**BHARATHIDASAN UNIVERSITY**  **TIRUCHIRAPPALLI - 620 024.**

**M.Sc. CHEMISTRY: CHOICE BASED CREDIT SYSTEM -**
**LEARNING OUTCOMES BASED CURRICULUM FRAMEWORK (CBCS - LOCF)**

**(Applicable to the candidates admitted from the academic year 2022-23 onwards)**

| Sem. | Courses | Title | Ins. Hrs. | Credit | Exam. Hrs | Marks | | Total |
|---|---|---|---|---|---|---|---|---|
| | | | | | | Int. | Ext. | |
| I | Core Course I (CC) | Inorganic ChemistryI | 6 | 5 | 3 | 25 | 75 | 100 |
| | Core Course II (CC) | Organic Chemistry I | 6 | 5 | 3 | 25 | 75 | 100 |
| | Core Choice Course I (CCC) | 1. Physical Chemistry I<br>2. Bio-Physical Chemistry | 6 | 5 | 3 | 25 | 75 | 100 |
| | Core Practical I (CP) | Inorganic Chemistry Practical | 6 | 3 | 6 | 40 | 60 | 100 |
| | Elective Course I (EC) | 1. Analytical Chemistry<br>2. Supramolecular Chemistry | 6 | 4 | 3 | 25 | 75 | 100 |
| | Value Added Course I (VAC) | Environmental Chemistry | - | 2* | 3 | 25 | 75 | 100* |
| | | **Total** | **30** | **22** | **-** | **-** | **-** | **500** |
| II | Core Course III (CC) | Physical Chemistry II | 6 | 5 | 3 | 25 | 75 | 100 |
| | Core Course IV (CC) | Inorganic Chemistry II | 5 | 5 | 3 | 25 | 75 | 100 |
| | Core Choice Course II (CCC) | 1. Organic Chemistry II<br>2. Bio-Organic Chemistry | 5 | 5 | 3 | 25 | 75 | 100 |
| | Core Practical II (CP) | Organic Chemistry Practical I | 6 | 3 | 6 | 40 | 60 | 100 |
| | Elective Course II (EC) | 1. Solid State Chemistry<br>2. Pharmaceutical Chemistry | 5 | 4 | 3 | 25 | 75 | 100 |
| | Non-Major Elective Course I | Chemistry of Pollution, Food and Cosmetics | 3 | 2 | 3 | 25 | 75 | 100 |
| | | **Total** | **30** | **24** | **-** | **-** | **-** | **600** |
| III | Core Course V (CC) | Organic Chemistry III | 6 | 5 | 3 | 25 | 75 | 100 |
| | Core Course VI (CC) | Physical Chemistry III | 5 | 5 | 3 | 25 | 75 | 100 |
| | Core Choice Course III (CCC) | 1. Inorganic Chemistry III<br>2. Inorganic Photo Chemistry | 5 | 5 | 3 | 25 | 75 | 100 |
| | Core Practical III (CP) | Physical Chemistry Practical | 6 | 3 | 6 | 40 | 60 | 100 |
| | Elective Course III (EC) | 1. Green Chemistry<br>2. Catalysis | 5 | 4 | 3 | 25 | 75 | 100 |
| | Non-Major Elective Course II | Chemistry in Day-To-Day Life | 3 | 2 | 3 | 25 | 75 | 100 |
| | | **Total** | **30** | **24** | **-** | **-** | **-** | **600** |
| IV | Core Course VII (CC) | Chemistry of Nanoscience and Nanotechnology | 6 | 5 | 3 | 25 | 75 | 100 |
| | Core Course VIII (CC) | Selected Topics in Chemistry | 6 | 5 | 3 | 25 | 75 | 100 |
| | Entrepreneurship / Industry Based Course | Industrial Chemistry | 6 | 5 | 3 | 25 | 75 | 100 |
| | Project | | 12 | 5 | - | 20 | 80 | 100 |
| | Value Added Course II (VAC) | Polymer Chemistry | - | 2* | 3 | 25 | 75 | 100* |
| | | **Total** | **30** | **20** | **-** | **-** | **-** | **400** |
| | | **Grand Total** | **120** | **90** | **-** | **-** | **-** | **2100** |

## SUMMARY OF CURRICULUM STRUCTURE OF PG PROGRAMMES

| Sl. No. | Types of the Courses | No. of Courses | No. of Credits | Marks |
|---|---|---|---|---|
| 1. | Core Courses | 8 | 40 | 800 |
| 2. | Core Choice Courses | 3 | 15 | 300 |
| 3. | Core Practicals | 3 | 9 | 300 |
| 4. | Elective Courses | 3 | 12 | 300 |
| 5. | Entrepreneurship/ Industry Based Course | 1 | 5 | 100 |
| 6. | Project | 1 | 5 | 100 |
| 7. | Non-Major Elective Courses | 2 | 4 | 200 |
| | **Total** | **21** | **90** | **2100** |
| | Value Added Courses * | 2* | 4* | 200* |

***The value added courses credit will not be included in the total CGPA.**
**These courses are extra-credit courses.**
**Instruction hours for these courses is 30 hours.**

**PROGRAMME OBJECTIVES:**

- To educate and prepare post graduate students from rural and urban area who will get employment on large scale in academic institutes, R & D and Quality control laboratories of Indian chemical/pharmaceutical industries as well as multinational and forensic Laboratories.
- To provide students with broad theoretical and applied background in all specialization of Chemistry with emphasis on qualitative and quantitative technique.
- To provide broad common frame work of syllabus to expose our young graduates to the recent and applied knowledge of interdisciplinary branches of chemistry involving applied organic, inorganic, physical, analytical, industrial, pharmaceutical, polymer, Nano science & technology.
- To conduct lesser written tests and to encourage on non-written tests.
- To focus on encouraging students to conduct various academic activities like midterm tests, online tests, open book tests, tutorial, surprise test, oral, seminar, assignments and seminar presentation.

**PROGRAMME OUTCOMES:**

- To attain profound Expertise in Discipline.
- To acquire the ability to function in multidisciplinary Domains.
- To achieve the ability to exercise Research Intelligence in investigations and Innovations.
- To learn Ethical Principles and be committed to Professional Ethics.
- To incorporate Self-directed and Life-long Learning.
- To obtain the capability to maneuver in diverse contexts with a Global Perspective.
- To attain Maturity to respond to others.

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**First Year** **CORE COURSE I** **Semester I**

**INORGANIC CHEMISTRYI**

**Code:** **(Theory)** **Credit: 5**

**COURSE OBJECTIVES:**

- To understand the basic concepts of main group elements.
- To learn the theories and mechanism of reactions of metal complexes.
- To study the concepts of photochemistry and its applications.

**UNIT – I MAIN GROUP CHEMISTRY:**

Chemistry of boron – borane, higher boranes, carboranes, borazines and boron nitrides. Chemistry of silicon – classification of silicates- silanes- silicon nitrides- silicones. P-N compounds, linear and cyclophosphazenes – S-N compounds – $S_2N_2$, $S_4N_4$, (SN)x, polythiazyl compounds – S-N cations and anions, S-P compounds – molecular sulphides such as $P_4S_3$, $P_4S_7$, $P_4S_9$ and $P_4S_{10}$.Ionic model –lattice energy – Born-Lande equation – Kapustinskii equation – high $T_c$ superconductors.

**UNIT – II PRINCIPLES OF COORDINATION CHEMISTRY:**

Studies of coordination compounds in solution – detection of complex formation in solution – stability constants – stepwise and overall formation constants. Simple methods (potentiometric, pH metric and photometric methods) of determining the formation constants. Factors affecting stability – statistical and chelate effects – forced configurations.

**UNIT – III THEORIES OF METAL-LIGAND BOND:**

Crystal field theory – splitting of d-orbitals under various geometries – factors affecting splitting – CFSE and evidences for CFSE (structural and thermodynamic effects). Spectrochemical series – Jahn-Teller distortion – spectral and magnetic properties of complexes – site preferences. Limitations of CFT – ligand field theory – MO theory – sigma- and pi-bonding in complexes – Nephelauxetic effect – the angular overlap model.

**UNIT – IV REACTION MECHANISM IN COORDINATION COMPLEXES:**

Kinetics and mechanism of reactions in solution – labile and inert complexes – ligand displacement reactions in octahedral and square planar complexes – acid hydrolysis, base hydrolysis and anationreactions. Trans effect – theory and applications – electron transfer reactions – electron exchange reactions – complementary and non-complementary types – inner sphere and outer sphere processes – application of electron transfer reactions in inorganic complexes – isomerisation and racemisation reactions of complexes. Molecular rearrangements of four- and six-coordinate complexes – interconversion of stereoisomers – reactions of coordinated ligands – template effect and its applications for the synthesis of macrocyclic ligands – unique properties.

**UNIT – V INORGANIC PHOTOCHEMISTRY:**

Electronic transitions in metal complexes, metal-centered and charge-transfer transitions – various photophysical and photochemical processes of coordination compounds. Unimolecular charge-transfer photochemistry of cobalt(III) complexes – mechanism of CTTM, photoreduction – ligand-field photochemistry of chromium(III) complexes – Adamson's rules, photoactive excited states, V-C model – photophysics and photochemistry of ruthenium – polypyridine complexes, emission and redox properties.

Photochemistry of organometallic compounds – metal carbonyl compounds – compounds with metal-metal bonding – Reinecke'ssalt chemical actinometer.

**UNIT – VI Bonding in Small Molecules (For Continuous Internal assessment only):**

Valence Bond (VBT) and Molecular Orbital (MO) Theories - Application to small molecules such as BeCl2, BCl3 and CCl4, SF4, ClF3, BrF3 , BrF5 , IF5, IF7 etc – Bonding in Noble gas compounds – XeCl2, XeF4, XeOF4, XeF6.

**REFERENCES:**


1. M. C. Day, J. Selbin and H. H. Sisler, Theoretical Inorganic Chemistry; Literary Licensing (LLC), Montana, 2012.
2. F. A. Cotton and G. Wilkinson, C. A. Murillo and M. Bochmann, Advanced Inorganic Chemistry; 6th Ed., A Wiley - Interscience Publications, John Wiley and Sons, USA, 1999.
3. J. E. Huheey, Inorganic Chemistry; 4th Ed., Harper and Row publisher, Singapore, 2006.
4. A. W. Adamson, Concept of Inorganic Photochemistry; John Wiley and Sons, New York, 1975.
5. S. F. A. Kettle, Physical Inorganic Chemistry – A Coordination Chemistry Approach, Spectrum; Academic Publishers, Oxford University Press, New York, 1996.
6. A. W. Adamson and P. D. Fleischauer, Concepts of Inorganic Photochemistry; R. E. Krieger Pubs, Florida, 1984.
7. J. Ferraudi, Elements of Inorganic Photochemistry; Wiley, New York, 1988.
8. F. Basolo and R. G. Pearson, Mechanism of Inorganic Reactions; 2nd Ed., John Wiley, New York, 1967.
9. R. K. Sharma, Inorganic Reactions Mechanism; Discovery Publishing House,NewDelhi.


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**First Year** **CORE COURSE II** **Semester I**

**ORGANIC CHEMISTRY I**

**Code:** **(Theory)** **Credit: 5**

**COURSE OBJECTIVES:**

- To learn the Nomenclature of Organic Compounds
- To learn stereochemistry of organic compounds.
- To understand the basic concepts of aromaticity.
- To know about oxidation and reducing reagents for organic synthesis.

**UNIT – I NOMENCLATURE OF ORGANIC COMPOUNDS, REACTIVE INTERMEDIATESAND ELECTRONIC EFFECTS:**

Nomenclature of heterocyclics having not more than two hetero atoms such as oxygen, nitrogen and sulphur - Nomenclature of heterocyclic compounds of fused ring system - Nomenclature of alicyclic, bicyclic and tricyclic compounds.

**Reactive Intermediates**: Classical and non-classical carbocations, carbanions-free radicals, carbenes, nitrenes, arynes and singlet oxygen- general methods of generation, detection, geometry, stability and reactivity of these intermediates.

**Electronic Effects**: Inductive effect - resonance effect – hyper conjugation (Baker-Nathan effect) hydrogen bonding (inter and intramolecular) and steric effects.

**UNIT – II METHODS OF DETERMINING REACTION MECHANISMS AND CORRELATION ANALYSIS**

Kinetics and non-kinetic methods of determination of reaction mechanisms - Thermodynamic and kinetic aspects of organic reactions ,energy profile diagrams - spectroscopic studies, isotopic effects - intermediate versus transition states - product analysis and its importance - crossover experiments-isotopic labelling studies.

**Correlation Analysis**: Linear Free Energy Relations-Hammet equation - significance - sigma and rho applications and limitations - Taft, Swain-Scott-Grunwald-Winstein equations and their applications, classification of solvents.

**UNIT – III STEREOCHEMISTRY I:**

Optical isomerism - Optical activity and chirality - elements of symmetry - Stereochemistry of overcrowded molecules (hexahelicene, ansa compounds, cyclophanes and trans cycloalkenes -Newmann, Sawhorse and Fischer projections - representation and interconversion - Absolute configuration – R & S notations for special molecules(allenes, spirans, biphenyls)R-Snomenclature of cyclic chiral compounds - molecules with more than one chiral center. Asymmetric synthesis - Optical purity-determination of enantiomeric excess by NMR – definition of terms like prochirality,enantiotopicanddiastereotopic atoms, groups and faces - stereoselective and stereospecific reactions.

**UNIT – IV STEREOCHEMISTRY II:**

**Geometrical isomerism** : E and Z nomenclature - determination of configuration of geometrical isomers (cyclisation, converting into compounds of known configuration, dipolemoment, converting into less symmetric compounds- spectroscopic methods) configuration of cyclic and bicyclic ring systems - cis- trans nomenclature of three, four and six membered substituted cyclic systems-decalins.

**Dynamic Stereochemistry**: Quantitative correlation between conformation and reactivity - Winstein-Eliel equation – Curtin- Hammet principle- conformation, reactivity and mechanism of cyclic systems and fused (decalin) ring systems-bridged(norbornane) systems-saponification of an ester - esterification of an alcohol - chromic acid oxidation of cyclohexanols - neighbouring group participation - deamination of 2- amino cyclohexanol.

**UNIT – V AROMATICITY AND REAGENTS IN ORGANIC SYNTHESIS:**

**Aromaticity**: Aromatic character: Five-, six-, seven-, and eight-membered rings-other systems with aromatic sextets – Huckel's theory of aromaticity,Craig's rule- concept of homoaromaticity and antiaromaticity. – NMR concept of aromaticity and antiaromaticity-non benzeniod aromatic compounds- systems with 2,4,8 and 10 electrons, systems of more than 10 electrons (annulenes), Mobius aromaticity. alternant and non-alternant hydrocarbons (azulene type) – aromaticity in heteroaromatic molecules, sdnones and fullerenes.

**Reagents in organic synthesis**: Oxidation: Baeyer-Villiger, Jacobsen epoxidation, Shi epoxidation, Jones reagent, DMP, TPAP, NOCl, Mn(OAc)3, Cu(OAC)2, Bi2O3,Swern oxidation. Reduction: Hydride transfer reagents from group III and group IV in reductions. (i) triacetoxyborohydride, L-selectride, K-selectride, Luche reduction (ii) stereo/enantioselectivity reductions (Chiral Boranes).

**UNIT – VI NAMEREACTIONS AND APPLICATIONS IN ORGANIC SYNTHESIS: (For Continuous Internal Assessment Only):**

Bamford-Stevens reaction – Barton-McCombie reaction (Barton Deoxygenation) – Baylis-Hillman reaction – Biginelli reaction – Corey-Chaykovsky reaction – Enamines and selective mono- and dialkylation via enamine reactions Henry reaction – Hosomi-Sakurai reaction – Hunsdiecker reaction – Julia olefination and its modifications – Mitsunobu reaction – Mukaiyama-Aldol addition – Nazarov cyclization – Peterson olefination – Prevost reaction – Prins reaction – Staudinger reaction Ugi reaction – Weinreb ketone synthesis – Wittig reaction and its modifications – Yamaguchi macrolactonization – Palladium based reactions: Fukuyama coupling – Heck reaction – Hiyama coupling – Sonogashira coupling – Stille coupling – Suzuki coupling – Tsuji-Trost Reaction.

**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 Edn.,Butterworths, 1997.
3. I. L. Finar, Organic Chemistry; Vol.II, 7th Ed., Pearson education Ltd, New Delhi, 2009.
4. J. March, "Advanced Organic Chemistry: Reactions, Mechanisms and Structure",4th ed., Wiley, 1992.
5. R.K. Bansal, "Organic Reaction Mechanisms", Tata McGraw Hill, 1975.
6. P. S. Kalsi, "Organic Reactions and their Mechanisms", New Age International Publishers.
7. E.L.Eliel, "Spectrochemistry of Carbon Compounds", McGraw Hill, 1962.
8. D. Nasipuri, Stereochemistry of Organic Compounds.
9. I.L. Finar, "Organic Chemistry", Vol.II, 5 th ed., ELBS 1975.
10. 10.R.T. Morrison and R.N.Boyd, "Organic Chemistry", 6 th ed., Allyn and Eacon,
11. F.A. Carey and R.J. Sunberg, "Advanced Organic Chemistry, Parts A & B, Plenum, 1984.


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**First Year** **CORE CHOICE COURSE I** **Semester I**

**1) PHYSICAL CHEMISTRY I**

**Code:** **(Theory)** **Credit: 5**

**COURSE OBJECTIVES:**

- To study the theories of kinetics, photochemistry and radiation chemistry.
- To understand the concepts of quantum mechanics and group theory.
- To learn the statistical thermodynamics.

## UNIT – I CHEMICALKINETICS I:

Theories of reaction rate based on statistical mechanics –statistical mechanics and chemical equilibrium-Transition state theory based on statistical mechanics-symmetry numbers and statistical factors- transmission coefficient- reaction coordinate – potential energy surfaces – kinetic isotope effect – Hinshelwood theory – Kassel, Rice and Ramsperger theory (KRRT) – Slater's treatment.

Principle of microscopic reversibility – steady-state approximation – chain reactions: thermal and photochemical reactions between hydrogen and halogens – explosions and hydrogen-oxygen reactions.

## UNIT – II FAST REACTION TECHNIQUES, PHOTOCHEMISTRY AND RADIATION CHEMISTRY

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

Photophysical processes of electronically excited molecules – Jablonskidiagram Stern-Volmer equation and its applications – experimental techniques in photochemistry – chemical actinometers – lasers and their applications.

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

## UNIT– III BASIC QUANTUM MECHANICS:

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 – decline of old quantum theory.

Schrödinger equation – postulates of quantum mechanics – operator algebra: linear operator, Hermitian operators, eigenfunctions and eigenvalues, angular momentum operator – commutation relations and related theorems – orthogonality and normalization.

Applications of wave mechanics to simple systems – particle in a box, one and three dimensional, particle with finite potential barrier – the quantum mechanical tunneling.

## UNIT – IV STATISTICALTHERMODYNAMICS:

Thermodynamic probability – probability theorems – relation between entropy and probability (Boltzmann-Planck equation), ensembles, phase space, Ergodic hypothesis, microstates and macrostates, Maxwell-Boltzmann distribution law. partition functions – translational, rotational, vibrational and electronic partition functions.

Relationship between partition functions and thermodynamic properties – calculation of equilibrium constants from partition functions – heat capacities of monatomic crystals – Einstein theory and Debye theory.

Quantum statistics – Bose-Einstein (B.E.) and Fermi-Dirac (F.D.) distribution equations – comparison of B.E. and F.D. statistics with Boltzmann statistics – applications of quantum statistics to liquid helium, electrons in metals and Planck's radiation law – concept of negative Kelvin temperature.

## UNIT– V GROUPTHEORY AND ITS APPLICATIONS:

Symmetry and group theory: Symmetry elements and operations – point groups – assignment of point groups to molecules – group postulates and types of groups – group multiplication tables, sub groups, similarity transformations – conjugate elements and classes.

Matrix representation of symmetry operations and point groups – reducible and irreducible representations – properties of irreducible representation.

The great orthogonality theorem – construction of character table ($C_2V$ & $C_3V$)– direct product – projection operators – symmetry of hybrid orbitals.

**Applications:** vibrational spectra – selection rules for fundamental vibrational transition – IR and Raman activity of fundamentals in $CO_2$, HO,$N_2F_2$–the rule of mutual exclusion and Fermi resonance.

## UNIT – VI COLLOIDS AND MICELLES(For Continuous Internal Assessment Only):

Colloids: Distinction between suspension, colloidal solutions and true solutions – lyophilc and lyophobic colloids – Tyndall effect – stability of colloids – coagulation – emulsions – various types. Micelles: Surfactant (amphipathic molecules) – micellization - critical micelle concentration – size of micelle – aggregation number – Thermodynamics of micellization– reverse micelles.

## REFERENCES:


1. F. A. Cotton, Chemical Applications of Group Theory; 3rd Ed., John Wiley and Sons, Singapore, 2003.
2. R. L. Flurry, Jr, Symmetry Groups: Theory and Chemical Applications;

Prentice Hall, New Jersy, 1980.
3. S. F. A. Kettle, Symmetry and Structure; 2nd Ed., John Wiley and Sons, Chichester, 1995.
4. A.K. Chandra, Introductory Quantum Chemistry; 4th Ed., Tata McGraw Hill, Noida, 1994.
5. D. A. Mcquarrie, Quantum Chemistry; University Science Books, Sausalito, 2008.
6. I. N. Levine, Quantum Chemistry; 5th Ed., Prentice Hall, New Jersey, 2000.
7. R.K. Prasad, Quantum Chemistry; 4th Ed., New Age International Publishers, New Delhi, 2014.
8. K. J. Laidler, Chemical Kinetics; 3rd Ed., Tata McGraw Hill, Noida, 1987.
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13. K. S. Gupta, Chemical Kinetics and Reaction Mechanism; RBSA Publishers, Jaipur, India, 1992.
14. P. W. Atkins, Physical Chemistry; 7th Ed., Oxford University Press, Oxford, 2001.
15. J. Rajaram and J. C. Kuriacose, Thermodynamics for Students of Chemistry - Classical, Statistical and Irreversible; Pearson Education, New Delhi, 2013.
16. HoriaMetiu, Physical Chemistry, Thermodynamics; Taylor and Francis, Singapore, 2006.
17. K. K. Rohatgi-Mukherjee, Fundamentals of Photochemistry; 3rd Ed., New Age International Pvt. Ltd., New Delhi, 2014.
18. J. W. T. Spinks and R. J. Woods, Introduction to Radiation Chemistry; 3rd Ed., John Wiley and Sons, New York, 1990.

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**First Year** **CORE CHOICE COURSE I** **Semester I**

**2) BIO-PHYSICAL CHEMISTRY**

**Code:** **(Theory)** **Credit: 5**

**COURSE OBJECTIVES:**

- To understand the basic concepts of biological system via physical nature
- To learn the fundamental concepts of bioenergetics and biomolecules
- To study the concepts of biopolymers and its applications.

**UNIT – I BIOLOGICAL CELL AND ITS CONSTITUENT:**

Biological cell, structure and functions of proteins, enzymes, DNA and RNA in living systems. Helix coil transition. Bioenergetics - Standard free energy change in biochemical reactions, exergonic, endergonic. Hydrolysis of ATP, synthesis of ATP from ADP.

**UNIT – II STATISTICAL MECHANICS IN BIOPOLYMERS:**

Chain configuration of macromolecules, statistical distribution end to end dimensions, calculation of average dimensions for various chain structures. Polypeptide and protein structures, introduction to protein folding problem.

**UNIT – III BIOPOLYMER INTERACTIONS:**

Forces involved in biopolymer interactions. Electrostatic charges and molecular expansion, hydrophobic forces, dispersion force interactions. Multiple equilibria - Various types of binding processes in biological systems. Hydrogen ion titration curves.

**UNIT – IV THERMODYNAMICS OF BIOPOLYMER SOLUTIONS:**

Thermodynamics of biopolymer solutions, osmotic pressure, membrane equilibrium, muscular contraction and energy generation in mechanochemical system.

**UNIT – V CELL MEMBRANE AND TRANSPORT OF IONS:**

Structure and functions of cellmembrane, ion transport through cell membrane, irreversible thermodynamic treatment of membrane transport. Nerve conduction. Biopolymers and their Molecular Weights - Evaluation of size, shape, molecular weight and extent of hydration of biopolymers b various experimental techniques. Sedimentation equilibrium, hydrodynamic methods diffusion, sedimentation velocity, viscosity, electrophoresis and rotational motions.

**UNIT – VI BASIC MOLECULAR DYNAMICS(For Continuous Internal Assessment Only):**

Equations of motion – potential functions – integration computations – Initial state – boundary conditions – equilibration – dynamics protocols – trajectories –

analyses of results – AMBER, CHARM, -simple applications to proteins and nucleic acids Miscellaneous topics

**REFERENCES:**


1. Principles of Biochemistry, A. L. Lehninger,Worth Publishers.
2. Biochemistry, L.Stryer, W.H. Freeman.
3. Biochemistry, J.DavidRawn, Neil Patterson
4. Biochemistry, Voet and Voet, John Wiley Publication.
5. Outlines of Biochemistry, E. E. Conn and P. K. Stumpf, John Wileyub
6. Bioorganic Chemistry: A Chemical Approach to Enzyme Action, H. Dugasand C.Penny,Springer-verlag
7. Macromolecules: Structure and Function, F.World. Prentice Hall.


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**First Year** **CORE PRACTICAL I** **Semester I**

**INORGANIC CHEMISTRY PRACTICAL**

**Code:** **(Practical)** **Credit: 3**

**COURSE OBJECTIVES:**

- To perform the semi-micro qualitative analysis.
- To estimate the metal ions using colorimeter.
- To Prepare the coordination complexes

1. **Semi-micro qualitative analysis** of a mixture containing two common cations (Pb, Bi, Ca, Cd, Fe, Cr, Al, Co, Ni, Mn, Zn, Ba, Sr, Ca, Mg, $NH_4$) and two less common cations (W, Tl, Se, Te, Mo, Ce, Th, Zr, Ti, V, U, Li).

2. **Photoelectric colorimetric estimation** of copper, ferric, nickel, chromium and manganese ions

3. **Preparation of complexes**

    1. Tris(thiourea)copper(I) chloride
    2. Tetraamminecopper(II) sulphate
    3. Potassium trisoxalatoferrate
    4. Potassium trisoxalatoaluminate(III)
    5. Potassium trisoxalatochromate(III)
    6. Hexamminecobalt(III) chloride

**REFERENCES:**


1. V. V. Ramanujam, Inorganic Semimicro Qualitative Analysis; 3rd Ed., National Pubs, London, 1988.
2. G. Svehla, Text Book of Macro and Semimicro Qualitative Inorganic Analysis; 5thEd., Longman group Ltd, London, 1987.
3. A. I. Vogel, Text Book of Quantitative Inorganic Analysis;6th Ed., Longman, New Delhi, 2000.


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**First Year** **ELECTIVE COURSE I** **Semester I**

**1) ANALYTICAL CHEMISTRY**

**Code:** **(Theory)** **Credit: 4**

**COURSE OBJECTIVES:**

1. To learn the instrumental methods
2. To learn the nature of errors and their types.
3. To understand the various techniques in chromatography.
4. To understand the principles and instrumentation of thermoanalytical and fluorescence techniques.
5. To studying detail the electroanalytical techniques.

**UNIT – I INSTRUMENTAL METHODS OF ANALYSIS:**

Principles and applications of extended X-ray absorption fine structure (EXAFS) – surface extended X-ray absorption (SEXAFS) – atomic absorption spectroscopy (AAS) – flame emission spectroscopy (FES) – turbidimetry – theory and applications. Instrumentation and sampling techniques in UV-visible and IR spectroscopy.

**UNIT – II DATA AND ERROR ANALYSIS:**

Various types of error – accuracy, precision, significant figures – frequency distributions, the binomial distribution, the Poisson distribution and normal distribution – describing data, population and sample, mean, variance, standard deviation, way of quoting uncertainty, robust estimators, repeatability and reproducibility of measurements.

Hypothesis testing, levels of confidence and significance, test for an outlier, testing variances, means t-Test, paired t-Test – analysis of variance (ANOVA) – correlation and regression.

Curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals – general polynomial equation fitting, linearizing transformations, exponential function fit – r and its abuse – multiple linear regression analysis, elementary aspects.

**UNIT – III CHROMATOGRAPHY:**

Solvent extraction – principles of ion exchange, paper, thin-layer and column chromatography techniques – columns, adsorbents, methods, $R_f$ values, McReynold's constants and their uses – HPTLC, HPLC techniques – adsorbents, columns, detection methods, estimations, preparative column – GC-MS techniques – methods, principles and uses.

**UNIT – IV THERMOANALYTICAL METHODS AND FLUORESCENCE SPECTROSCOPY:**

Principles – instrumentations and applications of thermogravimetry analysis (TGA), Differential Thermal Analysis (DTA) and Differential Scanning Calorimetry (DSC) – thermometric titrations – types – advantages.

Basic aspects of synchronous fluorescence spectroscopy – spectral hole burning – flow cytometry – fluorometers (quantization) – instrumentation – applications.

**UNIT – V ELECTROANALYTICAL TECHNIQUES:**

Electrochemical sensors, ion-sensitive electrodes, glass – membrane electrodes, solid-liquid membrane electrodes – ion-selective field effect transistors (ISFETs) – sensors for the analysis of gases in solution.

Polarography – principles and instrumentation – dropping mercury electrode – advantages –Ilkovic equation – applications of polarography – polarographic maxima – oscillographic polarography, AC polarography – cyclic voltammetry – advantages over polarographic techniques – chronopotentiometry – advantages – controlled potential coulometry – amperometric titrations: principles – techniques – applications – estimation of lead.

**UNIT – VI TYPES OF TITRATIONS (For Continuous Internal Assessment Only):**

Redox titration: Redox potentials, theory and feasibility of redox titration, calculation of potentials at different stages of titrations, redox indicators, their choice and applications. Precipitation titrations: Theory and types, Mohr, Volhard and Fajan's methods. Adsorption indicators: theory, choice and applications. Complexometric titrations: Theory, Stepwise and overall formation constants, Titrations involving chelates (EDTA). Metallochromic indicators: Theory and Choice, Masking and demasking methods and applications.

**REFERENCES**


1. D. B. Hibbert and J. J. Gooding, Data Analysis for Chemistry; Oxford University Press, UK, 2006.
2. J. Topping, Errors of Observation and Their Treatment; 4th Ed., Chapman Hall, London, 1984.
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**First Year** **ELECTIVE COURSE I** **Semester I**

**2) SUPRAMOLECULAR CHEMISTRY**

**Code:** **(Theory)** **Credit: 4**

**OBJECTIVES**

- To know the fundamentals of supramolecules.
- To learn co-receptor molecules and multiple recognition
- To study the supramolecular reactivity and catalysis.

**UNIT – I CONCEPTS OF SUPRAMOLECULAR CHEMISTRY:**

Concepts and languages of supramolecular chemistry – various types of non-covalent interactions – hydrogen bonds, C-H···X interactions, halogen bonds – π-π interactions, non–bonded interactions – various types of molecular recognition.

Crystal engineering of organic solids – hydrogen bonded supramolecular patterns involving water / carboxyl / halide motifs – concepts of different types of synthons based on non-covalent interactions – principles of crystal engineering and non-covalent synthesis – polymorphism and pseudopolymorphism– supramolecular isomorphism / polymorphism – crystal engineering of pharmaceutical phases.

**UNIT – II METALLO ORGANIC FRAMEWORKS:**

M.O.F (Metallo Organic Frameworks) – organometallic systems – combinations of different interactions to design molecular rods, triangles, ladders, networks, etc. – design of nanoporous solids – interligand hydrogen bonds in metal complexes – implications for drug design – crystal engineering of NLO materials, OLED.

**UNIT – III CO-RECEPTOR MOLECULES AND MULTIPLE RECOGNITION:**

Dinuclear and polynuclear metal ion cryptates– linear recognition of molecular length by ditopic co-receptors – heterotopic co-receptors – cyclophane receptors, amphiphilic receptors and large molecular cages – multiple recognition in metalloreceptors– supramolecular dynamics.

**UNIT – IV 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, dendrimers, gelators– classification and typical reactions – applications.

**UNIT – V SUPRAMOLECULAR DEVICES:**

Supramolecular devices and sensors – various types of supramolecular devices – an overview – supramolecular photochemistry – molecular and

supramolecularphotonic devices – light conversion and energy transfer devices – molecular and supramolecular electronic devices – electronic conducting devices – molecular wires, modified and switchable molecular wires – molecular and supramolecular ionic devices – tubular mesophases, molecular protonics– switching devices – electro-photo switch – ion and molecule sensors – role of supramolecular chemistry in the development of nanoscience and technology.

**UNIT – VI BIOLOGICAL SUPRAMOLECULAR SYSTEMS(For Continuous Internal Assessment Only):**

Ionophores, Porphyrin and other TetrapyrrolicMacrocycles, Coenzymes, Neurotransmitters, DNA and Biochemical Self-assembly.SupramolecularreactivityBiomimetic systems and Artificial receptors:

(a) Cation Binding Hosts - Podand, Crown Ether, Cryptand, Spherand; Nomenclature, Selectivity and Solution Behaviour; Alkalides, Electrides, Calixarenes and Siderophores.
(b) Anion binding hosts - Challenges and Concepts, Biological Receptors, Conversion of Cation Hosts to Anion Hosts, Neutral Receptors, Metal-Containing Receptors, Cholapods.
(c) Ion Pair Receptors - Contact Ion Pairs, Cascade Complexes, Remote Anion and Cation Binding Sites, Symport and Metals Extraction.
(d) Hosts for Neutral Receptors -Clathrates, Inclusion Compounds, Zeolites, Intercalates, Coordination Polymers, Guest Binding by Cavitands and Cyclodextrins, cucurbituril.

**REFERENCES:**


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5. J. M. Lehn, Transition Metals in Supramolecular Chemistry; John Wiley and Sons: New York, 1999.
6. G. R. Desiraju, Current Science; 2001, 81, 1038.
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   (ii) Crystal Engineering Communication http://www.rsc.org/Publishing/Journals/ce/index.asp


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**First Year** **VALUE ADDED COURSE I** **Semester I**

**ENVIRONMENTAL CHEMISTRY**

**Code:** **(Theory)** **Credit: 2***

**COURSE OBJECTIVES:**

1. To know the fundamentals of various environment.
2. To study the Energy Resources, Ecosystem, Biodiversity and its Conservation.
3. To learn environment related social issues

**UNIT – I ENERGY AND ENVIRONMENT:**

Energy resources and their exploitation, Sun as the source of energy- nature of its radiation, Conventional energy sources: coal, oil, biomass and nature gas, nonconventional energy sources: hydroelectric power, tidal, wind, geothermal energy, solar collectors, photovoltaic, solar ponds, nuclear-fission and fusion, magnetohydrodynamic power (MHD), Energy use pattern in different parts of the world and its impact on the environment. $CO_2$ emission in atmosphere.

**UNIT – II ECOSYSTEM, BIODIVERSITY AND ITS CONSERVATION:**

Biodiversity concepts and patterns, microbial diversity, Plant diversity, agrobiodiversity, soil biodiversity, economic value of biodiversity, biodiversity losses. Biodiversity hotspots and their characteristic flora and fauna, threatened plants and animals of India, ecosystem people and traditional conservation mechanisms, Biodiversity Convention and Biodiversity Act, IPRs, national and international programmes for biodiversity conservation.

**UNIT – III ENERGY RESOURCES AND MAINTENANCE:**

Renewable and non-renewable energy resources, growing energy need, solar radiation and its spectral characteristics, fossil fuels classification, composition. Physicochemical characteristics and energy content of coal, petroleum and natural gas. Principle of generation and conservation of conventional and non-conventional energy. Energy from biomass and biogas, an aerobic digestion, energy use pattern and future need projection in different parts of the world, energy conservation policies.

**UNIT – IV SOLID AND HAZARDOUS WASTE MANAGEMENT:**

Solid wastes: Definition, types, sources, characteristics and impact on environmental health. Waste generation rates. Concepts of waste reduction, recycling and reuse. Collection, segregation and transport of solid wastes Handling and segregation of wastes at source. Collection and storage of municipal solid wastes.

Hazardous wastes: Definition, sources and characteristics: Hazardous waste categorization, generation, collection, transport, treatment and disposal. Legislation on management and handling of municipal solid wastes and hazardous wastes.

**UNIT – V SOCIAL ISSUES:**

Urban issues - energy - water conservation - environmental ethics - global warming resettlement and rehabilitation issues - environmental legislations – environmental protection Act. 1986 - Air, water, wildlife and forest conservation Act – Population growth and explosion - Human rights and value education - environmental health - HIV/AIDS - Role of IT in environment and human health - women and child welfare -public awareness.

**UNIT – VI MECHANISM OF RADIATION ACTION ON LIVING SYSTEMS(For Continuous Internal Assessment Only):**

Stochastic and Non-stochastic effects; delayed effects, radioactivity from nuclear reactors, fuel processing and radioactive waste, hazards related to power plants, terrestrial and non-terrestrial radiation, dose from environment and nuclear radiations, ultraviolet radiations, pathway analysis and dose assessment, radiologic age dating, radioactivity risk assessment, criterion for safe exposure. Wildlife values and eco-tourism, wildlife distribution in India, problem in wildlife protection, role of WWF, WCU, CITES, TRAFFIC, Wildlife Protection Act 1972. In-situ conservation: sanctuaries, biospheres reserves, national parks, nature reserves, preservation plots. Ex-situ conservation: botanical gardens, zoos, aquaria, homestead garden; herbarium; In-vitro Conservation: germplasm and gene Bank; tissue culture: pollen and spore back, DNA bank.

**REFERENCES:**


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2. Jadhav H.V (1992): Elements of Environmental Chemistry, Himalaya.
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**First Year** **CORE COURSE III** **Semester II**

**PHYSICAL CHEMISTRY II**

**Code:** **(Theory)** **Credit: 5**

**COURSE OBJECTIVES:**

- To study the applications of quantum chemistry and group theory.
- To acquire knowledge about various spectroscopic techniques.

**UNIT – I QUANTUM CHEMISTRY –APPLICATIONS:**

Applications of wave mechanics – the harmonic oscillator, rigid rotator – hydrogen and hydrogen like atoms – shapes and nodal properties of orbitals – space quantization – approximation methods – methods of variation, application to hydrogen and helium atoms – perturbation method – non- degenerate systems – helium atom – effective nuclear charge.

Electron spin – many electron atoms – Pauli's principle – Slater determinants – atomic structure calculation – self-consistent field method – Hartree-Fock method for atoms – angular momentum in many electron systems –vector atom model-spin-orbit interaction, L-S and j-j coupling schemes.

**UNIT – II MOLECULAR QUANTUM MECHANICS:**

Born-Oppenheimer approximation-MO and VB treatments of hydrogen molecule-comparison– hybridization, solving wave equation for sp, $sp^2$ and $sp^3$ hybrid orbitals – Huckel's molecular orbital theory and its application to ethylene and butadiene - charge density, pi-bond order and free valence.

Computational Quantum chemistry- ab initio calculations(elementary treatment only)-valence shell ionization potentials.

**UNIT – III SPECTROSCOPYI:**

Interaction of electromagnetic radiation with molecular systems – time evolution of the systems under radiation – Einstein transition probability for induced absorption and spontaneous and stimulated emission – absorption coeffients-transition moment and oscillator strength.

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

**UNIT – IV SPECTROSCOPYII:**

Infrared spectra – diatomic molecules, simple harmonic and anharmonic oscillators – diatomic vibrating rotator rotation – vibration spectrum of carbon monoxide – interaction of rotation and vibration (breakdown of Born-Oppenheimer approximation) – influence of the rotation on the spectrum of

polyatomic molecules, linear and symmetric top molecules, parallel and perpendicular vibrations – influence of nuclear spin.

Raman spectra - rotational Raman spectra of linear and symmetric top molecules – vibrational Raman spectra – rotational fine structure-polarization of light and Raman effect. Laser Raman spectroscopy- principle-applications.

**UNIT – V SPECTROSCOPY III:**

Electronic spectra of diatomic molecules- vibrational coarse structure – intensity of vibrational lines in electronic spectra – Franck-Condon principle-predissociation-rotational fine structure- Fortratdiagram.Electronic spectra of poly atomic molecules.

Photoelectron Spectroscopy: Basic Principles – Koopman's theorem – UPES, XPES (ESCA and Auger Spectroscopy) – valence and core binding analysis, examples and applications of ESCA with two examples.

**UNIT – VI FUNDAMENTAL CONCEPTS OF QUANTUM CHEMISTRY(For Continuous Internal Assessment Only):**

Preliminary mathematics; Fundamental concepts and problems in trigonometric - Exponential functions - Matrices Vector Algebra - Differential equations – Integrations - Legendre differential equations - Legendre and associated Legendre Polynomials - Hermite and Associated Laguerre polynomials - Orthogonal functions and Sturm-Liouville problems.

**REFERENCES:**


1. A.K. Chandra, Introductory Quantum Chemistry; 4th Ed., Tata McGraw Hill, Noida, 1994.
2. D. A. Mcquarrie, Quantum Chemistry; University Science Books, Herndon, 2008.
3. J. P. Lowe, and K. A. Peterson, Quantum Chemistry; 3rd Ed., Academic Press, Cambridge, 2005.
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7. C. N. Banwell, Fundamentals of Molecular Spectroscopy; 4th Ed., McGraw Hill Education, Noida, 1994.
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10. P.K. Ghosh, Introduction to Photoelectron Spectroscopy; John Wiley, New York, 1989
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13. Puri, Sharma & Pathania, Principles of Physical chemistry, Vishal Publishing Co, 46th edition.


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**First Year** **CORE COURSE IV** **Semester II**

**INORGANIC CHEMISTRY II**

**Code:** **(Theory)** **Credit: 5**

**COURSE OBJECTIVES:**

- To understand the role of metal ions in biological process.
- To learn the basic concepts of chemotherapy.
- To learn the fundamentals of organometallic compounds and catalysis.

**UNIT – I GENERAL PRINCIPLES OF BIOINORGANIC CHEMISTRY:**

Occurrence and availability of inorganic elements in biological systems – Porphyrin and corrin systems in biology- Vitamin B12 – Structure and function.

Function and transport of alkali and alkaline earth metal ions: characterization of $K^+$, $Na^+$, $Ca^{2+}$ and $Mg^{2+}$ – complexes of alkali and alkaline earth metal ions with macrocycles – ion channels – ion pumps, catalysis and regulation of bioenergetic processes by the alkaline earth metal ions – $Mg^{2+}$ and $Ca^{2+}$.

Metals at the center of photosynthesis – primary processes in photosynthesis – photosystems I and II-light absorption (energy acquisition) – exciton transport (direct energy transfer) – charge separation and electron transport – manganese catalyzed oxidation of water to $O_2$.

**UNIT – II HEME AND NON-HEME PROTEINS AND ENZYMES:**

Heme and non-heme proteins – haemoglobin and myoglobin – oxygen transport and storage – electron transfer and oxygen activation – cytochromes, ferredoxins and rubredoxin – model systems, mononuclear non-heme iron enzymes.

Copper containing proteins – classification and examples – electron transfer – oxygen transport-oxygenation – oxidases and reductases – cytochrome oxidase – superoxide dismutase (Cu, Zn) – nickel containing enzyme: urease.

**UNIT – III METALS IN MEDICINE:**

Bioinorganic chemistry of quintessentially toxic metals – lead, cadmium, mercury, aluminium, chromium, copper and plutonium – detoxification by metal chelation – drugs that act by binding at the metal sites of metalloenzymes.

Chemotherapy – chemotherapy with compounds of certain non-essential elements – platinum complexes in cancer therapy – cisplatin and its mode of action – cytotoxic compounds of other metals.

Gold containing drugs as anti-rheumatic agents and their mode of action – lithium in psychopharmacological drugs – radiopharmaceuticals – technetium.

**UNIT – IV ORGANOMETALLICS:**

Hapticity - The 18 electron rule – applications and limitations – preparation, properties, structure and bonding in metal carbonyls, metal nitrosyls – metal alkenes (Zeise salt)- metal alkyne – metallocene (Ferrocene)- metal arenes- dinitrogen complexes – fluxional molecules.Isolobal concept and its applications.

**UNIT – V CATALYSIS IN ORGANOMETALLICS:**

Organometallic reactions – ligand association and dissociation – oxidative addition and reductive elimination – insertion reactions- reactions of coordinated ligands.

Hydrogenation of olefins (Wilkinson's catalyst), hydroformylation(Oxo process), olefin oxidation (Wacker process) and carbonylation of methanol (acetic acid synthesis)- epoxidation of olefin, polymerization of olefins (Ziegler Natta catalyst)- olefin metathesis.

**UNIT – VI METAL DRUG, DISCOVERY AND DESIGN (For Continuous Internal Assessment Only):**

Drug discovery and design - Therapeutic index and chemotherapeutic index - Structure - activity relationship - Factors governing drug design - Computer aided drug design - Gold-based drugs -treatment of cancer and rheumatoid - mechanism of interaction. Lithium containing drugs- uses - mode of interaction - side effects. Silver based drugs - anti-bacterial - antifungal agent - anticancer agent. Bismuth containing drugs - the treatment of acidity and related diseases.

**REFERENCES:**


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**First Year** **CORE CHOICE COURSE II** **Semester II**

**1) ORGANIC CHEMISTRY II**

**Code:** **(Theory)** **Credit: 5**

**COURSE OBJECTIVES:**

- To understand the nucleophilic and electrophilic substitution reactions.
- To learn the addition and elimination reactions.
- To study a variety of heterocycles.
- To know the chemistry of terpenoids, steroids and alkaloids.

**UNIT – I NUCLEOPHILIC SUBSTITUTION REACTIONS:**

Aliphatic nucleophilicsubstitution – mechanisms – $S_N1$, $S_N2$, $S_Ni$ – ion-pair in $S_N1$ mechanisms – neighbouring group participation, non-classical carbocations – substitutions at allylic and vinylic carbons.

Reactivity – effect of structure, nucleophile, leaving group and stereochemical factors – correlation of structure with reactivity – solvent effects – rearrangements involving carbocations– Wagner-Meerwein and dienone-phenol rearrangements.

Aromatic nucleophilic substitutions – $S_N1$, $S_NAr$, Benzyne mechanism – reactivity orientation – Ullmann, Sandmeyer and Chichibabin reaction – rearrangements involving nucleophilic substitution – Stevens – Sommelet-Hauser and von-Richter rearrangements.

**UNIT – II ELECTROPHILIC SUBSTITUTION REACTIONS:**

Aromatic electrophilic substitution reaction – orientation, reactivity and mechanisms based on transition state theory with suitable reactions – substitutions in thiophene and pyridine – N-oxide – quantitative treatment of the structural effects on reactivity.

Substituent effects – origins of Hammett equation – principles of Hammett correlation – effect of structure on reaction mechanisms Hammett parameters – $\sigma$and $\rho$, modified forms of Hammett equation, Taft Equation.

Aliphatic electrophilic substitution – $S_E2$, $S_Ei$ and $S_E1$mechanisms – diazonium coupling reactions – metals as electrophile in substitution reactions and decomposition of diazonium salts.

**UNIT – III ADDITION AND ELIMINATION REACTIONS:**

Addition to carbon-carbon multiple bonds – electrophilic, nucleophilic and free radical additions – orientation of the addition – stereochemical factors influencing the addition of bromine and hydrogen bromide, hydroxylation, 1,2-dihydroxylation – hydroboration leading to formation of alcohols – oxidation and ozonolysis.

Addition to carbonyl and conjugated carbonyl systems – mechanism – Grignard reagents – 1,2- and 1,4-additions (lithium dimethylcuprate) – addition to carbon-

oxygen double bond – Benzoin, Knoevenagel, Stobbe, Darzensglycidic ester condensation and Reformatsky reactions.

Elimination reactions – mechanisms; E1, E2, E1cB – stereochemistry of elimination, Hofmann's and Zaitsev's rules – competition between elimination and substitution – pyrolytic*cis*-elimination, Chugaev reaction – examples such as dehydration, dehydrohalogenation, Hofmann degradation, Cope elimination – Bredt's rule with examples.

**UNIT – IV HETEROCYCLES:**

Non-aromatic heterocycles– synthesis of tetrahydrofurans – pyrrolidines – tetrahydropyrans – piperidines.

Synthesis of heterocycles: aziridines – oxiranes – thiiranes – azetidines – oxetanes – oxazoles – imidazoles – thiazoles.

Synthesis and reactivity of aromatic heterocycles: pyrazoles – isothiazoles – triazoles – pyrimidines – purines – triazines–pyrazines.

**UNIT – V NATURAL PRODUCTS:**

Terpenoids:Introduction – biosynthesis of menthol, camphor – total synthesis: Takasago synthesis of menthol, Corey's synthesis of longifolene, Curran's synthesis of hirsutene.

Steroids:Introduction – partial synthesis of androsterone and testosterone (from Cholesterol) – total synthesis: Johnson's synthesis of progesterone and Vollhardt's synthesis of estrone.

Alkaloids: Introduction – biosynthesis of nicotine, camptothecin – total synthesis: Corey's synthesis of epibatidine, Comin's asymmetric synthesis of Camptothecin and Woodward's synthesis of reserpine.

**UNIT – VI PLANT PIGMENTS, PROSTAGLANDINS, PYRETHOIDS, ROTENONES AND PHEROMONES(For Continuous Internal Assessment Only):**

Occurrence, nomenclature and general methods of structure determination of Anthocyanidins.Synthesis of Cyanidin Chloride, Chalcones, Flavones, Quercetin.Occurrence, classification.Biogenesis, physiological effects and synthesis of PGE2 and PGF2z. Natural and synthetic of pyrethroids, Rotenones and pheromones.Synthesis of bombykol.

**REFERENCES**


1. S. H. Pine and J. B. Hendrickson, D. J. Cram and G. S. Hammond, Organic Chemistry; 5th Ed., McGraw Hill, Noida, 1987.
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**First Year** **CORE CHOICE COURSE II** **Semester II**

**2) BIO-ORGANIC CHEMISTRY**

**Code:** **(Theory)** **Credit: 5**

**COURSE OBJECTIVES:**

- To learn the preparation, properties of amino acids and proteins.
- To study the activity of enzymes and cofactors.
- To know basics of lipids and nucleic acids.
- To learn the concept of bioenergetics.
- To learn the principles of lead and analogue synthesis.

**UNIT – I AMINO ACIDS AND PROTEINS:**

Structure, classification, synthesis and properties of amino acids – biosynthesis of amino acids – peptides – N-terminal and C-terminal residue analysis – solid phase peptide synthesis.

Proteins – classification and properties (denaturation, isoelectric point and electrophoresis), primary, secondary, tertiary and quaternary structures of proteins – biological roles of proteins.

**UNIT – II ENZYMES AND COFACTORS:**

Chemical nature of enzymes – characteristics of enzymes – colloidal nature, catalytic nature.

Mechanism of enzymes – Michaelis-Menten hypothesis – Fischer's lock and key model – regulation of enzyme activity.

Structure and biological functions of coenzyme A, NAD+, FAD and vitamin B12.

**UNIT – III LIPIDS AND NUCLEIC ACIDS:**

Lipids – definition – simple lipids – fats and oils – compound lipids – phospholipids, glycolipids – physical properties – solubility, melting point, surface tension, emulsification and geometric isomerism – chemical properties – reaction involving -COOH group, -OH group and double bonds.

Nucleic Acid – definition – nucleosides and nucleotides – deoxyribonucleic acid (DNA) – internucleotides linkages – base composition – double helical structure.

**UNIT – IV BIOENERGETICS:**

Concept of energy – thermodynamic principles – first law, second law, combining the two laws – relationship between standard free energy change and equilibrium constant.

Standard free energy values of chemical reactions – Adenosine triphosphate (ATP) as universal currency of free energy in biological systems – ATP hydrolysis and equilibria of coupled reactions – inter conversion of adenine nucleotides.

**UNIT – V LEAD AND ANALOGUE SYNTHESIS:**

Designing organic synthesis – disconnection approach – synthons and synthetic equivalents – one group disconnections: alcohol, acid and ketone – functional group interconversions.

Asymmetric synthesis – basic principles – stereoselective and stereospecific reactions – reagents, catalysts and their applications (wherever applicable) in alkylation and hydrogenation – Jacobsen's catalyst – Evan's catalyst.

**UNIT – VI BIOORGANIC REACTIONS (For Continuous Internal Assessment Only):**

Timing of Bond formation and fission – Acyl group transfer – C-C bond formation and fission – Catalysis of proton transfer reactions – Transfer of hydride ion – Alkyl group. Transfer – Terpene biosynthesis – Merrifield state peptide synthesis – Sanger method for peptide and DNA sequencing

**REFERENCES:**


1. J. L. Jain, Fundamentals of Biochemistry; S. Chand and Co., New Delhi, 2007 [Unit- I, II, III, IV].
2. N. C. Price and L. Stevens, Fundamental of Enzymology; Oxford University Press, UK, 1999 [Unit-II].
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4. S. Warren, Designing Organic Synthesis: The Disconnection Approach; 2nd Ed., Wiley, New York, 2008 [Unit-V].
5. H. B. Kagan, Asymmetric Synthesis; Thieme Medical Publishers, Germany, 2009 [Unit – V].


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**First Year** **CORE PRACTICAL II** **Semester II**

**ORGANIC CHEMISTRY PRACTICAL I**

**Code:** **(Practical)** **Credit: 3**

**COURSE OBJECTIVES:**

- To perform the qualitative analysis of a given organic mixture.
- To estimate the organic compounds

**1. Qualitative analysis of an organic mixture containing two components (Separation followed by analysis of any one component)**

Mixtures containing two components are to be separated (pilot separation) and purified (bulk separation) – The physical constants are to be reported (analysis).

**2. Quantitative analysis of organic compounds**

Estimation of phenol, aniline, ketone and glucose.

**REFERENCES:**


1. J. Mohan, Organic Analytical Chemistry: Theory and Practice; Narosa, 2003.
2. V. K. Ahluwalia, P. Bhagat, and R. Agarwal, Laboratory Techniques in Organic Chemistry; I. K. International, 2005.
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**First Year** **ELECTIVE COURSE II** **Semester II**

**1) SOLID STATE CHEMISTRY**

**Code:** **(Theory)** **Credit: 4**

**COURSE OBJECTIVES:**

- To learn the band theory and defects of solids.
- To study the preparative methods and solid state reactions.
- To learn the applications of thermal and magnetic materials.
- To study the chemistry of organic solids and metal-organic frame work.

**UNIT – I THEORY OF SOLIDS AND CRYSTAL DEFECTS:**

Metallic state - free electron and band theories- Metals, insulators and semiconductors, electronic structure of solid-band theory, band structure of metals, insulators and semiconductor, intrinsic and extrinsic semiconductors, n- and p-type- doping semiconductor, p-n-junction, super conductors-general applications.

Defects in solids: Stoichiometry-Schotty defects and Frenkel defects - non-Stoichiometry defects- dislocations in solids-line-point defects.

**UNIT – II PREPARATIVE METHODS AND SOLID STATE REACTIONS:**

Preparative methods: Chemical Precursor methods, co-precipitation, sol-gel metathesis, self-propagating high temperature synthesis, ion exchange reactions, intercalation/deintercalation reactions; hydrothermal and template synthesis, high pressure synthesis. Types of solid state reactions (Solid-solid, solid-liquid, solid-gas)

**UNIT – III THERMAL AND MAGNETIC PROPERTIES OF SOLIDS:**

Electronic specific heat, lattice heat capacity, Hall effect, Einstein theory, Debye theory, Born's modification of the Debye theory - thermoelectric effects , Thomson, Peltier, Seeback.

Origin and classifications of magnetic substance, magnetic moment, ferromagnetic, antiferromagentic and ferromagnetic ordering, magnetic susceptibility, Curie and Cuire-Weiss law, super exchange, magnetic domains, and hysteresis.

**UNIT – IV ORGANIC SOLID STATE CHEMISTRY:**

Topochemical control of solid state organic reactions – intramolecular reactions – conformational effects – intermolecular reactions – molecular packing effects – photodimerization of 2-ethoxycinnamic acid (α form, β form, γ form) – photopolymerization of 2,5-distyrylpyrazine – photopolymerizations of diacetylenes.

Organic reactions within inorganic host structures – electrically conductive organic solids – organic metals, conjugated systems, doped polyacetylene, polyparaphenylene, polypyrrole – organic charge transfer complexes.

**UNIT – V METALLO ORGANIC FRAMEWORKS:**

M.O.Fs (Metallo Organic Frameworks) – organometallic systems – combinations of different interactions to design molecular rods, triangles, ladders, networks, etc. Design of nanoporous solids.

Interligand hydrogen bonds in metal complexes – implications for drug design – crystal engineering of NLO and OLED materials.

**UNIT – VI CRYSTAL ENGINEERING OF ORGANIC SOLIDS(For Continuous Internal Assessment Only):**

Hydrogen bonded supramolecular patterns involving water / carboxyl / halide motifs – concepts of different types of synthons based on non-covalent interactions – principles of crystal engineering and non-covalent synthesis – polymorphism and pseudopolymorphism – supramolecular isomorphism, polymorphism and crystal engineering of pharmaceutical phases.

**REFERENCES:**


1. A. R. West, Solid State Chemistry and Its Applications; 2nd Ed., John Wiley and sons, New York, 2014 (Unit III – V).
2. J. M. Lehn, Supramolecular Chemistry; VCH, Weinheim, 1995.
3. G. R. Desiraju, Crystal Engineering: The Design of Organic Solids; Elsevier, Amsterdam, 1989.
4. G. R. Desiraju, and T. Steiner, The Weak Hydrogen Bond in Structural Chemistry and Biology; Oxford University Press: Oxford, 2002.
5. G. A. Jeffrey, Introduction to Hydrogen Bonding; Oxford University Press, New York, 1997.
6. J. M. Lehn, Transition Metals in Supramolecular Chemistry; Vol 5, John Wiley and Sons, New York, 1999.
7. C. N. R. Rao, Current Science, 2001, 81, 1030.
8. Journals:
   (i) Crystal Growth and Design
   http://www.pubs.acs.org/journals/cgdefu/index.html
   (ii) Crystal Engineering Communication, http://www.rsc.org/Publishing/ Journals /ce/ ind


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**First Year** **ELECTIVE COURSE II** **Semester II**

**2) PHARMACEUTICAL CHEMISTRY**

**Code:** **(Theory)** **Credit: 4**

**COURSE OBJECTIVES:**

- To understand the basics of pharmaceutical chemistry.
- To study the antibiotics and their activity.
- To learn the analgesic and antipyretic activities.
- To know the activities of anaesthetics and local anaesthetics.
- To understand concept of clinical chemistry.

**UNIT – I BASICS OF PHARMACEUTICAL CHEMISTRY:**

Definitions – the terms – drugs, pharmacology, pharmacy, chemotherapy, therapeutics – pharmacologically active principles in plants – first aid – important rules of first aids, cuts, fractures, bleeding for blood, maintaining breathing burns and first aid box – tuberculosis (T.B.), jaundice, piles, typhoid, malaria, cholera – causes – symptoms, diagnosis – prevention and treatment – medicinally important compounds of iron – ferrous gluconate, ferrous sulphate and ferric ammonium citrate.

**UNIT – II ANTIBIOTICS:**

Definition – introduction – classification and biological actions – penicillin, chloramphenicol, streptomycin and tetracycline – structure, properties and therapeutic uses – chemical structure and pharmacological activity – effect of unsaturation, chain length, isomerism, halogens, amino groups, hydroxyl groups and acid groups.

**UNIT – III ANALGESIC AND ANTIPYRETICS:**

Narcotic analgesic – analgesic action of morphine – derivatives of morphine – heroin and apomorphine – synthetic analgesics – pethidine, methadone – non-narcotic analgesic – aspirin, paracetamol and phenacetin – analgin – preparation, properties and uses – ibuprofen and ketoprofen – structure and uses.

**UNIT – IV ANAESTHETICS AND LOCAL ANAESTHETICS:**

Characteristics of anaesthetics – classification of anaesthetics – general anaesthetics – volatile anaesthetics – ether, chloroform and halothane – advantages and disadvantages – non-volatile anaesthetics (intravenous anaesthetics) – methohexitone and propanidid – structure and uses – cocaine and amethocaine – structure and uses – benzocaine and procaine – structure, synthesis and uses.

**UNIT – V CLINICAL CHEMISTRY:**

Determination of sugar (glucose) in serum – *o*-toluidine method – diagnostic test for sugar in urine – Benedict's test – detection of diabetes – detection of

cholesterol in urine – detection of anaemia – estimation of haemoglobin (Hb concentration) – red cell count.

**UNIT – VI MOLECULAR MODELING AND COMPUTER AIDED DRUG DESIGN(For Continuous Internal Assessment Only):**

Basic features of molecular modeling, Molecular mechanics, *Ab initio*, DFT and semi-empirical methods-Energy minimization; Local and global energy minima, saddle point-Force fields, Monto Carlo simulation; Molecular docking- Molecular Dynamics; Introduction, basic principles, Mechanics and dynamics of Bio-macromolecules.

**REFERENCES:**


1. Jayashree Ghosh, AText Book of Pharmaceutical Chemistry; 5th Ed., S. Chand and Company Ltd., New Delhi, 2014.
2. S. Lakshmi; Pharmaceutical Chemistry; 1st Ed., S. Chand and Company Ltd., New Delhi, 1995.
3. Bhagavathi Sundari; Applied Chemistry; 1st Ed., MJP Publishers, Chennai, 2006.


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**First Year** **NON MAJOR ELECTIVE COURSE I** **Semester II**

**CHEMISTRY OF POLLUTION, FOOD AND COSMETICS**

**Code:** **(Theory)** **Credit: 2**

**COURSE OBJECTIVES:**

- To understand the principles of Green chemistry.
- To learn the various pollutions affecting the environment.
- To acquire basic knowledge about chemistry of food and cosmetics.

**UNIT – I AIR POLLUTION:**

Air- Introduction- Definition- Composition of air- Air pollution-Definition-Air pollutants-Types of Air pollution - Causes of Air pollution on human health-Prevention of Air pollution

**UNIT – II WATER POLLUTION:**

Water-Introduction-Definition-Sources of water-Types of water-Water quality parameters-Water pollution- Definition-Types of Water pollution- Causes of Water pollution on human health-Prevention of Water pollution.

**UNIT – III SOIL POLLUTION:**

Soil quality standards, monitoring and analysis of selected soil contaminants: pesticides, heavy metals, POP's, fluoride, cyanide, nitrate, phosphate, oil & grease, Geobiochemical impact of municipal solid waste, steel plants effluent, domestic sewage.

**UNIT – IV FOOD CHEMISTRY:**

Introduction to general Constituents of food, Proximate Constituents and their analysis, Additives- Introduction -Types - Study of preservatives colors and Antioxidants and method of estimation, adulteration - Introduction, Types, Test for adulterants.

Introduction of standards composition and analysis of following foods: Wheat, Bread, Biscuits, Jam, Jelly, Honey, Milk, Ice Cream, Butter, Cheese, Milk Powder, Oils and Fats, Tea, Coffee, Soft drinks, Alcoholic beverages, Cereal and pulses, Confectionery, Fruits, Vegetables, Egg, Fish, Meat.

**UNIT – V COSMETICS:**

Introduction of Cosmetics, evaluation of cosmetics materials, raw material and additives, Cosmetics colors, Perfumes in cosmetics, Cosmetics formulating, introduction, standards and methods of analysis, Creams, Face powders, Make-up, Shaving preparations, Bath preparations.

**UNIT – VI NOISE POLLUTION (For Continuous Internal Assessment Only):**

Noise pollution: Basics of acoustics and specification of sound; sound power, sound intensity and sound pressure levels; plane, point and line sources, multiple sources; outdoor and indoor noise propagation; psychoacoustics and noise criteria, effects of noise on health, annoyance rating schemes; special noise environments: Infrasound, ultrasound, impulsive sound and sonic boom; noise standards and limit values; noise instrumentation and monitoring procedure. Noise indices.Noise control methods.

**REFERENCES:**


1. Environmental Chemistry, S.E. Manahan, Lewis Publishers.
2. Environmental chemistry, Sharma and Kaur, Krishna Publishers.
3. Environmental Chemistry, A.K. De, Wiley Eastern.
4. Environmental Chemistry, Analysis, S.M. Khopkar, Wiley Eastern.
5. Standard Method of Chemical Analysis, F.J. Welcher Vol. III, Van Nostr and ReinholdCo.
6. Environmental Toxicology, Ed.J. Rose, Gordon and Breach Science Publication.
7. Environmental Chemistry, C. Baird, W.H. Freeman.
8. Analytical chemistry, G.D. Christian, J. Wiley.
9. Fundamentals of Analytical Chemistry, D.A.Skoog, D.m. Westand F.J. Holler, W.B. Saunders.
10. Analytical Chemistry - Principles, J.H. Kennedy, W. Saunders.
11. Analytical Chemistry-Principles, and Techniques, L.G. Hargis, Prentice Hall.
12. Principles of Instrumental Analysis, D.A. Skoog and J.L. Loary, W.B. Saunders.
13. Principles of Instrumental Analysis, D.A. Skoog, W.B. Saunders.
14. Quantitative Analysis, R.A. Day, Jr. and A.L. Underwood, Prentice Hall.
15. Environmental Solution Analysis, S.M. Khopkar, Wiley Eastern. Basic Concepts of Analytical Chemistry, S.M. Khopkar, Wiley Eastern.
16. Handbook of Instrumental Techniques for Analytical Chemistry, F. Settle, Prentice Hall.
17. Environmental Biotechnology, Indushekhar Thakur, I.K. International Pvt. Ltd.
18. Fundamental of Analytical Chemistry D.A. Skoog, D.m. West, F.J. Holler and S.R. Crouch, Thompson Learning Inc.
19. APHA, 1977, “Methods of air c Health Sampling Association Washingtonand – Analysis US.


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| Second Year | CORE COURSE V<br>ORGANIC CHEMISTRY III | Semester III |
|---|---|---|
| Code | (Theory) | Credit: 5 |

**COURSE OBJECTIVES:**

- To learn the Photochemistry and Pericyclic reactions
- To apply the various spectroscopic techniques of organic compounds
- To understand the Retro synthetic analysis and strategy.

**UNIT – I ORGANIC PHOTOCHEMISTRY:**

Fundamental concepts- Jablonski diagram- energy transfer- characteristics of photo reactions-photo oxidation-photo reduction- photo reactions of ketones and enones- Norrish type I and II- reactions- photo-chemistry of alkenes, dienes and aromatic compounds- photosensitization- photo additions- Barton reaction- PatternoBuchi reaction. Photo-Fries rearrangement –Zimmerman's di-π-methane rearrangement.

**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- sigmatropic rearrangements- selection rules with examples- 1,3 and 1,5 hydrogen shifts- Cope and Claisen rearrangements.

**UNIT – III ULTRAVIOLET AND VISIBLE SPECTROSCOPY & INFRARED SPECTROSCOPY:**

**Ultraviolet and visible Spectroscopy:** Basic principles of electronic transitions- correlation of energy change with electronic transitions- Applications of UV- visible spectroscopy- Woodward Fischer Scott rules- applications to conjucateddienes, trienes and polyenes- unsaturated carbonyl compounds- conjugated cyclic ketones- actophenones – benzene and its substituted derivatives- other aromatic hydrocarbons- heterocyclic systems- differentiation of position isomers- stereo-chemical factors affecting electronic spectra of biphenyl and binaphthyls- cis trans isomers- angular distortion- cross conjugation.

**Infrared Spectroscopy:** Factors influencing group frequencies- quantitative studies- finger print region - identification of functional groups- hydrogen bonding, intermolecular and intra molecular- solvent effect on vibrational frequencies.

**UNIT – IV NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY:**

$^{1}H$ NMR Spectroscopy – multiplicity – coupling constants – spin-spin splitting – vicinal and geminal coupling constants – Karplus equation – long range coupling constants, influence of stereochemical factors on chemical shift of protons.

Simplification of complex spectra – double resonance techniques, shifts reagents – chemical spin decoupling of rapidly exchangeable protons (OH, SH, COOH, NH, $NH_2$) – an elementary treatment of NOE phenomenon.

$^{13}C$ NMR Spectroscopy – broad band decoupling – off resonance decoupling – chemical shifts of common functional groups – FT NMR and its importance– DEPT spectra – identification of small compounds based on NMR data – 2D techniques: $^{1}H$–$^{1}H$ COSY, $^{1}H$–$^{13}C$ HETCOR – NOESY-Heteronuclear Multiple Bond correlation(HMBC).

**UNIT – V ORD,CD& MASS SPECTROMETRY:**

ORD& CD: Optical rotatory dispersion and circular dichroism – introduction to theory and terminology – cotton effect – ORD curves – axial haloketone rule and its applications – the octant rule –applications of ORD to determine absolute configuration of monocyclic ketones.

Mass Spectrometry: Resolution – ESI, EI, CI and FAB methods – base peak, isotopic peaks, metastable peaks – importance of metastable peaks, parent peak, recognition of molecular ion peak – fragmentation – general rules – pattern of fragmentation for various classes of compounds, McLafferty rearrangement – nitrogen rule.

Application of UV, IR, NMR and mass spectroscopy – structural elucidation of organic compounds – (minimum 15 problems should be worked out).

**UNIT – VI PHOTOCHEMISTRY OF ALKENES, KETONES AND AROMATIC COMPOUNDS (For Continuous Internal Assessment Only):**

Olefin photochemistry - conjugated olefins - Isomerisation and rearrangements - cis-trans isomerisation - valence isomerisation - rearrangement of 1,4 and 1,5 dienes - di- pi methane rearrangement - Cope and Claisen rearrangement - cycloaddition reactions - Photochemistry of Aromatic compounds - Arene photo isomerisation – Photo dimerization - Cycloaddition reactions – 1,2 cycloadditions – Photo oxygenation - ene reaction. Photo reduction - oxetane formation – Reactivity of π-π* excited ketones – Photochemistry of α, β- unsaturated ketones - dienone phenol photo rearrangement.

**REFERENCES:**


1. J. D. Coyle, Organic Photochemistry; Wiley, New York, 1998.
2. J. M. Coxon, and B. Halton, Organic Photochemistry; 2nd Ed., Cambridge, University Press, UK, 1987.
3. G. R. Chatwal, Organic Phtochemistry; 1st Ed., Himalaya Publications house, Bangalore, 1998.
4. S. Sankararaman, Pericyclic Reactions – A Textbook: Reactions, Applications and Theory; Wiley-VCH, New York, 2005.
5. P. M. Silverstein and F. X. Western, Spectroscopic Identification of Organic Compounds; 8th Ed., John Wiley, New York, 2014.
6. W. Kemp, Organic Spectroscopy; 3rd Ed., Palgrave, New York, 1991.
7. J. R. Dyer, Applications of Absorption Spectroscopy of Organic Compounds, PHI Learning, New Delhi, 2009.
8. Y. R. Sharma, Elementary Organic Spectroscopy – Principles and Chemical applications; S. Chand, New Delhi, 1992.
9. P. S. Kalsi, Spectroscopy of Organic Compounds; 6th Ed., New Age International Publishers, New Delhi, 2004.


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| Second Year | CORE COURSE VI<br>PHYSICAL CHEMISTRY III | Semester III |
|---|---|---|
| Code | (Theory) | Credit: 5 |

**COURSE OBJECTIVES:**

- To learn about the Electrochemistry
- To acquire knowledge about kinetics, surface Phenomena and catalysis
- To understand Classical Thermodynamics**.**

**UNIT – I ELECTRO CHEMISTRY I:**

Ion transport in solution – migration, convection and diffusion – Fick's laws of diffusion conduction – Debye-Huckel theory – ionic atmosphere – Debye- Huckel-Onsager equation – verification and extension – Debye-Falkenhagen effect and Wien effect, Debye-Huckel limiting law – activity coefficients and ionic strength – Bjerrum model.

The electrode – electrolyte interface – electrical double layer and multi layers – theories – electrocapillary curves – Lipmann equation and Lipmann potential-structure of semiconductor interface-Garrett-Brattain space charge model.

Electrokinetic phenomena -classification – Tiselius method of separation of proteins — electrocatalysis.

**UNIT – II ELECTROCHEMISTRYII:**

Dynamics of electron transfer – Marcus theory – tunneling – the rate of charge transfer – current density – Butler-Volmer equation – Taft equation –Polarization and overvoltage – mechanism of hydrogen evolution and oxygen evolution reactions.

Principles of electrode position of metals – corrosion and passivity – Pourbaix and Evans diagrams – methods of protection of metals from corrosion.

Power storage systems – fuel cells – construction and functioning – applications– photovoltaic cells.

**UNIT – III CHEMICAL KINETICSII:**

Factors determining reaction rates in solution- Transition state theory- influence of internal pressure- influence of solvation-reaction between ions-influence of solvent dielectric constant- single sphere activated complex-influence of ionic strength(Bronsted-Bjerrum equation)-primary and secondary salt effects.

Influence of hydrostatic pressure—Vant Hoff's equation—volume of activation.

Substituent and correlation effects-Hammett equation-LFER-Compensation effects-Taft equation- diffusion controlled reactions (full microscopic diffusion control).

**UNIT – IV SURFACE PHENOMENA AND CATALYSIS:**

Adsorption of gases on solids – Langmuir theory-BET theory of multilayer adsorption-derivation of BET equation-surface area determination-adsorption from solutions-Gibbs adsorption isotherm – solid-liquid interfaces – contact angle and wetting.

Homogeneous catalysis---General catalytic mechanism-Equilibrium and steady state treatments-acid-base catalysis-protolytic and prototropic mechanisms-Brønsted relations- Acidity functions.

Heterogeneous catalysis—role of surface-semiconductor catalysis-Kinetics of heterogeneous catalysis-- Langmuir- Hinshelwood mechanism, Langmuir-Rideal mechanism – Rideal-Eley mechanism.

Surfactants-micelle formation-CMC-Micellar catalysis.

**UNIT – V CLASSICAL THERMODYNAMICS:**

Third law – thermodynamics – significance – Nernst heat theorem and other forms of stating the third law – thermodynamic quantities at absolute zero – apparent exceptions to the third law.

Thermodynamics of systems of variable composition – partial molar properties chemical potential–Gibbs-Duhem equation and its applications (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.

Phase rule - Application of phase rule to the three component systems - systems of three liquids - solid-liquid system (Eutectic systems - two salts and water).

**UNIT – VI ELECTROCHEMISTRY III (For Continuous Internal Assessment Only):**

Electrochemical Cells: Electromotive force - measurement of EMF - the potentiometer - the electrochemical potential - the cell EMF and the cell reaction - reversible cells - types of half cells - classification of cells - the standard EMF of a cell - standard electrode potentials - calculation of the EMF of a cell - Nernst equation and its limitations - calculation of solubility products - standard free energies and entropies of aqueous ions - electrode concentration cells - electrolyte concentration cells - cells with liquid junctions - oxidation - reduction reactions, measurement of pH, concentration cells with transference – Electrochemical energy systems - Li-ion batteries-Methanol Fuel cells.

**REFERENCES:**


1. S. Glasstone, Introduction to Electrochemistry; Maurice Press, Philadelphia, 2008.
2. L. Antropov, Theoretical Electrochemistry; University Press of the Pacific, USA, 2001.
3. S. Glasstone, An Introduction to Electrochemistry; Read Books, New Delhi, 2007.
4. J. O'M Bockris and A. K. N. Reddy, Modern Electrochemistry; Vol. 1 and 2, 2nd Ed., Plenum Press, New York, 1998.
5. K. J. Laidler, Chemical Kinetics; 3rd Ed., Prentice Hall, New Jersey, 1987.
6. J. W. Moore and R. G. Pearson, Kinetics and Mechanism; 3rd Ed., John Wiley and Sons, New York, 1981.
7. M. Mortimer and P. G. Taylor, Chemical Kinetics and Mechanism; 1st Ed., Royal Society of Chemistry, UK, 2002.
8. Amdur and G. G. Hammes, Chemical Kinetics Principles and Selected Topics; 3rd Ed., McGraw Hill, New York, 2008.
9. R. G. Compton, Electrode Kinetics: Reactions; Elsevier Science Press, Chennai, 1987.
10. M.Gratzel and K. Kalyanasundaram, Kinetics and Catalysisin Microheterogeneous Systems; Academic Press, New York, 1991.
11. J. Rajaram and J. C. Kuriacose, Thermodynamics for Students of Chemistry - Classical, Statistical and Irreversible; Pearson Education, New Delhi, 2013.
12. R. K. Dave, Chemical Kinetics; Campus Books, 2000.
13. S. Glasstone, Thermodynamics for Chemists; 3rd Ed., Narahari Press, Bangalore, 2007.
14. Puri, Sharma & Pathania, Principles of Physical chemistry, Vishal Publish in Co, 46th edition.


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**Second Year** **CORE CHOICE COURSE III** **Semester III**

**1) INORGANIC CHEMISTRY III**

**Code** **(Theory)** **Credit: 5**

**COURSE OBJECTIVES:**

- To educate students on electronic and Raman spectroscopy.
- To acquire knowledge in NMR,EPR and NQR spectroscopy

**UNIT – I ELECTRONIC SPECTROSCOPY:**

Microstates, terms and energy levels for d1 – d9 ions in cubic and square fields intensity of bands – group theoretical approach to selection rules – effect of distortion and spin-orbit coupling on spectra – evaluation of 10Dq and β for octahedral complexes of cobalt and nickel – applications to simple coordination compounds – charge transfer spectra – electronic spectra of $[Ru(bipy)_3]^{2+}$.

**UNIT – II INFRARED AND RAMAN SPECTROSCOPY:**

Vibrations in simple molecules ($H_2O$, $CO_2$) and their symmetry notation for molecular vibrations – group vibrations and the limitations – combined uses of IR and Raman spectroscopy in the structural elucidation of simple molecules like $N_2O$, $ClF_3$, $NO^{3-}$, $ClO^{4-}$ effect of coordination on ligand vibrations – uses of groups vibrations in the structural elucidation of metal complexes of urea, thiourea, cyanide, thiocyanate and dimethyl sulfoxide.

Effect of isotopic substitution on the vibrational spectra of molecules – vibrational spectra of metal carbonyls with reference to the nature of bonding – applications of Raman spectroscopy – Combined application of Raman and IR spectroscopy in inorganic small molecules.

**UNIT - III NMR SPECTROSCOPY:**

Examples for different spin systems – chemical shifts and coupling constants (spin-spin coupling) involving different nuclei ($^1H$, $^{19}F$, $^{31}P$, $^{13}C$) interpretation and applications to inorganic compounds – Effect of quadrupolarnuclei ($^2H$, $^{10}B$, $^{11}B$) on the $^1H$ NMR spectra-Systems with chemical exchange-kinetic and thermodynamic parameters from NMR- satellite spectra – study of fluxional behaviour of molecules – NMR of paramagnetic molecules – isotropic shifts contact and pseudo-contact interactions – lanthanide shift reagents.

**UNIT – IV EPR SPECTROSCOPY:**

Theory of EPR spectroscopy – Isotropic and anisotropic system- Hyperfine splitting (methyl, p-benzosemiquinone, naphthalene radical )-spin densities and McConnell relationship –g values ($g^{\perp}$ and $g_{\parallel}$)- factors affecting the magnitude of g and A tensors in metal species – Zero-field splitting and Kramers degeneracy – spectra of V(II), Mn(II), Fe(II), Co(II), Ni(II) and Cu(II) complexes – applications of EPR to a few biological molecules containing Cu(II) and Fe(III) ions.

**UNIT – V MOSSBAUER SPECTROSCOPY AND NQR SPECTROSCOPY:**

Theory of MB spectra- Isomer shifts -quadrupole splitting – magnetic interactions – applications to iron and tin compounds.

NQR spectroscopy – characteristics of quadrupolar nucleus – effects of field gradient and magnetic field upon quadrupolar energy levels – NQR transitions – applications of NQR spectroscopy.

**UNIT – VI PHOTOELECTRON SPECTROSCOPY & X-RAY ABSORPTION SPECTROSCOPY(For Continuous Internal Assessment Only):**

Photoelectron spectroscopy (UV and X-ray) – Physical principle – Experimental details - Koopman's theorem - chemical shift and correlation with electronic charges – Applications of PES.

X-ray absorption spectroscopy (XAS) and Extended X-ray absorption fine structure (EXAFS) – Applications of X-ray absorption spectroscopy. X-ray Absorption Edges - X-ray Fluorescence - Measurement of X-ray Absorption Spectra -Theoretical Description of EXAFS Spectra - Single scattering, Multiple scattering – Data reduction and analysis - Applications: structure determination, Resolution of crystallographic disorder, Oxidation state, prediction of molecular symmetry, determinations of atoms present in the first coordination sphere (Edge & EXAFS analysis) – Structure of Metal clusters.

**REFERENCES:**


1. R.S. Drago, Physical Methods in Inorganic Chemistry; Affiliated East-West Press Pvt. Ltd., New Delhi, 2012.
2. R.S. Drago, Physical Methods in Chemistry; Saunders College Publications, Philadelphia, 1992.
3. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 6th Ed., Wiley-Eastern Company, New Delhi, 1999.
4. P.J. Wheatley, The Determination of Molecular Structure; 2nd Ed., Dover Publications, Mineola, 1981.
5. G. J. Leigh, N. Winterton, Modern Coordination Chemistry; Royal Society of Chemistry, UK, 2002.
6. E.A.V. Ebsworth, Structural Methods in Inorganic Chemistry; 3rd Ed., ELBS, Great Britain, 1987.
7. W. Kemp, Organic Spectroscopy; 3rd Ed., Palgrave, New York, 2011.
8. J. R. Dyer, Applications of Absorption Spectroscopy of Organic Compounds, PHI Learning, New Delhi, 2009.
9. Y.R. Sharma, Elementary Organic Spectroscopy – Principles and Chemical Applications; S. Chand and Co., New Delhi, 1992.
10. P.S. Kalsi, Spectroscopy of Organic Compounds; 6th Ed., New Age International Publishers, New Delhi, 2004.
11. D.N. Sathyanarayana, Electronic Absorption Spectroscopy and Related Techniques; University Press, Hyderabad, 2001.


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**Second Year** **CORE CHOICE COURSE III** **Semester III**

**2) INORGANIC PHOTO CHEMISTRY**

**Code** **(Theory)** **Credit: 5**

**COURSE OBJECTIVES:**

- To educate students on the principles of photochemistry
- To understand the various photochemical properties of transition metal complexes
- To acquire knowledge in charge transfer photochemistry
- To know the various photochemical reactions taking place on solid surfaces

**UNIT – I PRINCIPLES OF PHOTOCHEMISTRY:**

Absorption, excitation, photochemical laws, quantum yield. Absorption and emission for complexes with different ground state /excited state for ML6complexes.Potential energy function and energy levels for ML6complexes. Flash photolysis, stopped flow techniques. Energy dissipation by radiative and non-radiative processes, absorption spectra. Frank-Codon principle, photochemical stages – primary and secondary processes. Jablonski diagram for photochemical process.

**UNIT – II PHOTOCHEMICAL PROPERTIES OF TRANSITION METAL COMPLEXES:**

Photo physical process, Photochemical process, Photo substitution reactions, photoredox reactions, Photorearrangement reaction, Prompt and Delayed Photochemical reactions, Photolysis rules and ligand field theory.

**UNIT – III CHARGE TRANSFER PHOTOCHEMISTRY:**

Introduction, charge transfer absorption spectra, types of charge transfer excitations and their energy level scheme for charge transfer excitations, Types of reactions observed by charge transfer metal complexes.

**UNIT – IV LIGAND FIELD PHOTOCHEMISTRY OF TRANSITION METAL COMPLEXES:**

Photochemistry Cr(III) of complexes : Photo-substitutions, properties of ligand field excited states, Photoaquation reactions, photolysis rule , photoisomerization , photo racemization, photoanation reactions, sensitizer, energy transfer process, Mechanism of photosensitization, photo reactive excited state. The Doublet hypothesis, Role of quartet excited states, Photochemistry of Co(III) complexes : Introduction, energy level diagram, Photoaquations in Co(III) amine, Co(III) cyanide complexes, Fe(II) low spin complexes, Ru(II) ammine derivative complexes, Photo redox properties of Ce(III)and Ce(IV) complexes, photochemistry of Cu(II) (1,3 diketone) complexes.

**UNIT – V PHOTOCHEMICAL REACTIONS ON SOLID SURFACE:**

Introduction, photo electron transfer mechanism, energy level diagram of solid acceptor and donor levels, Examples of photo catalytic metal/mixed metal oxides and their applications, semiconductor supported metal oxides for photolysis of water, Decomposition of organic pollutants, experimental setup, end product of organic products, carbon dioxide reduction, nitrogen fixations, solar energy conversion and its storage. Chemiluminescence's in coordination complexes, Thexi state and Franck condon state.

**UNIT – VI REDOX REACTIONS BY EXCITED METAL COMPLEXES AND METAL COMPLEX SENSITIZERS(For Continuous Internal Assessment Only):**

Energy transfer under conditions of weak interaction and strong interaction-examples formation; condition of the excited states to be useful as redox reactants, excited electron transfer, metal complexes as attractive candidates, (2,2-bipyridine and 1,10-phenanthroline complexes), illustration of reducing and oxidising character of Ruthenium+2 (bipyridal complex, comparsion with Fe (bipy); role of spin-orbit coupling-life time of these complexes. Application of redox processes of electronically excited states for catalytic purposes, transformation of low energy reactants into high energy products, chemical energy into light.

Metal complex sensitizer, electron relay, metal colloid systems, semiconductor supported metal or oxide systems, water photolysis, nitrogen fixation and carbon dioxidereduction.

**REFERENCES:**


1. Adamson, A.W and Fleischauer, P.D (1975): Concepts of Inorganic Photochemistry, Wiley, New York
2. Ferraudi, G.J (1988): Elements of Inorganic Photochemistry, Wiley, New York.
3. Lever, A. B. P (1984): Inorganic Electronic Spectroscopy, Elsevier Science.
4. VeeraReddy, K (1998): Symmetry and Spectroscopy of Molecules, New Age International.
5. Huheey J. E (1983): Inorganic Chemistry, 3rd Edition, Harper and Row Publisher, Singapore.


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| **Second Year** | **CORE PRACTICALIII** | **Semester III** |
| | **PHYSICAL CHEMISTRY PRACTICAL** | |
| **Code** | **(Practical)** | **Credit: 3** |

To perform the various techniques of physical chemistry experiments.

a. Kinetics-acid hydrolysis of ester–comparison of strengths of acids.
b. Kinetics-persulfate-iodine reaction –determination of order, effective of ionic strength on rate constant.
c. Determination of molecular weight of substances by Rast method.
d. Determination of Critical Solution Temperature (CST) of phenol-water system and effect of impurity on CST.
e. Study of phase diagram of two components forming a simple eutectic.
f. Three component system
g. Conductometry – Acid-alkali titrations-Mixture of acids
h. Conductometry – precipitation titrations.
i. Conductometry – solubility product of sparingly soluble salts (PbSO4/BaSO4/PbCrO4/BaCrO4) and verification of Onsager equation
j. Potentiometric titrations – acid alkali titrations.
k. Potentiometry – determination of dissociation constant of weak acids.

**REFERENCES:**


1. B.P. Levitt, Findlay's Practical Physical Chemistry; 9th Ed., Longman, 1985.
2. J.N. Gurtu and R. Kapoor, Advanced Experimental Chemistry; Vol. 1-Physical, S. Chand and Co., New Delhi, 1987.
3. J.B. Yadav, Advanced Practical Physical Chemistry; 20$^{th}$Ed., GOEL Publishing House, Krishna Prakashan Media Ltd., Chennai, 2001.


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| Second Year | ELECTIVE COURSE III<br>1) GREEN CHEMISTRY | Semester III |
|---|---|---|
| Code | (Theory) | Credit: 4 |

**COURSE OBJECTIVES:**

- To learn the green chemistry and their principles.
- To learn the importance of greener reactions.
- To understand the phase-transfer catalyst in green chemistry.

**UNIT – I INTRODUCTION TO GREEN CHEMISTRY:**

Introduction to green chemistry – twelve principles of green chemistry – planning a green synthesis in a chemical laboratory – evaluating the type of reaction involved – rearrangement, addition, substitution, elimination and pericyclic reactions.

Selection of appropriate solvent – aqueous phase reaction – reactions in ionic liquids – organic synthesis in solid state – solid supported organic synthesis – selection of starting materials – use of protecting group – use of catalyst – use of microwaves and sonication.

**UNIT – II ADDITION AND CONDENSATION REACTIONS:**

Addition reactions – Michael addition in [aqueous medium and solid state] – Diels-Alder reactions in aqueous phase.

Condensation reactions – Aldol condensation of aldehydes with nitroalkanes and nitriles – Aldol condensation in solid phase – benzoin condensation under catalytic conditions – applications.

**UNIT – III OXIDATION AND REDUCTION REACTIONS:**

Oxidation reactions – Baeyer-Villiger oxidation in aqueous phase and solid state – enzymatic Baeyer-Villiger oxidation.

Reduction reactions – Clemmensen reduction – mechanism – limitations – applications

**UNIT – IV PHASE-TRANSFER CATALYST REACTIONS:**

Phase-transfer catalyst reactions – Heck reaction – Michael addition reaction – oxidation of toluene to benzoic acid – Reimer-Tiemann reaction – Baker-Venkataraman synthesis – Williamson ether synthesis – Dozen reaction.

**UNIT – V SONICATION REACTIONS:**

Sonication reactions – Barbier reaction – Reformatsky reaction – Simmons-Smith reaction – Strecker synthesis – Ullmann coupling reaction – Wurtz reaction – Bouveault reaction.

**UNIT – VI Emerging Green Technology, Alternative Energy Sources and Renewable Resources(For Continuous Internal Assessment Only):**

Design for Energy efficiency-Photochemical reactions- Advantages-Challenge faced by photochemical process. Microwave technology on Chemistry- Microwave heating –Microwave assisted reactions-Sono chemistry and Green Chemistry – Electrochemical Synthesis-Examples of Electrochemical synthesis.

Biomass –Renewable energy – Fossil fuels-Energy from Biomass-Solar Power-

Other forms of renewable energy-Fuel Cells-Alternative economics-Syngas economy- hydrogen economy-Bio refinery chemicals from fatty acids-Polymer from Renewable Resources –Some other natural chemical resources.

**REFERENCES:**


1. V.K. Ahluwalia, Green Chemistry; 2nd Ed., Ane Books Pvt Ltd., New Delhi, 2016.
2. P.T. Anastas and J. C. Warner, Green chemistry Theory and Practice; Oxford University Press, New York, 2005.
3. V.K. Ahluwalia and K. Agarwal, Organic Synthesis, Special Techniques; 2nd Ed., Narosa Publishing House, New Delhi, 2007.


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| Second Year | ELECTIVE COURSE III<br>2) CATALYSIS | Semester III |
|---|---|---|
| Code | (Theory) | Credit: 4 |

**COUSE OBJECTIVES:**

- To understand the basic concepts of catalysis
- To know the different methods of catalysis
- To learn the various techniques and mechanisms involved in catalysis.

**UNIT – I INTRODUCTION TO CATALYSIS:**

Activity, selectivity, promoters, stabilisers and poisons, Catalysts deactivation, Turn overnumber, inhibitors.

Thermodynamic consideration in catalysis: Energy factor, significance of activationparameters and application to kinetic systems.

Physical adsorption-Unimolecular adsorption- types of adsorption isotherms, Multimolecular adsorption-BET method, Harkins-Jura equation.Chemisorption of gases onmetals and oxides.

**UNIT – II HOMOGENEOUS AND HETEROGENEOUS CATALYSIS:**

Acid-base catalytic reactions, protolytic and protropic mechanisms, activation energy of theprocesses, catalytic activity and acid-base strength, acidity functions: Hammett-Zuckertreatments, linear free energy relationships.

Homogeneous catalysts for the polymerization of olefins, oxidative dehydrogenation, Ethylbenzene to styrene, Ziegler-Natta polymerization.

Partial oxidation: n- butane to maleic anhydride, propylene to acrolene, Fisher-Tropschsynthesis, catalytic reaction of cracking, shape selective catalysis: Zeolites-Alkylation of aniline with alcohols.

Catalysts for the production of petrochemicals- production of aromatics, para-xylene, cumene, linear alkylbenzenes and methanol.

Phase transfer catalysis – Rhodium water soluble catalyst systems with carboxylated and sulfonatedphosphines for hydroformylation reactions.

**UNIT –III PHOTOCATALYSIS:**

Thermal and photochemical reactions between $H_2$-$Cl_2$ and $H_2$-$Br_2$ and $H_2$- $I_2$ reactions, fluorescence, phosphorescence and quenching-Stern-Volmer equation.

Photocatalytic studies using non-stoichiometric oxides such as n-type and p-type semiconductors ($TiO_2$, ZnO, $Cr_2O_3$, doped and coupled semiconductors for the degradationof dyes)

**UNIT – IV ELECTROCATALYSIS:**

Solar energy conversion, electrochemical cells, photoelectrolysis of water and photocatalytic reactions

Photocatalytic reduction of dinitrogen, photocatalysisfor organic reactions oxidation, reduction, polymerization, substitution and isomerization reaction using $TiO_2$.

**UNIT – V BIOCATALYSIS: MECHANISM AND APPLICATION:**

Mechanisms: Covalent catalysis, acid-base and metal-ion catalysis, entropy and geometric effects, structural complementary of the active site to the transition state, prevention of the side reactions, the size of the enzymes.

Applications of enzymes in organic synthesis: Oxidoreductase: Oxidation - Alcohols, epoxides, sulfoxides, amino acids, lactones,

Oxidoreductase: Reduction-α-hydroxyaminoacid, Transferase: Amino acids, amines.

**UNIT – VI TECHNIQUES IN CATALYSIS (For Continuous Internal Assessment Only):**

Structural characterization-BET surface area method, pore volume, and pore size distribution-BJH method, t-plot method, XRD, SEM, TEM, AFM, STM, TPR and TPD. Special relevance to metal oxides with different structures

**REFERENCES:**


1. B. Viswanathan, S. Sivasanker and A.V. Ramaswamy, Catalysis: Principles and Applications, Narosa Publishing House, New Delhi, 2004
2. G.C. Bond, Heterogeneous catalysis: Principles and applications, Oxford University Press,Ely House, London W.I, 1974.
3. V. Murugesan, A. Banumathi and M. Palanichamy, Recent Trends in Catalysis, Narosa Publishing House, New Delhi, 1999.
4. K.J. Laidler, Chemical Kinetics, Tata Mcgraw-Hill Publishing Company Ltd, New Delhi, 1973.
5. D.K. Chakrabarty, Adsorption and Catalysis by solids, Wiley Eastern Limited, New Delhi, 1991.
6. J.M Thomas, W.J. Thomas, Principles and practice of Heterogeneous Catalysis, Wiley- VCH, New York, 1996.


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**Second Year** **NON-MAJOR ELECTIVE COURSEII CHEMISTRY IN DAY-TO-DAY LIFE (Theory)** **Semester III**

**Code** **Credit: 2**

**COURSE OBJECTIVES:**

- To acquire the fundamental concepts related to the chemistry in daily life
- To understand the importance of different types of commercial products for the environment
- To apply the basic concepts of chemistry in the manufacture of commercial products for the society
- To find the efficiency and the utility of the byproducts derived from the basic and applied concepts of chemistry
- To have knowledge about the basic concepts of various micronutrients, fertilizer, dyes, disinfectants and detergents.
- To introduce the properties, structural elucidation, applications and the demerits of the products of the applied chemistry.

**UNIT – I ESSENTIAL MICRONUTRIENTS:**

Carbohydrates - Proteins - Lipids - Nucleic acids and Vitamins – Definition, Sources, Classification, Applications and Diseases due to deficiency.

**UNIT – II SOIL NUTRIENTS AND FOOD ADDITIVES:**

Fertilizers – Pesticides - Insecticides – Definition, Classification, Characteristics and Uses. Additives –Definition, Characteristics, Uses and Abuse of additives in foods and beverages.

**UNIT – III DYES, PAINTS AND PIGMENTS:**

Dyes – Definition, Classification based on mode of application and structure, Applications. Paints – Definition, Ingredients, Characteristics, uses and drying process. Pigments -Varnishes - Definition, Characteristics, Types and Uses.

**UNIT - IV SOAPS, DETERGENTS AND DISINFECTANTS:**

Soaps and Detergents - Definition, Ingredients, Classification, Characteristics and Uses. Disinfectants – Definition, Characteristics and Uses. Perfumes - Definition, Characteristics, Raw materials and perfumes used in soaps - Cosmetics.

**UNIT – V CERAMICS,CEMENT AND GLASS:**

Ceramics: General properties, porous and non-porous wares. Manufacturing process, extrusion, turning, drying, decoration). Porcelain and china.

Cement: Types, manufacture, additives, setting, properties & testing of cement.

Glass: Manufacture, properties, shaping of sheets & plate glasses. Annealing, finishing. Special glasses.

**UNIT – VI PLASTICS AND POLYMERS (For Continuous Internal Assessment Only):**

Introduction to polymers, types of polymers. Plastic in daily use: HDPE, LDPE, PVC, PET, PP. Environmental Hazards of plastics. Recycling of plastics International universal recycling codes and symbols for identification. Biodegradable plastics. Alternatives: Paper news print, writing paper, paper boards, cardboards and Natural materials: Wood, cotton, jute, coir.

**REFERENCES:**


1. B. K. Sharma: introduction to Industiral Chemistry, Goel Publishing, Meerut (1998)
2. Medicinal Chemistry by AshtoushKar.
3. Drugs and Pharamaceutical Sciences Series, Marcel Dekker, Vol. II, INC, New York
4. Analysis of Foods – H.E. Cox: 13. Chemical Analysis of Foods – H.E. Coxandpearson.
5. Foods: Facts and Principles. N. Shakuntala Many and S. Swamy, 4th ed. New Age International (1998)
6. Physical Chemistry – P l Atkins and J. de Paula – 7 th Ed. 2002, Oxford University Press.
7. Handbook on Feritilizer Technology by Swaminathan and Goswamy, 6th ed. 2001, FAI.
8. K. Bagavathi Sundari (2006), Applied Chemistry, MJP Publishers.
9. Des W. Connell (2016). Basic Concepts of Environmental Chemistry, Second edition, Taylor & Francis Group.
10. Ley E. Manahan (2009), Fundamentals of Environmental Chemistry, Third Edition, CRC Press, Taylor & Francis Group


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**Second Year** | **CORE COURSE VII** | **Semester IV**

**CHEMISTRY OF NANOSCIENCE AND NANOTECHNOLOGY**

**Code** | **(Theory)** | **Credit: 5**

**COURSE OBJECTIVES:**

- To know the synthetic methods of nanomaterials.
- To understand the characterization of nanomaterials.
- To understand carbon clusters and nanostructures.
- To learn nanotechnology and nanodevices.

**UNIT – I SYNTHETIC METHODS OF NANOMATERIALS:**

Definition of nanodimensional materials – historical milestones – unique properties due to nanosize, quantum dots, classification of nanomaterials.

General methods of synthesis of nanomaterials – hydrothermal synthesis, solvothermal synthesis – microwave irradiation– sol-gel and precipitation technologies – combustion flame – chemical vapour condensation process – gas-phase condensation synthesis – reverse micelle synthesis – polymer-mediated synthesis – protein microtubule-mediated synthesis – synthesis of nanomaterials using microorganisms and other biological agents – sonochemical synthesis – hydrodynamic cavitation.

Inorganic nanomaterials – typical examples – nano $TiO_2$/ZnO/CdO/CdS, organic nanomaterials – examples – rotaxanes and catenanes

**UNIT – II CHARACTERISATION OF NANOSCALE MATERIALS:**

Principles of Atomic Force Microscopy (AFM) – Transmission Electron Microscopy(TEM)

Resolution and Scanning Transmission Electron Microscopy (STEM) – Scanning Tunneling Microscopy (STM) – Scanning Nearfield Optical Microscopy (SNOM).

Scanning ion conductance microscope, scanning thermal microscope, scanning probe microscopes and surface plasmon spectroscopy.

**UNIT – III REACTIONS IN NANOPARTICLES:**

Reactions in nanospace – nanoconfinement – nanocapsules

Cavitands, cucurbiturils, zeolites, M.O.Fs, porous silicon, nanocatalysis-homogeneous and heterogeneous nanocatalysis.

**UNIT – IV CARBON CLUSTERS AND NANOSTRUCTURES:**

Nature of carbon bond – new carbon structures – carbon clusters – discovery of $C_{60}$–alkali doped $C_{60}$–superconductivity in $C_{60}$–larger and smaller fullerenes. Carbon nanotubes – synthesis –single walled carbon nanotubes – structure and characterization – mechanism of formation – chemically modified carbon nanotubes – doping – functionalizing nanotubes – applications of carbon nanotubes.

Nanowires –synthetic strategies – gas phase and solution phase growth –growth control – properties.

**UNIT – V NANOTECHNOLOGY AND NANODEVICES**

DNA as a nanomaterial – DNA – knots and junctions, DNA – nanomechanical device designed by Seeman.

Force measurements in simple protein molecules and polymerase – DNA complexes– molecular recognition and DNA based sensor.

Protein nanoarray, nanopipettes, molecular diodes, self-assembled nanotransistors, nanoparticle mediated transfection.

**UNIT – VI NANOMEDICINE (For Continuous Internal Assessment Only):**

Principles of nanomedicine – impact of nanotechnology in medicine- nanomedical perspective and the medical applications- nanoparticles delivery for cancer therapy – Bioactive nanomaterials in medicine- Nanodiagnostics - Nanoarrays for diagnostics- nanoparticles for molecular diagnosticsself-assembled protein nanoarrays- protein nanobiochip - Nanobiosensor-CNT biosensor-DNA biosensor.

**REFERENCES:**


1. C. N. R. Rao, A. Muller and A. K. Cheetham (Eds), The Chemistry of Nanomaterials: Vol. 1 and 2; Wiley-VCH; Germany, Weinheim, 2004.
2. C. P. Poole, Jr: and F. J. Owens, Introduction to Nanotechnology; Wiley Interscience, New Jersey, 2003.
3. K. J. Klabunde (Ed), Nanoscale Materials in Chemistry; 2nd Ed., Wiley- Interscience, New York, 2009.
4. T. Pradeep, Nano: The Essentials in Understanding Nanoscience and Nanotechnology; 1st Ed., Tata McGraw Hill, New York, 2007.
5. H. Fujita (Ed.), Micromachines as Tools in Nanotechnology; Springer-Verlag, Berlin, 2003.
6. BengtNölting, Methods in Modern Biophysics; 3rd Ed., Springer-Verlarg, Berlin, 2009.
7. H. Gleiter, Nanostructured Materials: Basic Concepts, Microstructure and Properties, Elsevier, Chennai, 2000.
8. W. Kain and B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life; 2nd Ed., John-Wiley R Sons, New York, 2013.
9. T. Tang and P. Sheng (Eds), Nanoscience and Technology, Novel Structures and Phenomena; Taylor andFrancis, New York, 2003.
10. A. Nabok, Organic and Inorganic Nanostructures; Artech House, Boston, 2005.
11. E.A. Rietman, Molecular Engineering of Nanosystems; Springer-Verlag, New York, 2001.
12. Home page of Prof. Ned Seeman - http://seemanlab4.chem.nyu.edu/
13. Nanoletters - http://pubs.acs.org/journals/nalefd/index.html
14. Nanotation - http://www.acsnanotation.org/


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**Second Year** **CORE COURSE VIII** **Semester IV**

**SELECTED TOPICS IN CHEMISTRY**

**Code** **(Theory)** **Credit: 5**

**COURSE OBJECTIVES:**

- To acquire the knowledge about crystallographic techniques.
- To understand the retro-synthetic methods.
- To study Natural products and macromolecules.
- To learn the principles and applications of nuclear chemistry.

## UNIT – I CRYSTALLOGRAPHY:

Crystal symmetry elements- crystal classes- crystal systems- unit cell- Bravais lattices –space groups- differences between point group and space group- screw axis-glide planes relationship between molecular symmetry and crystallographic symmetry-the concept to reciprocal lattice and its application-x-ray diffraction by single crystal- structure factor- systematic absence- determination of space groups-Fourier synthesis-heavy atom method- a brief account of Cambridge Structural Database (CSD) and Protein Data Bank(PDB).

Neutron diffraction by crystals–magnetic scattering –measurement techniques – comparison with X-ray diffraction elucidation of structure of magnetically ordered unit cell.

## UNIT – II RETRO SYNTHETIC ANALYSIS:

Introduction to disconnections – synthons and synthetic equivalents – synthon approach – electron donors (nucleophiles) – electron acceptors (electrophiles)

Introduction of functional groups – umpolung reactions – one group disconnections: alcohols, olefins, ketones, acids – two group disconnections: 1,2-, 1,3-, 1,4- and 1,5-difunctional compounds – convergent syntheses.

Functional group interconversion – functional group addition – carbon-heteroatom bonds – methods for 3- and 4-membered rings - synthesis of mono- and difunctional open chain molecules – mono and bicyclic molecules with substituents.

## UNIT – III NATURAL PRODUCTS:

**Carbohydrates**-polysaccharides-structure of starch, and cellulose, configuration of carbohydrates-photosynthesis

**Proteins& peptides**: Naturally occurring amino acids – their classifications – acid-base properties and their importance – primary, secondary, tertiary and quaternary structures of proteins –protection of N-terminal and C-terminal groups of proteins -Merifield's solid state peptide synthesis.

**Nucleic acids**: chemistry of nucleic acids-structure of DNA, properties, biological implications of DNA, replication of DNA- structure of RNA- types of RNA- their functions –determining the base sequence of DNA.

**UNIT - IV: MACROMOLECULES**

Introduction – structure – classification of polymers –polymerisation methods – importance of polymers.

Molecular weight of polymers – number average and weight average – determination of molecular weight by osmometry – light scattering, viscosity and sedimentation methods.

Kinetics of polymerisation reactions, polycondensation reactions, ionic and free radical polymerisation, copolymerisation – coordination polymers, conducting polymers, Ziegler-Natta catalyst.

**UNIT – V NUCLEAR CHEMISTRY:**

Nuclear reactions, nuclear cross section, Q-Values, coloumbic barrier, threshold energy and excitation function – different types of nuclear reactions-transmutation, stripping and pick-up reactions-isotope distribution analysis-neutron activation analysis.

Projectile capture and particles emission, spallation, fragmentation, nuclear fission, nuclear fusion – proportional counter, Geiger-Muller counter, scintillation counter and Cherenkov counter – linear accelerator, cyclotron and synchrotron.

**UNIT – VI RECENT TRENDS IN FORENSIC SCIENCE(For Continuous Internal Assessment Only):**

Environmental Forensics: Definition, Legal processes involving environmental forensic science. Geo-forensics Global Positioning System; Basic principles and applications. Biometrics in Personal Identification: Introduction, Concepts of Biometric Authentication, Role in person Identification, Techniques and Technologies (Finger Print Technology, Face Recognition, IRIS, Retina Geometry, Hand Geometry, Speaker Recognition, Signature Verification and other forensic related techniques). Bioterrorism: Definition, Concepts of Biosecurity and microbial forensics, Weapons of mass destruction (WMD), mass-casualty weapons (MCW), NBC and CBRNE, Dirty Bombs.

**REFERENCES:**


1. W. Clegg, Crystal Structure Determination; Oxford University press, UK, 1998.
2. G.H Stout and L. H. Jensen, X-ray Structure Determination: A Practical Guide; John Wiley and Sons, New York, 1992.
3. J.P. Glusker and K. N. Trueblood, Crystal Structure Analysis: A Primer; 3rd Ed., Oxford University Press, UK, 2010
4. Web Pages: Cambridge Structural Database(CSD)- http://www.ccdc.cam.ac.uk/products/csd/ProteinData Bank(PDB) http://www.rcsb.org/pdb/home/home.do
5. S. Warren, Designing Organic Synthesis: The Disconnection Approach; 2nd Ed., Wiley, New York, 2008.
6. F. A. Carey and R. J. Sundberg, Advanced Organic Chemistry, Parts A and

B, 5th Ed., Springer, Germany, 2007.
7. W. Carruthers and I. Coldham, Modern Methods of Organic Synthesis, 4th Ed., Cambridge University Press, Cambridge, 2004.
8. O.P. Agarwal, Chemistry of Organic Natural Products, Vol. I & II, Goel Publications, 1997.
9. I.L. Finar, "*Organic Chemistry*",Volume-II,5thEd., (**2006)**
10. C.E. Carraher, Polymer chemistry, 6th Ed, Marcel Dekker, New York, 2003.
11. F. W. Billmeyer, Jr., A Text Book of Polymer Science, 3rd Ed., John Wiley, 1994.
12. V.R. Gowariker, N. V. Viswanathan, and J. Sreedhar, Polymer Science; 1st.Ed., New Age Publishers, New Delhi, 1986.
13. G. Friedlander, E. S. Macias, J. W. Kennedy and J. M. Miller, Nuclear and Radiochemistry; 3rd Ed., John Wiley and Sons, London, 1981.
14. S. Glasstone, Source Book on Atomic Energy, Krieger Publishing Company, New Delhi, 2014.
15. H.J. Arnikar, Essentials of Nuclear Chemistry; 4th Ed., New Age International Publishers, New Delhi, 2005.

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| **Second Year** | **ENTREPRENEURSHIP / INDUSTRY BASED COURSE INDUSTRIAL CHEMISTRY** | **Semester IV** |
| **Code** | **(Theory)** | **Credit: 5** |

**COURSE OBJECTIVES:**

- To know the basic ideas of an industry and industrial wastes.
- To understand the petroleum and petrochemicals.
- To understand the functions of portland cement.
- To study the principles of pulp and paper.
- To know the preparation of soaps, detergents and perfumes.

**UNIT – I BASIC IDEAS AND INDUSTRIAL WASTES:**

Basics idea about unit operation – flow chart – chemical conversion – batch versus continuous processing – chemical process selection – design – chemical process control.

Types of industrial wastes – treatment of wastes or effluent with organic impurities – treatment of wastes or effluent with inorganic impurities – treatment of some important chemical wastes.

**UNIT – II PETROLEUM AND PETROCHEMICALS:**

Introduction – saturated hydrocarbons from natural gas – uses of saturated hydrocarbons – unsaturated hydrocarbons – acetylene, ethylene, propylene, butylene – aromatic hydrocarbons – toluene and xylene.

Preparation of rectified spirit from beat – methylated spirit – preparation of absolute alcohol from rectified spirit – petrochemicals in India.

**UNIT – III MANUFACTURE OF CEMENT:**

Introduction – types of cement – high alumina cement, water proof cement, slag cement, acid resisting cement, white cement, coloured cement, Pozzolana cement.

Setting of cement – properties of cement – testing of cement – uses of cement – concrete – cement industries in India.

**UNIT – IV PULP AND PAPER AND MANUFACTURE OF PAPER**

Introduction – manufacture of pulp – types of pulp – sulphate or craft pulp, soda pulp, Rag pulp – beating, refining, filling, sizing and colouring.

Calendaring – uses – paper industries in India.

**UNIT – V SOAPS, DETERGENTS AND PERFUMES:**

Introduction – types of soaps – hard and soft soaps – manufacture of soap (hot and continuous process only) – cleansing action of soap – detergents – surface active agents – biodegradability of surfactants, amphoteric detergents.

Introduction – production of natural perfumes – flower perfumes – jasmine, rose and lily – production of synthetic perfumes – muscone and nitro-musks.

**UNIT – VI DYES(For Continuous Internal Assessment Only):**

Introduction-sensation of colour-colour and constitution-nomenclature-basic operations in dyeing-classification of dyes according to the mode of application-synthesis, reaction and applications of diphenyl methane dyes-triphenylmethane dyes-phthalein dyes- xanthene dyes-acridine dyes-Sulphur dyes-cyanine dyes.

**REFERENCES:**


1. B. K. Sharma, Industrial Chemistry; 8th Ed., Goel Publishing House, New Delhi, 1997. (Unit–I, II, III, IV and V)
2. R. N. Shreve, and J. A. Brink Jr. Chemical Process Industries; 4th Ed., McGraw Hill, Toronto, 1977. (Unit–I, II, III, IV and V)
3. A. C. S. Brain, Production and Properties of Industrial Chemicals; Reinhold, New York, 1989. (Unit–I)


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**Second Year** **PROJECT** **Semester-IV**

**Code:** **Credit: 5**

Each candidate shall be required to take up a Project Work and submit it at the end of the final year. The Head of the Department shall assign the Guide who, in turn, will suggest the Project Work to the student in the beginning of the final year. A copy of the Project Report will be submitted to the University through the Head of the Department on or before the date fixed by the University.

The Project will be evaluated by an internal and an external examiner nominated by the University. The candidate concerned will have to defend his/her Project through a Viva-voce.

**ASSESSMENT /EVALUATION /VIVA-VOCE:**

**1. PROJECT REPORT EVALUATION (Both Internal & External):**

I. Plan of the Project - 20 marks

II. Execution of the Plan/collection of Data / Organisation of Materials / Hypothesis, Testing etc and presentation of the report. - 45 marks

III. Individual initiative - 15 marks

**2. VIVA-VOCE / INTERNAL& EXTERNAL** - 20 marks

**TOTAL** **- 100 marks**

**PASSING MINIMUM:**

| | **Vivo-Voce 20 Marks** | **Dissertation 80 Marks** |
|---|---|---|
| Project | 40% out of 20 Marks (i.e. 8 Marks) | 40% out of 80 marks (i.e. 32 marks) |

A candidate shall be declared to have passed in the Project work if he/she gets not less than 40% in each of the Project Report and Viva-voce but not less than 50% in the aggregate of both the marks for Project Report and Viva-voce.

A candidate who gets less than 40% in the Project must resubmit the Project Report. Such candidates need to defend the resubmitted Project at the Viva-voce within a month. A maximum of 2 chances will be given to the candidate.

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| **Second Year** | **VALUE ADDED COURSE II POLYMER CHEMISTRY** | **Semester IV** |
| **Code** | **(Theory)** | **Credit: 2** |

**COURSE OBJECTIVES:**

- To know the basic concepts of polymers.
- To study the Structure and Properties of Polymers.
- To learn the applications of polymers.

**UNIT- I CONCEPTS IN POLYMERS:**

Introduction to polymers and polymerization **-** Classification –Addition-condensation -Linear, branched and cross linked polymers.

Thermoplastic and thermosetting polymers - Elastomers, Fibers and Resins **-** Chemical and geometrical structure of polymers.

Techniques of polymerization - emulsion, bulk, solution and suspension.

**UNIT – II STEREOISOMERISM IN POLYMERS:**

Types of stereoisomerism in polymers –Monosubstitutedethylenes (Site of steric isomerism, Tacticity).

Disubstitutedethylenes (1,1-disubstituted ethylenes, 1,2-disubstituted ethylenes),1,3- Butadiene and 2-Substituted 1,3-Butadienes (1,2- and 3,4-Polymerizations,1,4-Polymerizations).

Stereoregular polymers: Significance of stereoregularity (isotactic, syndiotactic, and atacticpolypropenes), Cis- and trans-1,4-poly-1,3-dienes, Cellulose and amylose.

**UNIT – III STRUCTURE AND PROPERTIES OF POLYMERS:**

Morphology and order in crystalline polymers- Configurations of polymer chains. Crystal structures of polymers - Strain-induced morphology.

Crystalline melting point, Tm- melting points of homogeneous series, effect of chain flexibility and other steric factor, entropy and heat of fusion.

The glass transition temperature, Tg, relationship between Tm and Tg - Effect of molecular weight, diluents, chemical structure, chain topology, branching and crosslinking.

**UNIT – IV CHARACTERIZATION METHODS:**

Average molecular weight concept - Number, weight and viscosity average molecular weights.

Measurement of molecular weights - End group, viscosity, lightscattering, osmotic and ultracentrifugation methods.

Analysis and testing of polymers- Chemical analysis, spectroscopic methods, thermal Analysis.

**UNIT – V COMMERCIAL, NATURAL AND SPECIALITY POLYMERS:**

Commercial Polymers: Polyethylene, Polyvinyl chloride, Polyamides, Polyesters, Phenolicresins, Epoxy resins and silicone polymers.

Natural Polymers: Importance of natural polymers –rubber- vulcanization- Application and structures of starch, cellulose and chitosin derivatives.

Speciality Polymers: Bio polymers - Biodegradable polymers – Biomedical polymers - Poly electrolytes - High temperature and fire retardant polymers- Polymer blend.

Polymer composites -Polymer nanocomposites.

**UNIT – VI POLYMER DEGRADATION AND STABILIZATION(For Continuous Internal Assessment Only):**

Chemical degradation, physical degradation, ageing, crazing, degradation by microorganisms, Biodegradable polymers, Mechanism of degradation, secondary chain reaction, Self-reaction, depolymerisation, metal catalysed degradation, Thermal oxidation, Photo oxidation, Mechanical degradation, Degradation by ionizing radiation, ozone attack. Degradation of special polymers: Polyolefins, PVC, PS, PMMA. Stabilization: Chain breaking antioxidants, bound antioxidants, Radiation protection, Stabilization against biodegradation.

**REFERENCES:**


1. V. R. Gowarikar, B. Viswanathan, J. Sridhar, Polymer Science - Wiley Eastern, 1986, I Edition.
2. G. S. Krishenbaum, Polymer Science Study Guide, Gordon Breach Science publishing, New York, 1973, I Edition.
3. P. Bahadur, N. V. Sastry, Principles of Polymer Science, Narosa Publishing House.
4. G. S. Misra – Introduction to Polymer Chemistry, Wiley Eastern Ltd.
5. F. W. Bill Meyer. Text book of polymer science, III Edition, John Wiley and sons, New York.
6. P. J. Flory. Principles of Polymer Chemistry, Cornell Press (recent edition).
7. G. Odian, Principles of Polymerization, McGraw Hill Book Company, New York, 1973.
8. A. Rudin, The Elements of Polymer Science and Engineering. Academic Press, New York, 1973.
9. C. E. H. Brawn, The Chemistry of High Polymers, Butter worth & Co., London, 1948.


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