene, codinene, α-santonin, abietic acid and sqalene.

Vitamins: Struture and synthesis of Vitamins A, B1, B2, B6 and B12 (Strutural features only) C, E, and H and K.

Unit V:

Aromatic electrophilic substitution – orientation –reactivity-mechanism of nitration, halogenations, Friedel-Craft’s reaction and sulponation –partial rate factors- ortho/para ratio – Quantitative treatment of reactivity of reactivity of the electrophile (the selectivity relationship) – Aromaticnucleophilic substitution reactions - SNAr, SN1 and benzyne mechanisms.


Suggested Readings:


Semester II

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<th>14PCHC22</th>
<th>Coordination and Organometallic Chemistry</th>
<th>Hours-5 / Credits – 5</th>
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</table>

Objectives:
- To ascertain theories of bonding and geometries in coordination compounds.
- To understand the reaction mechanism of coordination compounds.
- To study the role of metal ions in biological systems.
- To know the role of enzymes and co enzymes in biological systems.
- To learn the reaction mechanism, structure, synthesis of inorganic Complexes.

UNIT I – Coordination compounds:


UNIT II – Reaction mechanism of coordination compounds:
UNIT III – Bioinorganic chemistry I


UNIT – IV: Bioinorganic chemistry II:


UNIT – V Complexes of π-acceptor ligands:

Synthesis, structure and bonding in metal carbonyls, nitrosyls, dioxygen complexes and dinitrogen complexes-Application of EAN rule.
Synthesis properties, structure and bonding inFerrocene, Arene, Olefin, acetylene and allyl complexes.

Catalysis using organometallic compounds: Oxidative addition – reductive elimination – insertion reaction-Catalytic mechanism in the following reactions-hydrogenation of olefins (Wilkinson catalytic) – Tolmann catalytic loops-hydroformylation (oxo process) – acetic acid from ethanol-oxidation of alkenes to aldehydes and ketones (Wacker process)- catalysis in the formation of synthesis of gas-olefin polymerization (Ziegler-Natta) – Cycloooligomerization of acetylenes (Reppe’s catalyst or Wilke’s catalyst) Olefin isomerization using Ni catalyst.

Suggested Readings:

6. Y. Mido, Chemistry in Aqueous and nonaqueous solvents, Discovery publishers house, NewDelhi, 1969.
SEMESTER II

| 14PCHC23 | Group theory and spectroscopy | Hours-5 / Credits – 4 |

Objectives:

- To identify and concerned with the symmetry found in molecules and solids.
- To assign the modes of molecular vibrations to irreducible representations of point groups to which a molecule belongs.
- To determine which orbitals used for hybridization in chemical bondings and selection rules.
- To deals with the transitions that a molecule undergoes between its energy levels.
- To verify Quantum mechanical calculations on atoms, molecules.

UNIT I: Group Theory:

Molecular Symmetry elements and symmetry operations- Matrices-Matrix representation of symmetry operations and transformation matrices- Group- definition and properties of a group- Symmetry point groups- representation of a group- reducible and irreducible representations- Great orthogonality theorem- characters- construction of character tables- \( \text{C}_2\text{V}, \text{C}_3\text{V}, \text{C}_4\text{V} \) and \( \text{D}_{2\text{d}} \)- Direct product concept.

UNIT II: Application of Group Theory to spectroscopy and Molecular Problems:

Symmetry of normal modes of vibrations, application of group theory to normal modes of vibrations and to normal mode analysis- Symmetry properties of integrals- application for spectral selection rules of vibration spectra- IR and Raman active fundamentals. Symmetry of molecular orbitals and Symmetry selection rules for electronic transitions in simple molecules like ethylene, formaldehyde and benzene. Group theory and quantum mechanics- wave functions as the basis of irreducible representations- Group theory applied to hybridization- HMO theory- HMO calculations and delocalization energy for cyclopropenyl, butadiene and benzene systems.

UNIT III: Molecular Spectroscopy I:

Electromagnetic spectrum- Types of molecular energies- Absorption and emission of radiation- Einstein’s coefficient- induced emission and absorption- Rotational spectra of rigid diatomic molecules- isotope effect in rotational spectra- Microwave spectrometer- Informations derived from rotational spectra.
Infrared spectroscopy - vibrational energy of a diatomic molecule - Infrared selection rules - diatomic vibrating rotator - vibrations of polyatomic molecules - overtone, combination and difference bands - concept of group frequencies - coupling interaction - Fermi resonance - Fourier transform infrared spectroscopy

UNIT IV: Molecular Spectroscopy II:


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

UNIT V: Spin Resonance Spectroscopy:

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

ESR - principles of ESR - Total Hamiltonian - hyperfine structure - ESR spectra of free radicals in solution - Anisotropic systems - systems in triplet state - Zerofield splitting in ESR and Kramer's degeneracy.

Suggested Readings:

5) A. Streitweiser, Molecular Orbital Theory for Organic Chemistry, John Wiley & Sons.
16) D. Shaw, Fourier Transform NMR Spectroscopy, Elsevier.

Semester II

Major Elective

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<th>14PCHE21</th>
<th>Analytical Chemistry</th>
<th>Hours-5 / Credits – 5</th>
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Objectives:

- To recollect the mathematical significant among the students
- Make the students to infer the various laboratory techniques
- Create the knowledge to manipulate the electro chemical system
- To know the temperature dependent substances

UNIT I: Precipitation Techniques:


UNIT II: Error Analysis:


UNIT III: Electroanalytical Methods:

UNIT IV: Thermoanalytical Methods:

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

Unit-V: Spectroanalytical Methods:

Colorimetry: Beer and Lambert’s law –terminology –conditions for a satisfactory colorimetric analysis –methods of colour measurement or comparison -principles of colorimetric determinations of NH₃, Cr, Fe, Mn – simultaneous spectrophotometric determination of Cr &Mn.

Nephelometry and turbidometry : -determination of sulphate and phosphate .

Fluorimetry: principle –application of flourimetry in the determination of Ca ,Cd and Zn and determination of codein and morphine in a mixture.

Flame spectrometry :theory- interferences- AAS-applications in the determination of Mg²⁺, Ca²⁺ in tap water, V in lubricating oil, trace lead in a Ferrous alloy and trace elements in contaminated soil.

Suggested Reading:

Objective:

- To study the different spectrosopes such as UV spectroscopy, IR spectroscopy and mass spectroscopy.
- To study about NMR spectroscopy through various aspects.
- To know chirooptical and analytical techniques in organic compounds and study about chromatography.
- To know about steroids and prostaglandins, also about certain alkaloids and antibiotics.

Unit I: Spectroscopy I:


IR Spectroscopy: Molecular vibrations – vibrational frequency – factors influencing group frequencies – quantitative studies.


Unit II: Spectroscopy II:


C\(^{13}\) NMR Spectroscopy: Basic principle of FT technique – Relaxation time – assignment of signals – Off resonance decoupling - calculation of chemical shifts for aromatic and aliphatic compounds – DEPT \(^{13}\)C spectra - \(^{13}\)C-\(^{13}\)C correlation COSY, HETCOR, ROESY, NOESY and TOCSY- technique.
Unit III: Chiro optical and Analytical techniques:

ORD and CD – Principle- cotton effect- type of ORD curves- \( \alpha \)-halo ketone rule- octant rule-applications to determine the configuration and conformation of simple mono cyclic and bi cyclic ketone and comparison of ORD and CD.

Chromatographic techniques: column- TLC, paper, GLC, HPLC, exclusion and ion exchange .

Unit IV :

Steroids: Classification – configurational and conformational aspects of A/B cis and A/B trans steroids- complete chemistry and stereo chemistry of cholesterol (includes bile acids) chemistry of ergosterol and vitamin D\(_2\) – male sex hormones – androsterone- testosterone- female sex hormone- oestrone, equilenin and progesterone – a basic idea about adrenocortical hormones – cortisone (synthesis not included)

Prostaglandins. General study of prostaglandins- structure – chemistry of PGE1 and PGF1 \( \alpha \)

Unit V:


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

Suggested Readings:

Objectives;

➢ To understand the Rearrangement mechanisms.
➢ To grow their spectroscopic knowledge about how to find out the NMR, ESR, IR, UV active compounds.
➢ To know the shift reagents’s uses.
➢ To compare the orbital degeneracy of various molecules.
➢ To improve their ability to understand the spectral datas.

Unit I: Electronic spectra of transition metal complexes and photochemistry:

- Photochemistry-photoredox and substitution reactions occurring in Co(III) and Cr(III) complexes-Photochemistry of ruthenium polypyridyls.

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

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

Mossbauer and Photoelectron spectroscopy (PES):
Mossbauer effect resonance absorption-Doppler effect-Doppler velocity-Experimental technique of measuring resonance absorption-isomer shift-magnetic hyperfine splitting-application of Mossbauer spectroscopy in the study of Iron and Tin complexes.

Photoelectron spectroscopy:

UNIT III: Application of spectroscopy to the study of Inorganic compounds II:

NMR Spectroscopy: 
-\(^{31}\)P - \(^{19}\)F and \(^{15}\)N-NMR-Introduction-applications in structural problems-evaluation of rate constants-monitoring the course of reaction-NMR of Fluxional molecules-NMR of paramagnetic molecules-contact shifts and shifts Reagents.

ESR spectroscopy:
Principles-presentation of the spectrum-hyperfine splitting-evaluation of g and A tensors-factors affecting magnitude of g values-zero field splitting-Kramer’s
degeneracy-ESR of d³ Octahedral complexes –anisotropy –hyperfine splitting constants-
application of ESR in the study of transition metal complexes – John Teller distortion
studying in Cu(II) complexes – Evaluation of spin orbit coupling

UNIT IV: Nano chemistry

Basic Idea of nano chemistry –defining nanoassemblies-measurements-examples-
potential uses –Zero dimensional, one dimensional and two dimensional arrangements.
Nano tubes: Structure and characterization single walled carbon nano tubes –Nano tubes
properties –applications of Nano tubes.
Nano Wires-Vapour phase-oxide assisted – carbo thermal growth of Nano wires-properties.
Nano Rods: Seed mediated growth of inorganic Nano tubes and Nano rods.
Nano structured Polymers: Conducting polymers –block –copolymers-Nano cages

UNIT V: Molecular Rearrangements and reaction of coordinated ligands

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

Suggested Readings:
   York, 1967.
3. S.F. Kettle, Coordination chemistry. An approach, Spectrum Academic Publishers,
4. R.S. Drago, Physical Methods in chemistry, Sanders Golden Sunburst series, W.B.
6. ChatwalBhagi and Agarwal, Bioinorganic chemistry, sultan chand co., New delhi,
7. M.A. O. Hill and P. Day (Eds), Physical Methods in Advanced Inorganic chemistry,
   Interscience, Newyork, 1968.
Objectives

- To assign the formulation of Quantum mechanics for wave mechanical treatment of atom.
- To know about the probabilities of finding the particles at various locations in space.
- To get a key factors of which is the quantization of energy.
- To get a knowledge about the instrumentation used in nanoscience.
- To give a detailed notes about the large molecules and their properties.

Unit I: The Birth of Quantum Mechanics
Plank’s explanation about Black body radiation – De Broglie concept of matter waves, Compton effect - Heisenberg’s uncertainty principle and complementary- operators- linear operator – method of getting the following quantum mechanical operator- position, momentum, kinetic energy, potential energy, total energy, angular momentum, raising and lowering and spin angular momentum

Postulates of quantum mechanics- hermicity and proving the quantum mechanical operators are hermitian- commutators – eigen function and eigen value- introducing dirac notation- expansion theorem. Orthogonality and normalization of wave function

Unit II: Application of Quantum mechanics to simple systems:

Unit III: Approximation methods in Quantum mechanics:
need for approximation methods- schrodinger equation for He atom and other many electron system- the time independent perturbation theory( first order only)- application to hydrogen atom- variation theorem- application to hydrogen and helium atom- Hartee- fock- self consistent field (HFSCF) method of many electron system and its application to helium atom- electron spin and pauli’s principle-antisymmetric nature of the wave functions- Slater determinants- electronic configuration of many electron system- Born-Openheimer approximation –VB and MO theories, MO treatment of hetero nuclear and homo nuclear diatomic molecules.
Unit IV: Instrumentation in nano chemistry

Microscopic techniques for the characterization of nano materials- UV-VISIBLE and Fluorescence spectroscopy- AFM, SEM, TEM, X-RAY diffraction and micro analysis


Suggested Readings:

Objective

- To get a knowledge about carbohydrates, amino acids, and nucleic acids.
- To analyse photochemistry and free radical formation in organic compounds.
- To understand the mechanisms involved in certain molecular rearrangements.
- To know about green chemistry and microwave synthesis.
- To study about methods involved in various synthesis.

UNIT I: Proteins, amino acids, Nucleic acids and Carbohydrates:


Introduction to carbohydrates

Pyronose and furanose, forms of aldohexoses and keto hexoses – methods used for determination of ring size – conformation of aldohexopyranoses- structure and synthesis of maltose, lactose sucrose and cellobiose.

UNIT II: Photochemistry & Free radicals:


UNIT III: Molecular rearrangements:

Mechanism of the following rearrangement reactions: Wagner-Meerwin, Pinacol-Demzanov, Bechmann, Hoffmann, Curtius, Wolff, Baeyer-villiger, Stevens, Sommellet-
Hauser, Favorskii, Benzil-bezillic acid, Claisen, Cope, Fries, Dienone-phenol, di-pi methane, hydroxiamino-p-aminephenol and benzidine rearrangement – Photochemical rearrangement.

UNIT IV: Green Chemistry I:

Principles of green chemistry – planning a green synthesis in a laboratory – general interest for solvent free processes- solvent free technique- Microwave synthesis: Introduction and characteristics of microwave heating – interaction of microwave radicatin with the material – difference between conventional heating and microwave heating. Dielectric polaroization – dipoloar polarization – application and advantages of microwave heating over conventional heating.

UNIT V: Synthetic methods:

Planning a synthesis – Relay approach and convergent approach to total synthesis – Retro-synthetic analysis of simple organic compounds – Functional groups interconversions(FGI) – Activating and blocking groups in synthesis – stereoselective problems of geometrical and optical isomerism-Umpolung-synthesis- Robinson annelation- A schematic analysis of the total synthesis of the following compounds: 2,4-dimethyl-2-hydroxypentanoic acid, Trans-9-methyl-1-decalone and Isonootkatone.

Suggested Readings:

1. A.I. Lehninger, Biochemistry, Nath Publications.
7. P.De. Mayo, Molecular Rearrangements.
Objectives:

- To understand the fission and fusion mechanisms
- To grow their computer knowledge about browsing, programming
- To know the radioactive element’s uses
- To compare the processes of nuclear power reactor and breeder reactor
- Classify the various reactors

Unit I: STRUCTURE OF NUCLEUS AND RADIOACTIVE DECAY
Composition of the nucleus-nuclear size, shape and density—principal, radial and magnetic quantum numbers—magnetic and electric properties of nucleus—elementary treatment of shell (independent particle) model—nuclear configuration-parity and its conversion—mass defect and binding energy-nuclear forces theory.

Relative decay: Group displacement law—decay series—rate of disintegration—half life—average life—units of radioactivity—secular and transient equilibria—Theories of alpha decay, beta decay, gamma emission, positron decay, nuclear isomerism, internal conversion and electron capture—Auger effect.

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

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

Applications of radioactive isotopes: characteristics of tracer isotopes—chemical investigations—age determination—medical field—agriculture—industry—analytical applications—isotope dilution analysis—neutron activation analysis—biological effects of radiation—waste disposal management

Unit IV: ELECTROANALYTICAL & THERMOANALYTICAL METHODS:


**Thermoanalytical methods:** Instrumentation and applications of thermogravimetry – Differential Thermal Analysis and Differential scanning colorimetry.

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

Unit V: COMPUTERS IN CHEMISTRY: History and development of computers, Mainframe, micro and super computer systems - CPU and other peripheral devices – Evolution of programming language and higher level language, Syntax and structure of C language.


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

**Suggested Readings:**

Semester IV

| 14PCHC43 | Chemical kinetics, Surface, Biophysical and Photochemistry | Hours-5 / Credits – 4 |

Objectives

- To concerns with measurements of rates of reactions.
- To determine the factors which influence rates of reactions.
- To study the rates of catalyst in rate of reactions.
- To get the knowledge about the adsorption on solids and liquid surface.
- To study the various chemical reactions by absorption of light radiations.

UNIT I: CHEMICAL KINETICS I

Potential energy surfaces: Chain reactions-general characteristics- Steady state approximations-Study of kinetics of Chain reactions like H₂-Br₂ reaction-decomposition of N₂O₅ and acetaldehyde.

Unimolecular reaction rate theories-the simple Lindemann treatment- Hinshelwood’s theory-Rice, Ramsperer and Kessel (RRK) theory-Advanced Unimolecular theory-Marcus theory or Rice, RamspererKessel and Marcus (RRKM) theory-Slater’s theory. Principle of microscopic reversibility and detailed balancing- Reactions in solution- influence of solvent dielectric constant, ionic strength (Bronsted-Bjerrum equation)-primary and secondary salt effects and pressure on reaction rates in solution-Significance of volume of activation.

UNIT II: CHEMICAL KINETICS II AND CATALYSIS:

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


UNIT III: SURFACE CHEMISTRY

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

UNIT IV: BIOPHYSICAL CHEMISTRY

Basic concepts of non-equilibrium thermodynamics- Onsager reciprocal relationship- Its application to biological systems- High energy metabolites- ATP and its role in bioenergetics- transfer of potential and coupled reaction- Biological energy conversion in catabolism and anabolism- role of singlet oxygen in biology- Biophysical applications of Mossbauer effect- NMR imaging- Applications of spin labeling in membrane research- Molecular recognition – An introduction to supra- molecular chemistry and photochemistry.

UNIT V: PHOTO AND RADIATION CHEMISTRY:


Recommended Books:

5) Margaret Robson Wright, Fundamental Chemical kinetics-An Explanatory introduction to the concepts,Horwood Publishing Ltd.,West Sussex 1999
9) N.J. Turro, Modern Molecular Photochemistry,Benjamin Cummings.
Objectives:

- To know the types of polymers and mechanism of polymerization.
- To ascertain the preparation and uses of individual polymer.
- To study the properties and molecular weight determination of polymers.
- To understand polymerization techniques.
- To know the polymer processing.

Unit – I CLASSIFICATION OF POLYMERS AND CHEMISTRY OF POLYMERISATION

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

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

Unit – II INDIVIDUAL POLYMERS

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

Unit – III PROPERTIES OF POLYMERS

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

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

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

Unit IV

POLYMERIZATION TECHNIQUES, DEGRADATION AND USES OF POLYMERS

Polymerization techniques: Bulk, solution, suspension, emulsion, melt condensation and interfacial polycondensation polymerizations.
Degradation: Types of degradation-thermal, mechanical, ultrasonic and photodegradation-photostabilizers-oxidative degradation-antioxidants-hydrolytic degradation.
Uses of polymers in electronics and biomedicine.

Unit – V POLYMER PROCESSING

Polymer processing: Plastics (thermo and thermosetting), elastomers, fibres, compounding, plasticisers, colorants, flame retardants.
Compression and injection mouldings-film extrusion and calendaring-die casting and rotational casting-thermofoaming-reinforcing.

Reference Books

Semester III
Non-Major Elective

<table>
<thead>
<tr>
<th>14PCHE31</th>
<th>Environmental Science</th>
<th>Hours-5 / Credits – 5</th>
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Objectives

- To know the basics of chemistry and their needs.
- To understand about organic, inorganic & physical chemistry.
- To get an new idea about macromolecules.
- To know the environmental chemistry and pollution

Unit:I Introduction and Classification


Unit:II Air pollution

Introduction - sources of air pollution - air pollutants - classification and effects of air pollutants - oxides of nitrogen, sulphur and carbon - acid rain - effects and control - hydrogen sulphide - effects and control - carbon mono oxide - effects and control - photochemical smog - effects and control - fly ash - effects and control - green house effects - global warming - effects and control - ozone layer - ozone depletion - chlorofluoro carbons - effects and control.

Unit:III Water pollution


Unit:IV Soil pollution

Unit: V Analysis of pollutants


Suggested Readings:
4. N. Manivasakam, physio-chemical Examination of water, Sewage and Industrial Effluents, Pragati Prakashan Publ., Meerut, 1985

Semester I

Inorganic qualitative and quantitative analysis and preparations

1. Semi micro qualitative analysis: analysis of mixtures containing one familiar and one less familiar cations from the following: W, Pb, Tl, Se, Te, Mo, Cu, Bi, Cd, Ce, Th, Zr, Ti, V, Cr, Mn, Al, U, Ni, Co, Zn, Ca, Ba, Sr, Li and Mg.

2. Estimation of one metal in the presence of another by EDTA (demonstration)

3. In organic preparations; Preparations of atleast 6 (six) in organic complexes.

4. Quantitative analysis: separation and estimation of mixture by volumetric and gravimetric methods.
   Cu, Ni; Cu, Zn: Ba, Ca; Fe, Ni; Fe, Cu.

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

Organic preparation, Qualitative and Quantitative analysis

Qualitative analysis

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

1. Quantitative analysis:
   a. Estimation of glucose by lane and eynon method and Bertrand method
   b. Estimation of glycine
   c. Estimation of formalin
   d. Estimation of methyl ketone

2. Organic preparations: (only for class work)
   About 3 (five) two-stage preparation:
   a. P-Nitro aniline from acetanilide benzophenone
   b. P-Bromo aniline from acetanilide Aniline
   c. m-Nitro benzoic acid from methyl benzoate

Semester III

Physical chemistry practical: conductometric and potentiometric titrations and kinetic adsorption and spectral experiments.

I. Conductometric experiments
   i. Double displacement & acid base titrations
      a) NH₄Cl → NaOH → Mixture of CH₃COOH & HCL
      b) NH₄Cl → NaOH → Mixture of NH₄Cl & HCL
   ii. Precipitation titration
      a) Na₂CO₃ → Pb(NO₃)₂ → Na₂CO₃
      b) K₂SO₄ → BaCl₂ → K₂SO₄

II. Adsorption experiments
   Adsorption of oxalic acid/acetic acid on charcoal

III. Kinetic experiments
   i. Kinetics of alkali hydrolysis of ester by potentiometric method
   ii. Perdisulphate and iodide ion reaction: Study of primary salt effect and determination of the concentration of given KNO₃

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

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

VI. Experiments based on UV-Visible and Infra red spectrophotometers.
Semester IV  Project.