# D.K.M. COLLEGE FOR WOMEN

# (AUTONOMOUS), VELLORE-1

## DEPARTMENT OF CHEMISTRY

## SYLLABUS FOR MASTER DEGREE COURSE IN

## CHEMISTRY

## WITH EFFECT FROM 2019 - 2020

# PROGRAMME EDUCATIONAL OBJECTIVES

The purpose of the postgraduate chemistry program at this institution is

**PEO1:** To offer students a more quantitative significant foundation in the principles of Chemistry by conducting academic, industrial and scientific research via the academic conferences, workshops and to produce graduating national provisionally qualified personal who are necessary for the service of the community, government plans and programs of development, education and industry

**PEO2:** To prepare students for their careers as professionals in the field of chemistry, biochemistry and related fields in various industries, colleges and for professional schools including medical, dental, law and business programs by stepping them into the modern laboratory methods and principles using state-of-the-art scientific equipment.

# PROGRAM OUTCOMES

After completion of this program, the students will be able

**PO1:** To understand and apply the concepts of chemical and scientific theories with mastery approach.

**PO2:** To analyze quantitative and qualitative data, employ critical thinking and scientific inquiry.

**PO3:** To develop research oriented learning with analytical and integrative problem solving approaches.

**PO4:** To demonstrate their interpretational skills with understanding the theory background and contemporary chemical instrumentation.

**PO5:** To get specific placements in Colleges, R & D synthetic division of various chemical industries, allied division and to develop laboratory competence in relating chemical structure to spectroscopic phenomena.

**PO6:** To pursue global level research opportunities like Ph.D programme, postdoctoral fellowship, Junior and Senior research fellowship and also the targeted approach of CSIR – NET/SET/Competitive examinations.

**PG Department of Chemistry with effect from 2019-2020**
**CBCS PATTERN**
**The course of study and Scheme of Examination**

| S. No. | Study components | | Ins. Hrs/ Week | Credit | Title of the paper | Maximum marks | | |
|---|---|---|---|---|---|---|---|---|
| | Course Title | | | | | CIA | Sem.. Exam | Total |
| **SEMESTER I** | | | | | | | | |
| 1 | Core | Paper I | 4 | 4 | Structure and bonding of Inorganic compounds | 25 | 75 | 100 |
| 2 | Core | Paper II | 4 | 4 | Substitution reactions and stereochemistry | 25 | 75 | 100 |
| 3 | Core | Paper III | 4 | 4 | Chemical kinetics and electrochemistry | 25 | 75 | 100 |
| 4 | Elective | Paper I | 3 | 3 | (Choose any one out of three)<br>a.Bioinorganic Chemistry and Separation Techniques<br>b. Drug Design<br>c. Green Chemistry | 25 | 75 | 100 |
| 5 | Core | Practical I | 5 | 0 | Organic Chemistry Practical – I | - | - | - |
| 6 | Core | Practical II | 5 | 0 | Inorganic Chemistry Practical – I | - | - | - |
| 7 | Core | Practical III | 5 | 0 | Physical Chemistry Practical – I | - | - | - |
| 8 | Optional | Self Study Paper | - | 2* | Environmental Chemistry for sustainable world | 25 | 75 | - |
| | | | **30** | **15** | | | | **400** |
| **SEMESTER II** | | | | | | | | |
| 9 | Core | Paper IV | 3 | 3 | Coordination chemistry | 25 | 75 | 100 |
| 10 | Core | Paper V | 3 | 3 | Organic Reaction mechanisms and Rearrangements | 25 | 75 | 100 |
| 11 | Core | Paper VI | 4 | 4 | Quantum Chemistry and Analytical Techniques | 25 | 75 | 100 |
| 12 | Elective | Paper II | 3 | 3 | (Choose any one out of three)<br>a. Modern Synthetic Strategies and Renewable Energy Resources | 25 | 75 | 100 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | | | | | b. Pharmaceutical Chemistry<br>c. Heterocyclic chemistry | | | |
| 13 | | Compulsory paper | 2 | 2 | Human rights | 25 | 75 | 100 |
| 14 | Core | Practical I | 5 | 5 | Organic Chemistry Practical – I | 40 | 60 | 100 |
| 15 | Core | Practical II | 5 | 5 | Inorganic Chemistry Practical – I | 40 | 60 | 100 |
| 16 | Core | Practical III | 5 | 5 | Physical Chemistry Practical – I | 40 | 60 | 100 |
| | | | **30** | **30** | | | | **800** |
| *** Optional Internship Training during summer Vocation with an extra credit:1-3** | | | | | | | | |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| **SEMESTER III** | | | | | | | | |
| 17 | Core | Paper VII | 4 | 4 | Nuclear Chemistry and Organometallic Chemistry | 25 | 75 | 100 |
| 18 | Core | Paper VIII | 4 | 4 | Spectroscopy and Applications | 25 | 75 | 100 |
| 19 | Core | Paper IX | 4 | 4 | Thermodynamics and group theory | 25 | 75 | 100 |
| 20 | Elective | Paper III | 3 | 3 | (Choose any one out of three)<br>a. Material Chemistry<br>b.Basic Pharmacology<br>c. Industrial Chemistry | 25 | 75 | 100 |
| 21 | Core | Practical IV | 5 | 0 | Organic Chemistry Practical – II | - | - | - |
| 22 | Core | Practical V | 5 | 0 | Inorganic Chemistry Practical – II | - | - | - |
| 23 | Core | Practical VI | 5 | 0 | Physical Chemistry Practical – II | - | - | - |
| 24 | Optional | Self Study Paper | - | 2* | Online course | - | - | - |
| | | | **30** | **15** | | | | **400** |
| **SEMESTER IV** | | | | | | | | |
| 25 | Core | Paper X | 6 | 5 | Photochemistry, Heterocycles and Natural products | 25 | 75 | 100 |
| 26 | Elective | Paper IV | 3 | 3 | (Choose any one out of three) | 25 | 75 | 100 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | | | | | a. Scientific Research Methodology<br>b.Supramolecular Chemistry<br>c. Nanoscience and Technology | | | |
| 27 | | Compulsory paper | - | 2 | Comprehensive Viva | - | 100 | 100 |
| 28 | Core | Practical IV | 5 | 5 | Organic Chemistry Practical – II | 40 | 60 | 100 |
| 29 | Core | Practical V | 5 | 5 | Inorganic Chemistry Practical – II | 40 | 60 | 100 |
| 30 | Core | Practical VI | 5 | 5 | Physical Chemistry Practical – II | 40 | 60 | 100 |
| 31 | Core | Project | 6 | 5 | Project with Viva Voce | 25 | 75<br>D:60;<br>V-15 | 100 |
| | | | **30** | **30** | | | | **700** |
| | | **Total** | **120** | **90** | | | | **2300** |

# PG DEPARTMENT OF CHEMISTRY

| Subject | Papers | Credit | Total Credits | Marks | Total Marks |
|---|---|---|---|---|---|
| Main Paper | 10 | 7x4<br>5x1<br>3x2 | 39 | 100 | 1000 |
| Main Practical | 6 | 5 | 30 | 100 | 600 |
| Elective Paper | 4 | 3 | 12 | 100 | 400 |
| Compulsory Paper | 2 | 2 | 4 | 100 | 200 |
| Project | 1 | 5 | 5 | 100 | 100 |
| **Total** | **23** | **-** | **90** | **-** | **2300** |

# PAPER-I: STRUCTURE AND BONDING OF INORGANIC COMPOUNDS

| Semester | Subject Code | Category | Instruction Hours | | | | | | Credits |
|---|---|---|---|---|---|---|---|---|---|
| | | | Lecture | | Theory | | Practical | | |
| | | | Per Week | Per Semester | Per Week | Per Semester | Per Week | Per Semester | |
| I | | Core | 4 | 60 | 4 | 60 | 0 | 0 | 4 |

## COURSE OBJECTIVES

- To provide knowledge of basic and advanced concepts in bonding and enable the students to identify the structure and bonding of simple molecules.
- To provide an understanding of the various types of solid state packing, types of chemical forces, structure of inorganic chain cluster compounds and the bonding in boron compounds.

## COURSE OUTCOMES

- On the successful completion of course, students will be able to

| CO Number | CO statement | Knowledge level |
|---|---|---|
| **CO1** | Gain the knowledge on hybridization, structure and bonding in inorganic molecules | **K2 & K3** |
| **CO2** | Gain the knowledge on structure and packing in solids | **K2 & K3** |
| **CO3** | Acquire knowledge about the crystal lattices and the diffraction methods | **K3** |
| **CO4** | Have a better understanding of boron compounds and clusters. | **K2 & K4** |
| **CO5** | Notify different types of inorganic chains and cluster compounds | **K3 & K4** |

*CO-Course Outcomes

Knowledge level K1-Remember; K2-Understand; K3-Apply; K4-Analyze

**MAPPING WITH PROGRAM OUTCOMES:**

| COS | PO1 | PO2 | PO3 | PO4 | PO5 | PO6 |
|---|---|---|---|---|---|---|
| **CO1** | M | M | S | M | S | M |
| **CO2** | M | S | M | S | M | M |
| **CO3** | M | M | S | S | M | M |
| **CO4** | M | M | S | S | M | S |
| **CO5** | M | M | M | M | S | S |

**UNIT I: Chemical Bonding** **12 hours**

V.B. approach to bonding-Hitler-London, Pauling and Slater refinements, Concept of hybridization and structure of molecules, VSEPR theory shapes of molecules. M.O. approach to covalent bonding – symmetry and overlap of atomic orbitals – symmetry of molecular orbitals – sigma and pi bonding – energy levels in homo and heteronuclear diatomic systems – bond length, bond order and bond energy, Application to small molecules such as $BeCl_2$, $BCl_3$ and $CCl_4$, $SF_4$, etc, ionic character in a covalent bond - The concept of multicentre bonding. Pseudo halogens: Structure and bonding in $ClF_3$, $BrF_3$ , $BrF_5$ , $IF_5$ and $IF_7$ . Oxides and oxyacids of halogens, Bonding in Noble gas compounds – $XeCl_2$, $XeF_4$, $XeOF_4$ and $XeF_6$.

**UNIT II: Chemistry of Solid State I: Structure** **12 hours**

Weak Chemical forces: van der Waals forces, Hydrogen bonding – Close packing of atoms and ions HCP and BCC types of packing voids – radius ratio – derivation – its influence on structures – Lattice energy – Born – Lande equation – Kapustinski equation – Madelung constant.

Representative structures of AB and $AB_2$ types of compounds – rock salt, cesium chloride, wurtzite, zinc blende, rutile, fluorite, antifluorite, cadmium iodide and nickel arsenide – Structure of graphite and diamond – Spinels – normal and inverse types and perovskite structures.

**UNIT III: Chemistry of Solid State II: Diffraction Methods** **12hours**

Band theory of solids – non – stoichiometry- point defects – linear defects – effects due to dislocations-electrical properties of solids – conductor, insulator, semiconductor – intrinsic – impurity semiconductors – optical properties – lasers and phosphors – elementary study of liquid crystals.

Difference between point group and space group – screw axis – glide plane – symmetry elements – relationship between molecular symmetry and crystallographic symmetry – The Concept of reciprocal lattice – X– ray diffraction by single crystal – rotating crystal – powder diffraction. Neutron diffraction: Elementary treatment – comparison with X-ray diffraction – Electron diffraction –Basic principle – Crystal Growth methods: From melt and solution (hydrothermal, Gel methods).

**UNIT IV: Boron Compounds and Clusters** **12 hours**

Chemistry of boron – Preparation, properties and structure of boranes, higher boranes - types of boranes closo, nido, arachno. ($B_2H_6$, $B_4H_{10}$, $B_5H_{11}$, $B_6H_{10}$, $B_{10}H_{14}$) linear and cyclic borazines ($B_3N_3H_6$), boron nitrides (BN)x and borates ions — STYX numbers, Wade's rules .

Carboranes ($C_2B_9H_{11}^{2-}$), Metallocarboranes (1,2-$C_2B_{10}H_{12}$), Metalloboranes ( $BnHn^{2-}$) – preparation, properties and Structure – a general study. Metal clusters: Chemistry of low molecularity metal clusters only – Structure of $Re_2Cl_8$; multiple metal – metal bonds.

**UNIT V: Inorganic Chain and Cluster Compounds** **12 hours**

Types of inorganic polymers – comparison with organic polymers – silanes, higher silanes ( $Si_2H_6$, $Si_4H_{10}$) – multiple bonded systems – silicon carbides, siloxanes. P– N compounds, cyclophosphazenes and cyclophosphazanes – S–N compounds – $S_4N_4$, $S_4N_4H_4$ and $(SN)_x$.

Isopoly acids – polyvanadates, polymolybdates, polytungstates – heteropolyacids and their salts – structure of silicates - applications of Paulings rule of electrovalence - isomorphous replacements in silicates – ortho, meta and pyrosilicates – one dimensional, two dimensional and three dimensional silicates – silazenes - preparation, properties and structure.

**Distribution of Marks**: Theory-80% and Problems-20%

**TEXT BOOKS**

| S. No. | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| 1. | J.E. Huheey | Inorganic Chemistry – Principles, Structure and Reactivity | Harper Collins, New York, IV Edition | 1993 |
| 2. | D. E. Douglas, D.H. McDaniel and J. J. Alexander | Concepts and Models in Inorganic Chemistry | 3rd Ed | 1994 |
| 3. | M. C. Day, J. Selbin | Theoretical Inorganic Chemistry | 2nd Ed, East West Press | 1985 |
| 4. | L. Pauling | The Nature of the Chemical Bond | 3rd Ed., Cornell University Press | 1960 |
| 5. | F.A. Cotton and G. Wilkinson | Advanced Inorganic Chemistry – A Comprehensive Text | John Wiley and Sons, V Edition | 1988 |
| 6. | D.F. Shriver, P.W. Atkins | Inorganic Chemistry | 3rd Ed | 1999 |
| 7. | A.G. Sharpe | Inorganic Chemistry | Pearson Education | 2008 |
| 8. | N. H. Ray | Inorganic Polymers | Academic Press | 1978 |
| 9. | A. R. West | Basic Solid State | John Wiley | 1991 |

| | | | | |
|---|---|---|---|---|
| | | Chemistry | | |
| 10. | E. L. Mutteri | Polyhedral Boranes | Academic Press, NY | 1975 |

**REFERENCE BOOKS**

| S.No | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| 1. | S.F.A. Kettle | Coordination Chemistry | EIBS | 1973 |
| 2. | K. Burger | Coordination Chemistry | Burter Worthy | 1973 |
| 3. | K.F. Purcell and J.C. Kotz | Inorganic Chemistry | WB Saunders Co., USA | 1977 |

**TEACHING METHODOLOGY:**

- PowerPoint presentation
- Models
- Group discussion
- Seminar and Assignments
- Animated videos
- Board and chalk

**SYLLABUS DESIGNERS:**

1. Dr.P.N.Sudha, Principal, Department of Chemistry
2. Dr.M.Nagarathinam, Head & Associate Professor, Department of Chemistry
3. Dr.S.Santha Lakshmi, Assistant Professor, Department of Chemistry
4. Dr.S.Sashikala, Assistant Professor, Department of Chemistry
5. Dr.N.Dhanam, Assistant Professor, Department of Chemistry
6. Dr. K. Vijayalakshmi, Assistant Professor, Department of Chemistry
7. Dr. T. Gomathi, Assistant Professor, Department of Chemistry
8. Mrs. J. Saranya, Assistant Professor, Department of Chemistry
9. Mrs. R. Bharathi Priyadharsini, Assistant Professor, Department of Chemistry

# PAPER-II: SUBSTITUTION REACTIONS AND STEREOCHEMISTRY

| Semester | Subject Code | Category | Instruction Hours | | | | | | Credits |
|---|---|---|---|---|---|---|---|---|---|
| | | | Lecture | | Theory | | Practical | | |
| | | | Per Week | Per Semester | Per Week | Per Semester | Per Week | Per Semester | |
| I | | Core | 4 | 60 | 4 | 60 | 0 | 0 | 4 |

**COURSE OBJECTIVES:**

- Understanding the fundamental mechanism involved in electrophilic reactions, nucleophilic reactions and reactions that involve transient species.
- Understanding the basic aspects of stereochemistry such as chirality, nomenclature, stereoselectivity Vs stereospecificity, asymmetric synthesis and the conformational analysis of six membered ring systems.

**COURSE OUTCOMES:**

- On the successful completion of course, students will be able to achieve excellency in education as follows

| CO Number | CO statement | Knowledge level |
|---|---|---|
| **CO1** | Gain knowledge about aromaticity, isotopic labeling techniques, kinetic isotope effect and the ambident nuclesophiles | **K2 & K4** |
| **CO2** | Get clear idea about the nucleophilic attack on saturated carbon atoms leading to substitution reactions, different mechanisms of nucleophilic substitution , effect of solvent on the rate of reaction, neighbouring group participation and the alkylation of active methylene compounds. | **K2 & K3** |
| **CO3** | Use various reagents in a logical manner in organic synthesis, understand various types of aromatic electrophilic substitution, nucleophilic substitution reaction and their mechanism | **K3 & K4** |
| **CO4** | Gain knowledge about basic principles of stereochemistry, to apply various concepts such as stereochemistry and fundamental principles of stereoselectivity in organic chemistry and also to identify and differentiate prochirality and chirality at centers, axis, planes and helices and determine the absolute configuration. | **K2 & K3** |
| **CO5** | Acquire good foundation about conformational analysis and to differentiate the reactive intermediates can be differentiated by their unique properties through various reaction pathways to develop new and notable aromatic organic compounds | **K3 & K4** |

*CO-Course Outcomes

Knowledge level K1-Remember; K2-Understand; K3-Apply; K4-Analyze

**MAPPING WITH PROGRAM OUTCOMES**

| COS | PO1 | PO2 | PO3 | PO4 | PO5 | PO6 |
|---|---|---|---|---|---|---|
| **CO1** | M | S | S | M | M | M |
| **CO2** | M | S | M | M | S | M |
| **CO3** | M | M | M | S | S | M |
| **CO4** | M | S | S | S | S | M |
| **CO5** | M | M | S | S | S | M |

**UNIT-I: Aromaticity and Reaction Mechanism 12 hours**

Aromaticity of benzenoid, heterocyclic and non – benzenoid compounds – Huckel's rule –Annulenes. Kinetic and Non kinetic methods of determining organic reaction mechanisms – Isolation and trapping of intermediates – Isotopic labeling studies – Primary Kinetic Isotopic effect. Generation of Kinetic and Thermodynamic enolates – Hammett equation-simple problems and Taft equation. Siginificance of reaction as well as substituent constants – Ambident nucleophiles such as $CN^-$, $NO_2^-$, phenoxide and ambident dianions – Williamsons ether synthesis.

**UNIT-II: Aliphatic Nucleophilic Substitution 12 hours**

Mechanism of nucleophlic substitution reaction: $S_N1$, $S_N2$ and $S_Ni$ mechanisms – Solvent and leaving group effects and neighbouring group participation (NGP) – Substitution at carbonyl, vinylic and bridgehead system – Substitution with ambident nucleophiles- "O" Vs "C"alkylation. Role of LDA – crown ethers and phase transfer catalysts (PTC) in nucleophilic substitution reactions.

Generation of enolates – enolate selectivity (Kinetic Vs Thermodynamic) – alkylation of enolates and stereochemistry of enolate alkylation – Mechanism of ester hydrolysis – Alkylation of active methylene compounds. Asymmetric alkylation (Evans, Enders and Meyers procedures) – Preparation and synthetic utility of enamines, Finkelstein reaction – Wurtz coupling.

**UNIT-III: Aromatic Electrophilic and Nucleophilic Substitution Reactions 12 hours**

Aromatic electrophilic substitution: mechanism of nitration, sulfonation, Friedel – Crafts alkylation and acylation reactions – Synthesis of di and trisubstituted benzenes from benzene or monosubstituted benzenes (symmetrical tribromo benzene, 2-amino 5-methylphenol, 3 - nitro 4-bromobenzoic acid, 3, 4-dibromonitrobenzene, 1,2,3 – trimethylbenzene) – Hammett and Hammett-Taft equation – Haworth reaction (for

naphthalene), Scholl reaction, Vilsmeier-Haack formylation, Gattermann reaction, Reimer–Tiemann and Bischler – Napieralski reactions.

Aromatic nucleophilic substitution in aryl halides by Meisenheimer complex mechanism and benzyne mechanism. Reactions of aryldiazonium salts – Zeigler alkylation, Vicarious Nucleophlic Substitution (VNS), Chichibabin and Schiemann reactions.

**UNIT-IV: Stereochemistry** **12 hours**

Chirality, Symmetry elements, Asymmetric and Dissymmetric chiral molecules – Calculation of number of optical isomers – Stereochemistry of mono and disubstituted cyclopropane, cyclobutane, cyclopentane and cyclohexane – Stereochemistry of tri-substituted cyclopentane, trisubstituted pentane and tetrasubstituted hexane. Description of various types of optically active compounds including allenes, cumulenes, spiranes, biphenyls, *trans* – cyclooctene.

Compounds containing two asymmetric centers; Erythro and threo isomers – Conversion of Fischer projection into perspective forms – Erythro and Threo – Inter conversion of Fischer to Sawhorse and Newman projections – Zig-Zag representation of glucose – Interpretation of homotopic, enantiotopic and diastereotopic atoms and faces – Pro-chiral carbon – Concept of *Re*- and *Si*- faces – R and S nomenclature of simple compounds – allenes, spiranes and biphenyls – Stereospecific and Stereoselective reactions – Asymmetric Synthesis-Crams rule and Felkin-Anh model. E-Z nomenclature of olefins.

**UNIT-V: Reactive Intermediates and Conformational Analysis** **12 hours**

Organic reactive intermediates: Generation, stability and reactivity of carbocations, carbanions, free radicals, carbenes, carbenoids, benzynes and nitrenes.

Conformation of some simple 1, 2 – disubstituted ethane derivatives – Conformational analysis of disubstituted cyclohexane and their stereochemical features (geometric and optical isomerism (if shown) by these derivatives) – Conformation and reactivity of substituted cyclohexanol (oxidation and acylation) – cyclohexanone. (reduction) and cyclohexane carboxylic acid derivatives (esterification and hydrolysis) – Conformation and stereochemistry of cis and trans decalin and 9 – methyldecalin.

**Distribution of Marks**: Theory-80% and Problems-20%

**TEXT BOOKS**

| S.No | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| 1. | S.M. Mukherji and S.P. Singh | Organic Reaction Mechanism | McMillan India Ltd., Chennai | 1990 |
| 2. | Stanley Pine | Organic Chemistry | V Edition, Tata McGraw-Hill Pub., | 1990 |
| 3. | Jerry March | Advanced organic reaction mechanism and structure | Tata McGraw-Hill Pub.,5th edition | 2001 |
| 4. | Mc Murray | Organic Chemistry | V-edition, Thomson Asia Pvt., Ltd. | 2001 |
| 5. | Graham Solomons | Organic Chemistry | John Wiley & Sons Ltd., | 2000 |
| 6. | P.S. Kalsi | Stereochemistry, Conformation analysis and Mechanism | 2nd Edition, Wiley Eastern Limited, Chennai. | 1993 |
| 8. | P.S. Kalsi | Stereochemistry and Mechanism through solved problems | Wiley Eastern Ltd | 1994 |
| 9. | R.K. Bansal | Organic Reaction Mechanism | IV Edition, New Age Int.,(P) Ltd., | 2003 |
| 11. | Peter Sykes | A Guidebook to mechanism in organic chemistry | Orient Longman Ltd. | 1999 |

**REFERENCE BOOKS**

| S.No | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| 1. | F. Carey and R. J. Sundberg | Advanced Organic Chemistry-Part A and B | Springer Science + Business Media, 5 th Ed | 2007 |
| 2. | M. B. Smith and Jerry March | Advanced Organic Chemistry | John Wiley & Sons, 5th Ed | 2001 |
| 3. | J. Clayden, N. Greeves and S. Warren | Organic Chemistry | Oxford University Press 2nd Ed | 2012 |
| 4. | M. B. Smith | Organic Synthesis | Academic Press, 3rd Ed | 2011 |
| 5. | R. O. C. Norman and J. M. Coxon, | Principles of Organic Synthesis | Chapman & Hall, 3rd Ed | 1993 |

| | | | | |
|---|---|---|---|---|
| 6. | Stuart Warren | Organic Synthesis: Disconnection Approach | Wiley India (P) Ltd | 2007 |
| 7. | I. L. Finar | Organic Chemistry Vol 2: Stereochemistry and the Chemistry of Natural product | Dorling Kindersley India (P) Ltd | 2009 |
| 8. | E. N. Eliel | Stereochemistry of Carbon Compounds | Tata McGraw Hill Ed, Reprint | 2008 |
| 9. | D. Nasipuri | Stereochemistry of Organic Compounds | New Age International (P) Ltd, Reprint | 2005 |
| 10. | E. L. Eliel and S. H. Wilen | Stereochemistry of Organic Compounds | Wiley India Ed | 2008 |

**TEACHING METHODOLOGY:**

- PowerPoint presentation
- Models
- Group discussion
- Seminar and Assignments
- Animated videos
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# PAPER-III: CHEMICAL KINETICS AND ELECTROCHEMISTRY

| Semester | Subject Code | Category | Instruction Hours | | | | | | Credits |
|---|---|---|---|---|---|---|---|---|---|
| | | | Lecture | | Theory | | Practical | | |
| | | | Per Week | Per Semester | Per Week | Per Semester | Per Week | Per Semester | |
| I | | Core | 4 | 60 | 4 | 60 | 0 | 0 | 4 |

## COURSE OBJECTIVES

- To understand the kinetics of chemical kinetics and explore the reaction kinetics of fast reactions .
- To learn the various techniques, mechanism of involved in catalysis and understanding of the Ionic activity, ionic interactions, Debye-Hückel-Bjerrum model, Debye-Hückel limiting law, Debye-Hückeleory of strong electrolytes, electrical double layer, electrocapillary phenomena, surfactants, design and applications of the batteries, Fuel Cells, Corrosion and its Protection.

## COURSE OUTCOMES:

- On the successful completion of course, students will be able to

| CO Number | CO statement | Knowledge level |
|---|---|---|
| **CO1** | Learn the reaction rate theories and reactions in solution and to explore the knowledge in kinetics | **K2 & K4** |
| **CO2** | Solve problems on rate/rate constants/efficiency for unimolecular and bimolecular reactions and Plot equations and functions representing kinetic behaviour. | **K2 & K4** |
| **CO3** | Gain clear concepts about transition in jablonski diagram and photo catalysis reaction | **K2 &K3** |
| **CO4** | Acquire knowledge about strong electrolytes and based on Debye-Huckel limiting law certain problems can be solved. | **K3 & K4** |
| **CO5** | Understand the designs of batteries, Fuel cells and ion selective electrodes | **K2 & K3** |

* CO-Course Outcomes

Knowledge level K1-Remember; K2-Understand; K3-Apply; K4-Analyze

## MAPPING WITH PROGRAM OUTCOMES

| COS | PO1 | PO2 | PO3 | PO4 | PO5 | PO6 |
|---|---|---|---|---|---|---|
| **CO1** | S | S | M | S | S | M |
| **CO2** | M | S | S | M | M | S |
| **CO3** | M | M | S | M | M | M |
| **CO4** | M | M | M | S | M | M |
| **CO5** | M | M | S | S | S | M |

**UNIT-I: Chemical Kinetics** **12 hours**

Effect of temperature on reaction rates – collision theory of reaction rate: Lewis rigid sphere theory – molecular beams – collision cross sections – effectiveness of collisions – Potential energy surfaces – partition function and activated complex –Absolute reaction rate theory – Thermodynamic terms-Significance of entropy and volume of activation – Reactions in solution: factors determining reaction rates in solutions, effect of dielectric constant and ionic strength, – Bronsted –Bjerrum equation – Primary and Secondary salt effect, influence of solvent on reaction rates.

**UNIT-II: Chemical Dynamics and Catalysis** **12 hours**

Acid base catalysis – Mechanism of acid base catalyzed reaction, Bronsted Catalysis Law – Enzyme catalysis and its mechanism, Michaelis – Menten equation, effect of pH and temperature on enzyme catalysis – Mechanism of enzyme inhibition kinetics of surface reactions – Unimolecular reactions-Bimolecular reactions-Langmuir Hinshelwood and Elay–Rideal mechanism, Rice – Ramsperger – Kassel(RRK) theory. Rice-Ramsperger – Kassel – Marsus (RRKM) theory.

Study of fast reactions by stopped flow techniques – relexation method, flash photolysis and the nuclear magnetic resonance method.

Linear free energy relationship – Hammett equation – Taft equation-Separation of polar, resonance and steric effects.

**UNIT-III: Introduction to Photochemistry** **12 hours**

Jablonski diagram, Primary and Secondary Processes, quantum yield and its determination – chemical actinometer. Excimers and exciplexes – Kinetics of collisional quenching – Stern Volmer equations. Photochemical reactions - photoredox, photosubstitution, photoisomerization and photosensitized reactions - photovoltaic and photogalvanic cells. Chemiluminescence, Photoassisted electrolysis of water, Photosynthesis, solar energy conversions. Semiconductor photocatalysis – lasers.

Radiation Chemistry – linear energy transfer, G – value, dosimeters, radiolysis of water, solvated electrons.

**UNIT IV: Electrochemistry – I** **12 hours**

Deviation from ideal behavior ion – solvent and ion – ion interactions – Debye–Hückel – Bjerrum model, Ion association and triple ion formations – Expression for the mean activity coefficient – Debye – Hückel limiting law and its applications – Diverse ion effect – Van't Hoff factor and its relation to colligative properties – Debye – Hückel theory of strong

electrolytes –Debye – Hückel length and potential around a central ion and its interpretation – Transport of ions in Solution: Electrolytic conduction- Debye – Hückel – Onsager treatment of strong electrolytes- ionic atmosphere- Anomalous conductance of nonaqueous electrolytes.

**UNIT V: Electrochemistry- II** **12 hours**

Diffusion – Fick's law of diffusion – electrokinetic phenomena-membrane potential. Electrical double layer – Electrocapillary phenomena – Surfactants – Lipmann's equation – Electrokinetic phenomena – Zeta potential and its applications – Structure of electrical double layer – Helmholtz – Perrin, Guoy – Chapmann and Stern models – Butler –Volmer equation for one electron transfer reaction - equilibrium and exchange current densities and symmetry factor – transfer coefficient – Cyclic voltammetry and Stripping voltammetry – principle – instrumentation- Corrosion and passivation of metals – Pourbaix diagram – Evans diagram – Batteries and Fuel cells-Ion selective electrodes.

**Distribution of Marks**: Theory-80% and Problems-20%

**TEXT BOOKS**

| S. No | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| 1. | R. G. Frost and Pearson | Kinetics and Mechanism | Wiley New York, | 1961 |
| 2. | C. Capellos and B. H. J. Bielski,. | Kinetic Systems | Wiley Interscience, New York | 1968. |
| 3. | K. J. Laidler | Chemical Kinetics | Harper and Row, New York, | 1987 |
| 4. | Rajaram and J.C.Kuriacose | Kinetics and Mechanism Of Chemical Transformations | Macmillan India Ltd. | 1993 |
| 5. | G. M. Harris | Chemical Kinetics | D. C. Healthand Co, | 1966 |
| 6. | A. W. Anderson | Physical Chemistry of Surfaces | Wiley - Interscience, Newyork | 1990 |
| 7. | Paula, Peter Atkins and Julio de | Elements of Physical chemistry | 5th Ed, Oxford U. P | 2012 |
| 8. | John O'M Bockris, Amula K. N. Reddy, and Maria Gamboa–Aldeco | Modern Electrochemistry 2A, 2nd Ed, | Kluwer Academic / Plenuim Publishers, NewYork | 2000 |
| 9. | Mordechay Schlesinger | Modern Aspects of Electrochemistry | Issue 43, Springer, Netherlands | 2009 |
| 10. | G. L. Agarwal | Basic Chemical Kinetics | Tata McGraw Hill | 1990 |

| | | | | |
|---|---|---|---|---|
| 11. | K. J. Laidler | Chemical Kinetics | Tata Mc Graw Hill | 1990 |
| 12. | Robert J Silbey, Robert A Alberty and Moungi G Bawendi | Physical Chemistry | 4th Ed,NJ Hoboken: Wiley | 2015 |
| 13. | N. J. Turro | Modern molecular photochemistry | Benjamin/Cummings , Menlo Park, California | 1978 |
| 14. | Revise G. W. Castellan, | Physical Chemistry | Narosa publishing House ,New Delhi, Ed, | 2011 |
| 15. | Gordon. M. Barrow | Physical Chemistry | Tata McGraw Hill Edition, New York, | 2011 |
| 16. | L. R. Puri, Y. R. Sharma and R. S. Pathania, | Principles of Physical Chemistry | Vishal Publishing Co, 4th edition edition | 2012. |
| 17. | J. N. Gurtu and A. Gurthu, | Advanced Physical Chemistry | Pragathi Prakashan, Meerut, Revised, | 2014 |

**REFERENCE BOOKS**

| S.No | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| 1. | S.Glasstone | Introduction To Electrochemistry | Affliated East West Press, New Delhi, | 1960 |
| 2. | J.O.M.Bokris and A.K.N.Reddy | Electrochemistry, Vols.1 and 2 Plenum | New York, | 1977 |

**TEACHING METHODOLOGY:**

- PowerPoint presentation
- Group discussion
- Seminar and Assignments
- Animated videos
- Board and chalk

**SYLLABUS DESIGNERS:**

1. Dr.P.N.Sudha, Principal, Department of Chemistry
2. Dr.M.Nagarathinam, Head & Associate Professor, Department of Chemistry
3. Dr.S.Santha Lakshmi, Assistant Professor, Department of Chemistry
4. Dr.S.Sashikala, Assistant Professor, Department of Chemistry
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## ELECTIVE-PAPER-A: BIOINORGANIC CHEMISTRY AND SEPERATION TECHNIQUES

| Semester | Subject Code | Category | Instruction Hours | | | | | | Credits |
|---|---|---|---|---|---|---|---|---|---|
| | | | Lecture | | Theory | | Practical | | |
| | | | Per Week | Per Semester | Per Week | Per Semester | Per Week | Per Semester | |
| I | | Elective | 3 | 45 | 3 | 45 | 0 | 0 | 3 |

**COURSE OBJECTIVES:**

- To have a knowledge about protein metallo biomolecules, role of metal ions in biological process, storage and transport of metal ions in biological system, chemical toxicology and uses of inorganic compounds as therapeutic agents.
- To learn about polymeric bio-organic molecules such as carbohydrates, proteins, nucleic acids, antibiotics, vitamins and to understand about various types of separation techniques for organic and biomolecules.

**COURSE OUTCOMES:**

- On the successful completion of course, students will be able to

| CO Number | CO statement | Knowledge level |
|---|---|---|
| **CO1** | To identify the occurrence, active site structure and functions of some transition metal ion containing metalloproteins or enzymes | **K2 & K3** |
| **CO2** | Gain better knowledge about the structure of metallo enzymnes, importance of transport and storage metals in biological systems. | **K2 & K3** |
| **CO3** | Acquire the skill of relating all the biomolecules in various biological systems and can gain knowledge about the biological importance of proteins, nucleic acids and carbohydrate | **K3 & K4** |
| **CO4** | Gain clear knowledge about the chemistry and physiological action of antibiotics, vitamins and carotenoids | **K3 & K4** |
| **CO5** | To apply principles of separation and isolation techniques in organic reactions leading to the separation and purification of various products | **K2 & K3** |

* CO-Course Outcomes

Knowledge level K1-Remember; K2-Understand; K3-Apply; K4-Analyze

**MAPPING WITH PROGRAM OUTCOMES**

| COS | PO1 | PO2 | PO3 | PO4 | PO5 | PO6 |
|---|---|---|---|---|---|---|
| **CO1** | M | M | M | M | S | S |
| **CO2** | M | M | S | S | S | M |
| **CO3** | M | S | S | S | M | M |
| **CO4** | M | S | S | M | M | M |
| **CO5** | S | S | S | S | S | S |

**UNIT-I: Metallo Proteins** **9 hours**

**Iron containing proteins:** Metalloporphyrins – Haemoglobin and myoglobin – Structures and work functions – synthetic oxygen carriers – Cytochrome – structure and work function. Non – heme oxygen carriers – Electron carrier proteins – Iron sulphur proteins – Ferridoxin and Rubredoxin – Magnesium containing proteins: Chlorophyll – structure – photosynthetic sequence – Copper containing proteins: Classification – blue copper proteins – structure of blue copper electron transferases – copper protein as oxidases – cytochrome c oxidase – mechanistic studies of cytochrome c oxidase

**UNIT II: Metallo Enzymes** **9 hours**

**Metalloenzymes:** Carboxy peptidase A – structure and function ; Carbonic anhydrase – inhibition and poisoning – Corrin ring system – Vitamin $B_{12}$ ( cyanocobalamin ) and $B_{12}$ coenzymes – *In vivo* and *In vitro* nitrogen fixation – nitrogen cycle.

**Essentials of trace elements and chemical toxicology:** Trace elements in biological system – sodium, potassium, calcium, zinc and copper – Metal ion toxicity - classes of toxic metal compounds – detoxification.

**Metals in medicine:** Antiarthritis drugs – Au and Cu in rheumatoid arthritis – Li in psychiatry – Pt, Au and metallocenes in anticancer drugs- metals in radiodiagnosis and magnetic resonance imaging.

**Transport and storage of metals:** Mechanism – Fe, Cu, Zn and V storage and transport – metallothioneins – Molecular mechanism of iron transport across the membrane – sodium and potassium ion pumps.

**UNIT-III: Biomolecules** **9 hours**

**Amino acids and Proteins:** Amino acids and Protein structure, peptides and their synthesis – (tripeptide using the amino acids glycine, alanine, lysine, cysteine, glutamic acid and arginine) – Analysis of N– terminal and C – terminals in a polypeptide. Sanger method, Edman degradation and Enzymatic analysis. Merrified synthesis – Primary, secondary and tertiary structure of proteins.

**Nucleic acids and Carbohydrates: C**hemistry of nucleic acids, nucleosides and nucleotides – Structure RNA and DNA and their biological importance – Pyranose and furanose forms of aldohexose and ketohexose – methods used for the determination of ring size – conformation of aldohexopyranose – structure and synthesis of lactose and sucrose. A brief study of starch and cellulose.

**UNIT-IV: Antibiotics, Vitamins and Carotenoids** **9 hours**

**Biomolecules: Antibiotics and vitamins:** A detailed study of structure, stereochemistry and synthesis of penicillin, cephalosporin – Chemistry and physiological action of ascorbic acid, thiamin, riboflavin and pyridoxine – Elementary aspect of vitamin A, E, K and $B_{12}$ - Synthesis of vitamin $A_1$ using Reformarsky method, Wittig reaction method, jansen method, Attenburrow method, Isler method – Synthesis of Vit- $A_2$ -Carotenoids – introduction – synthesis of α-carotene, β-carotene, γ-carotene and lycopene.

**UNIT V: Separation Techniques** **9 hours**

Basic aspects of thin-layer chromatography (TLC), column chromatography and flash vacuum column chromatography – Principles, theory, instrumentation and applications of Ion – exchange column Chromatography, Gel-permeation Chromatography, Gas chromatography and High Performance Liquid chromatography (HPLC) – Interpretation of chromatogram and separation of components from the mixture.

**Distribution of hours:** Theory-100%; Problems-Nil

**TEXT BOOKS**

| S.No | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| 1. | S. J. Lippard and J. M. Berg | Principles of Bioinorganic Chemistry | BergPanima Publishing Corporation | 1997 |
| 2. | W. Kaim and B. Schwederski | Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, (An Introduction and Guide), | John Wiley and Sons | 1994 |
| 3. | J. E. Huheey, E. A. Keiter and R. L. Keiter. | Inorganic Chemistry, Principles of Structure and Reactivity | Pearson Education | 2004 |
| 4. | F. A. Cotton and G. Wilkinson, | Advanced Inorganic Chemistry | Wiley Eastern | 1998 |
| 5. | Geoffrey L. Zubay, William W. Parson and Dennis E. Vance | Principles of Biochemistry | McGraw-Hill Education | 1995 |
| 6. | David L. Nelson and Michael M. Cox | Principles of Biochemistry | WH Freeman | 2017 |

| | | | | |
|---|---|---|---|---|
| 7. | John McMurray | Organic Chemistry | International Edition8th Ed | 2017 |
| 8. | I.L.Finar, | Organic Chemistry Vol 2, Stereochemistry and the Chemistry of Natural Product | Dorling Kindersley India (P) Ltd | 2009 |
| 9. | B. S. Furniss, A. J. Hannaford, P. W. G. Smith and A. R. Tatchell, | Vogel's text book of Practical Organic Chemistry | Pearsons Education (Singapore) PTE Ltd, 3rd Indian Reprint | 2005 |
| 10. | Douglas A. Skoog, F. James Holler and Stanley R. Crouch | Principles of Instrumental Analysis | CENAGE Learning, 7th Ed | 2018 |
| 11 | D. A. Skoog and D. M. West | Fundamentals of Analytical Chemistry | Holt Rinehart and Winston Publications, 4th Ed | 1982 |
| 12 | Douglas A. Skoog, Donald M. West, F. James and Stanley R. Crouch, | Fundamentals of Analytical Chemistry | 8th Ed | 2004 |
| 13 | Lloyd R. Snyder, Joseph J. Kirkland and John W. Dolan, | Introduction to Modern Liquid Chromatography | Wiley 3rd Ed | 2009 |

**REFERENCE BOOKS**

| **S.No** | **Authors** | **Title** | **Publishers** | **Year of publication** |
|---|---|---|---|---|
| **1.** | Gurdeep Charwal, | Chemistry of natural products | Himalaya publishing house | 2018 |
| **2.** | O.P. Agarwal, | Chemistry of natural products | GOEL Publishing house | 2015 |
| **3.** | I.L. Finar, | Organic chemistry, Stereochemistry and chemistry of natural products | Volume II, Pearson Education | 2002 |

**TEACHING METHODOLOGY:**

- PowerPoint presentation
- Group discussion
- Seminar and Assignments
- Animated videos
- Board and chalk

**SYLLABUS DESIGNERS:**

1. Dr.P.N.Sudha, Principal, Department of Chemistry
2. Dr.M.Nagarathinam, Head & Associate Professor, Department of Chemistry
3. Dr.S.Santha Lakshmi, Assistant Professor, Department of Chemistry
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## ELECTIVE PAPER-B: DRUG DESIGN

| Semester | Subject Code | Category | Instruction Hours | | | | | | Credits |
|---|---|---|---|---|---|---|---|---|---|
| | | | Lecture | | Theory | | Practical | | |
| | | | Per Week | Per Semester | Per Week | Per Semester | Per Week | Per Semester | |
| I | | Elective | 3 | 45 | 3 | 45 | 0 | 0 | 3 |

**COURSE OBJECTIVES:**

- To understand the concepts of drug design, drug metabolism, mechanism of drug – receptor binding and its structure activity relationship qualitatively and quantitatively.
- To enhance the knowledge in the various areas of molecular modelling, molecular docking and drug design techniques with detail concepts of all the mentioned areas.

**COURSE OUTCOME:**

- On completion of the course, the student should be able to:

| CO Number | CO statement | Knowledge level |
|---|---|---|
| **CO1** | Learn about the ligands based on its electronic level using computational quantum chemistry | **K2, K3 & K4** |
| **CO2** | Justify the role and importance of the various disciplines involved in the different phases of drug discovery and development, identification of gobal reactivity indicators of compounds using computer methodologies and molecular modeling including artificial intelligence methods. | **K2, K3 & K4** |
| **CO3** | Get clear idea about the use of computational chemistry in structure based drug design, drug development as a process involving target selection, lead discovery using computer-based methods and computational chemistry/high-throughput screening. | **K3 & K4** |
| **CO4** | Describe the safety evaluation, bioavailability, clinical trials, essentials used for drug development and also acquire knowledge about molecular recognition, computer aided drug design and toxicology as applied to the development of new medicines | **K2, K3 & K4** |
| **CO5** | Get knowledge about molecular docking, simulation and dynamic in drug designing and development process. | **K2, K3 & K4** |

*CO-Course Outcomes

Knowledge level K1-Remember; K2-Understand; K3-Apply; K4-Analyze

**MAPPING WITH PROGRAM OUTCOMES**

| COS | PO1 | PO2 | PO3 | PO4 | PO5 | PO6 |
|---|---|---|---|---|---|---|
| **CO1** | S | S | S | M | M | M |
| **CO2** | M | S | M | M | S | M |
| **CO3** | M | S | M | S | S | M |
| **CO4** | M | S | S | S | S | M |
| **CO5** | M | M | S | S | S | S |

**UNIT-I Electronic Structure methods** **9 hours**

Quantum chemical methods - semi-empirical and ab initio methods - Conformational analysis, energy minimization, comparison between global minimum conformation and bioactive conformation - Predicting the mechanism of organic reactions using electronic structure methods - Complete and constrained conformational search methods, their advantages and disadvantages - Theoretical aqueous solvation calculations for design of ligands - Conformational interconversion, transition-state determination and their role in designing rigid analogs.

**UNIT-II Molecular modeling** **9 hours**

Molecular Mechanics, Quantum Mechanics, Energy minimization, geometry optimization, conformational analysis, global conformational minima determination - approaches and problems - Bioactive vs. Global minimum conformations - Automated methods of conformational search - Advantages and limitations of available software - Molecular graphics - Molecular properties, reactivity, Homo, Lumo, Electrostatic potential - Solvent accessible surface - Computer methodologies behind molecular modeling including artificial intelligence methods.

**UNIT-III DRUG DESIGN** **9 hours**

Drug design strategies-rational drug design: Inhibitors of ACE; structure based drug design: Anti HIV agents; ligand based approach - Design of agonist and antagonist: β2-Agonists and the treatment of asthma - Discovery of the H2–receptor antagonist - Transition state analogues - Pro drug concept - prodrugs of ampicillin, elanapril and propranolol.

SAR: Qualitative versus quantitative approaches - advantages and disadvantages - Random screening - Non-random screening.

**UNIT-IV Qsar and Drug Metabolism** **9 hours**

QSAR - Electronic effects - Hammett equation - lipophilicity effects - Hansch equation, stericeffects - Taft equation - Experimental and theoretical approaches for the determination of physico-chemical parameters - parameter inter-dependence.

Adsorption, distribution, metabolism and elimination - Methods of drug administration, drug solubility and lipophlicity, clogP. cell membrane permeability, blood brain barrier Lipinski's rule of five – Metabolism - first pass metabolism, chemical and metabolic stability-bioavailability and bioequivalence - concept of drug half life -therapeutic window.

**UNIT – V Molecular docking and dynamics** **9 hours**

Rigid docking, flexible docking, manual docking - Advantages and disadvantages of Flex-X, Flex-S, Autodock and Dock softwares, with successful examples.

Molecular dynamics: Dynamics of drugs, biomolecules, drug-receptor complexes, Monte

Carlo simulations and Molecular dynamics in performing conformational search and docking - Estimation of free energy from dynamical methods

**Distribution of Marks**: Theory-80% and Problems-20%

**TEXT BOOKS**

| S. No | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| 1. | Burger | Medicinal Chemistry and Drug Discovery | 5th Edn | 1995 |
| 2. | R. B. Silverman | Chemistry of Drug Design and Drug action | Acad. press | 2004 |
| 3. | Graham Patrick | An Introduction to Medicinal Chemistry | 2nd Edn. Qxford | 2010 |
| 4. | N. K. Jain | Advances in Controlled and Novel Drug Delivery | CBS | 2001 |
| 5. | Lednicer | The Organic Chemistry of Drug Synthesis | Vol.1, 5th Edition, John Wiley & Sons | 2001 |
| 6. | Foye's | Principles of Medicinal Chemistry, | Sixth Edition, Wolters Kluwer | 2008 |
| 7. | G.R. Chatwal | Medicinal Chemistry | Himalaya Publishing House | 2007 |
| 8. | V.K. Ahluwalia and M. Chopra | Medicinal Chemistry | Ane Book Pvt. Ltd. | 2008 |

**REFERENCE BOOKS**

| S.No | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| 1. | R.B. Silverman | Organic Chemistry of Drug Design and Drug Action | Academic Press | 2012 |
| **2.** | William H, Malick JB | Drug Discovery and Development | Humana Press Clifton. | 2004 |

**TEACHING METHODOLOGY:**

- Board and chalk

- PowerPoint presentation
- Models
- Group discussion
- Seminar and Assignments
- Animated videos

**SYLLABUS DESIGNERS:**

1. 1. Dr.P.N.Sudha, Principal, Department of Chemistry
2. Dr.M.Nagarathinam, Head & Associate Professor, Department of Chemistry
3. Dr.S.Santha Lakshmi, Assistant Professor, Department of Chemistry
4. Dr.S.Sashikala, Assistant Professor, Department of Chemistry
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## ELECTIVE PAPER-C: GREEN CHEMISTRY

| Semester | Subject Code | Category | Instruction Hours | | | | | | Credits |
|---|---|---|---|---|---|---|---|---|---|
| | | | Lecture | | Theory | | Practical | | |
| | | | Per Week | Per Semester | Per Week | Per Semester | Per Week | Per Semester | |
| I | | Elective | 3 | 45 | 3 | 45 | 0 | 0 | 3 |

**COURSE OBJECTIVES**

- To understand the green chemistry strategies for designing the chemical synthesis.
- To make the students knowledgeable about solvent - free synthesis, ultrasound and microwave assisted green synthesis

**COURSE OUTCOME**

- On completion of the course, the student should be able to:

| CO Number | CO statement | Knowledge level |
|---|---|---|
| **CO1** | Gain knowledge about the basic principles and designing of safer chemicals to produce biodegradable products | **K2 & K3** |
| **CO2** | Get clear idea about the solvent - free green synthesis, ultrasound and microwave assisted green synthesis | **K3 & K4** |
| **CO3** | Understand polymer supported catalytic reactions and ionic liquids as green solvents in synthesizing various products | **K3 & K4** |
| **CO4** | Acquire knowledge about the phase transfer catalysis in green synthesis | **K2 & K3** |
| **CO5** | Gain clear knowledge about industrial case studies such as reverse tanning, vegetable tanning and chrome tanning | **K3 & K4** |

* CO-Course Outcomes
Knowledge level K1-Remember; K2-Understand; K3-Apply; K4-Analyze

**MAPPING WITH PROGRAM OUTCOMES**

| COS | PO1 | PO2 | PO3 | PO4 | PO5 | PO6 |
|---|---|---|---|---|---|---|
| **CO1** | S | S | S | M | M | M |
| **CO2** | S | S | M | M | S | M |
| **CO3** | M | S | S | M | S | M |
| **CO4** | M | S | S | M | S | M |
| **CO5** | M | M | S | S | S | S |

**UNIT- I: Basic Principles of Green Chemistry** **9 hours**

Basic principles - prevention of waste/by-products, maximum incorporation of the reactants (starting materials and reagents) into the final product, prevention or minimization of hazardous products, designing safer chemicals, energy requirements for synthesis, selection of appropriate solvent, selection of starting materials, use of protecting groups, use of catalyst and products designed should be biodegradable.

**UNIT- II: Ultrasound and Microwave Assisted Green Synthesis** **9 hours**

Ultrasound: Introduction, instrumentation, the phenomenon of cavitation - Sonochemical esterification, substitution, addition, alkylation, oxidation, reduction and coupling reactions - Microwaves: Introduction, concept, reaction vessel/ medium, specific effects, atom efficiency (% atom utilization), advantages and limitations - N-alkylation and alkylation of active methylene compounds and Diels –Alder reactions. Reactions in water and reaction in organic solvents - Solvent - free reactions and deprotection of esters.

**UNIT- III: Ionic-Liquids as Green Solvents** **9 hours**

Introduction - structure, synthesis and applications of some important ionic liquids in organic synthesis - Polymer supported reagents in green synthesis - Introduction - properties and advantages of polymer supported reagents and choice of polymers - Substrate covalently bound to the support - Synthesis of oligosaccharides - intramolecular cyclisation - Selective chemical reactions on one aldehyde group of symmetrical aldehydes - Asymmetric synthesis - Reagent linked to a polymeric material - Preparation of sulfonazide polymer and application in diazotransfer reaction - Synthesis of polymer bound per acid and its applications - synthesis of polystyrene tin dichloride resin and its applications - Polymer supported catalytic reactions - Preparation of polymer supported $AlCl_3$ and applications - polymer supported photosensitizers.

**UNIT- IV: Phase Transfer Catalysis In Green Synthesis** **9 hours**

Introduction - mechanism of phase transfer catalyst reaction - types and advantages of phase transfer catalyst - types and applications of phase transfer reaction - Nitriles from alkyl or acyl halides, alkyl fluorides, alcohols, azides from alkyl halides - generation of dichlorocarbenes - addition to olefins - elimination reaction - alkylation reactions - Willamson synthesis - Benzoin condensation - Darzen reaction - Michael reaction - Wittig reaction - oxidation under PTC condition and reduction.

**UNIT-V: Industrial Case Studies** **9 hours**

Methyl Methacrylate (MMA) - Greening of Acetic acid manufacture - Vitamin-C - Leather manufacture -Types of Leather- Difference between Hide and Skin - Tanning – Reverse tanning -Vegetable tanning - Chrome tanning - Fat liquoring – Dyeing – Application - Polyethylene-Ziegler Natta Catalysis - Metallocene Catalysis - Ecofriendly Pesticides and Insecticides.

**Distribution of marks :** Theory -100%

**TEXT BOOKS**

| S.No | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| **1.** | V.K.Ahluwalia and M. Kidwai | New Trends in Green Chemistry | II Edn., Anamaya publishers New Delhi | 2007 |
| **2.** | Mike Lancaster | Green Chemistry and Introductory text | II Edition | 2002 |
| **3.** | V. K. Ahluwalia and R. Aggarwal, Narosa | Organic Synthesis, Special Techniques | New Delhi | 2003 |
| **4.** | Mike Lancaster | Green Chemistry – an introduction text | Royal Society of Chemistry, UK | 2002 |
| **5.** | W. B. Weber, G. W. Gokel, Springer, Berlin,. | Phase Transfer Catalysis in Organic Synthesis | Springer | 1977 |

**REFERENCES BOOKS**

| S.No | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| **1.** | R. Sanghi and M. Srivastava | Green Chemistry - Environment Friendly Alternatives | New Delhi | 2003 |
| **2.** | P. T. Anastas and J. C. Warner | Green Chemistry - Theory and Practice | Oxford University press. Oxford | 1988 |
| **3.** | N. K. Mathur, C. K. Narang and R. E. Williams | Polymers as Aids in Organic Synthesis | Academic Press, NY | 1980 |

| | | | | |
|---|---|---|---|---|
| **4.** | E. V. Dehmlov, S. S. Dehmlov | Phase Transfer Catalysis | 2nd Edn., Verlagchemie, Wienhein | 1983 |

**TEACHING METHODOLOGY:**

- Board and chalk
- PowerPoint presentation
- Models
- Group discussion
- Seminar and Assignments
- Animated videos

**SYLLABUS DESIGNERS:**

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9. Mrs. R. Bharathi Priyadharsini, Assistant Professor, Department of Chemistry

**SELF STUDY PAPER (OPTIONAL)**

**ENVIRONMENTAL CHEMISTRY FOR A SUSTAINABLE WORLD**

| Semester | Subject Code | Category | Instruction Hours | | | | | | Credits |
|---|---|---|---|---|---|---|---|---|---|
| | | | Lecture | | Theory | | Practical | | |
| | | | Per Week | Per Semester | Per Week | Per Semester | Per Week | Per Semester | |
| I | | Self study Paper (Optional) | - | - | - | - | - | - | 2* |

## COURSE OBJECTIVES

- To provide an insight into the chemical reactions and to apply the principles in analysing pollution in water, air and soil environment.
- To provide an understanding on the fate of chemicals on the environment and suggest relevant interventions.

## COURSE OUTCOMES

- On the successful completion of course, students will be able to

| CO Number | CO statement | Knowledge level |
|---|---|---|
| **CO1** | Gain the knowledge on atmosphere of earth, global warming and greenhouse gases | **K1 & K2** |
| **CO2** | Gain the knowledge on contaminants, their natural pathways of degradation and their abatement | **K2 & K3** |
| **CO3** | Acquire knowledge about the various physicochemical parameters which affect the environment | **K3** |
| **CO4** | Have a better understanding of soil and water quality parameters by analysing the contaminated samples | **K2 & K4** |
| **CO5** | Gain knowledge on the various industrial wastewater treatment methods | **K3 & K4** |

*CO-Course Outcomes

Knowledge level K1-Remember; K2-Understand; K3-Apply; K4-Analyze

**MAPPING WITH PROGRAM OUTCOMES:**

| COS | PO1 | PO2 | PO3 | PO4 | PO5 | PO6 |
|---|---|---|---|---|---|---|
| **CO1** | M | S | M | M | M | M |
| **CO2** | M | S | M | M | M | M |
| **CO3** | M | S | M | M | M | S |
| **CO4** | M | S | M | M | M | S |
| **CO5** | M | S | M | M | M | S |

**UNIT – I : Atmospheric Chemistry**

The atmosphere of Earth-Contaminant behavior in the environment-Green house effect - Global Warming -Acid rain and - Ozone layer depletion.

Fundamental concepts in chemistry – Elements and compounds – Atomic structure – Formation of molecules – Solutions: normality, molality and molarity – Ionization – radicals – Expressing concentrations.

**UNIT II: Contaminants and Their Natural Pathways of Degradation and Their Abatement**

Carbon Cycle, Nitrogen Cycle, Sulphur Cycle, CO formation in atmosphere, Organic Pollutants, Pollution from Combustion Systems, Coal, Combustion, Photochemical Smog and Indoor Air Pollution

**UNIT- III: Physicochemical Parameters**

pH – Electrical conductivity – Total solids – Total suspended solids – Dissolved oxygen – Carbonates – bicarbonates – Hardness – Calcium – Magnesium – Total alkalinity – Fluoride – Iron – Nitrate – Nitrite –Phosphate Biochemical Oxygen Demand (BOD) – Chemical Oxygen Demand (COD). Biological Parameters: Macrophytes – Phytoplankton – Zooplankton – Primary Productivity. Bacteriological measurements-Standard Plate count method – MPN (Most Probable number)

**UNIT-IV: Soil and Water Analysis**

Nature of soil – Soil macro and micronutrients – Soil structure and texture – Soil water – Soil air – Soil Temperature – Soil organic matter .Water - Characteristics of bodies of water-Properties of water – Hydrogen Bonding – covalent bonding – ionic bonding –Water sampling: Sampling stations-Collection of water samples – Handling and Preservation. Water analysis: Physical parameters: Colour – Temperature – Transparency – Turbidity.

**UNIT - V: Industrial Chemistry**

Classification of Industries Based on Environmental Impacts, Criteria for Selection of Site for Establishment of Industry, Socio-economic and Environmental Impacts of Industries, Legal and Statutory Requirements, Manufacturing Process and the Sources of Wastes, Characterization & Treatment of Industrial Waste with respect to Paper and Pulp, Tannery, Textile, Dairy, Sugar, Petrochemical, Pharmaceutical, Oil Refinery and Power Plants-Thermal, Gas Based and Hydroelectric.

**Distribution of Marks**: Theory-90% and Problems-10%

**TEXT BOOKS**

| S.No | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| 1. | Manahan,Stanley E. | Fundamentals of Environmental Chemistry | Boca Raton, CRC Press, LLC | 2001 |
| 2. | Sonja Krause, Herbert M. Clark, James P. Ferris, Robert L | Strong Chemistry of the Environment | Elsevier Science & Technology | 2002 |
| 3. | Eugene R. Weiner 2000 CRC Press, LLC | Applications of Environmental Chemistry | CRC Press, LLC | 2000 |
| 4. | Clair N.Sawyer, Perry L. McCarty, Gene F.Parkin, | Chemistry for environmental engineering and science | McGraw Hill, 5th Edition | 2002 |

**SYLLABUS DESIGNERS:**

1. Dr.P.N.Sudha, Principal, Department of Chemistry
2. Dr.M.Nagarathinam, Head & Associate Professor, Department of Chemistry
3. Dr.S.Santha Lakshmi, Assistant Professor, Department of Chemistry
4. Dr.S.Sashikala, Assistant Professor, Department of Chemistry
5. Dr.N.Dhanam, Assistant Professor, Department of Chemistry
6. Dr. K. Vijayalakshmi, Assistant Professor, Department of Chemistry
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8. Mrs. J. Saranya, Assistant Professor, Department of Chemistry
9. Mrs. R. Bharathi Priyadharsini, Assistant Professor, Department of Chemistry

# PAPER-IV: COORDINATION CHEMISTRY

| Semester | Subject Code | Category | Instruction Hours | | | | | | Credits |
|---|---|---|---|---|---|---|---|---|---|
| | | | Lecture | | Theory | | Practical | | |
| | | | Per Week | Per Semester | Per Week | Per Semester | Per Week | Per Semester | |
| II | | Core | 3 | 45 | 3 | 45 | 0 | 0 | 3 |

## COURSE OBJECTIVES:

- To learn about thermodynamic and stereochemical aspects of complex formation, various theories of complexes, magnetic properties, term symbols and energy level diagram of weak and strong field ligands, charge transfer spectra and spectral properties of lanthanides and actinides.
- To learn about various mechanisms of substitution and electron transfer reactions and to study the recent development in the catalysis

## COURSE OUTCOMES:

- On the successful completion of course, students will be able to

| CO Number | CO statement | Knowledge level |
|---|---|---|
| **CO1** | Get better understanding of stability constant, types of macrocyclic ligands and nomenclature of chiral complexes | **K2 & K4** |
| **CO2** | Identify the principles, structure and reactivity of selected coordination complexes with the help of crystal field theory and molecular orbital theory | **K2 & K3** |
| **CO3** | Interpret their electronic spectra, magnetic properties and can gain knowledge about the distortion in co-ordination complexes concept of sigma and pi bonding in complexes | **K2 & K4** |
| **CO4** | Get clear knowledge about the ISM, OSM, reaction mechanism of coordination compounds and the application of substitution reactions in the synthesis of Platinum and Cobalt complexes | **K3 & K4** |
| **CO5** | Identify the bonding aspects of simple organometallic compounds, different types of organometallic reactions and to explain different catalytic reactions | **K2 & K3** |

* CO-Course Outcomes

Knowledge level K1-Remember; K2-Understand; K3-Apply; K4-Analyze

**MAPPING WITH PROGRAM OUTCOMES**

| COS | PO1 | PO2 | PO3 | PO4 | PO5 | PO6 |
|---|---|---|---|---|---|---|
| **CO1** | M | M | M | M | S | S |
| **CO2** | M | M | S | S | S | M |
| **CO3** | S | S | S | S | S | S |
| **CO4** | M | S | S | M | M | M |
| **CO5** | M | S | S | S | M | M |

**UNIT-I: Stability of Complexes** **9 hours**

Stability of complexes – Factors affecting stability of complexes – Thermodynamic aspects of complex formation – Stepwise and overall formation constants – Stability correlations – statistical factors and chelate effect – Determination of stability constant and composition of the complexes – Formation curves and Bjerrum's half method – Potentiometric method – Spectrophotometric method – Ion exchange method – Polorographic method and Continuous variation method (Job's method)

Stereochemical aspects – Stereoisomerism in inorganic complexes – Isomerism arising out of ligand distribution and ligand conformation – Chirality and nomenclature of chiral complexes; Application of ORD and CD in the identification of complexes.

Macrocyclic ligands – Porphyrins, Corrins, Schiff's bases and crown ethers.

**UNIT-II: Metal – Ligand Bonding** **9 hours**

Crystal field theory – Splitting of d – orbitals under various geometries – factors affecting splitting, CFSE, evidences for CFSE (Structural and thermodynamic effects), spectrochemical series – Jorgensen relation – site preferences – Jahn Teller distortion – Dynamic and Static J.T. effect – Application of CFT – Magnetic properties – spectral properties and Kinetic properties – Limitations of CFT – Evidences for Metal – Ligand overlap.

MOT – MO theory and energy level diagrams concept of Weak and strong fields – Sigma and pi bonding in octahedral, square planar and tetrahedral complexes – Nephlauxetic effect – Magnetic properties of complexes – Comparison of CFT and MOT of bonding in octahedral complexes.

**UNIT-III: Electronic Spectra of Complexes** **9 hours**

Spectroscopic term symbols for $d^n$ ions – derivation of term symbols and ground state term symbol – Hund's rule – Selection rules – breakdown of selection rules – spin orbit coupling, band intensities, weak and strong field limits – correlation diagram – Energy level

diagrams – Orgel diagram for weak field Oh and Td complexes – Splitting of energy level due to Jahn-Teller distortion – Modified orgel diagram – Limitiations of orgel diagram Tanabe–Sugano(T-S) diagrams – Evaluation of Dq and B values for $d^2$ –$d^8$ complexes – charge transfer – spectra – Complications in band classification between Lf(d-d) and CT bands – Comparison between d-d bands and CT bands – Numerical problems – Lanthanides and Actinides – Spectral properties-Lanthanide contraction.

**UNIT IV: Electron Transter Reactions 9 hours**

Electron transfer reactions – Potential energy well diagram – Inner sphere (ISET) and outer sphere (OSET) electron transfer processes – Differences between ISM and OSM – Role of bridging ligand with ISET reaction – formation and rearrangement of precursor complexes – Nature of bridging ligand – fission of successor complexes – Complementary and non complementary ET reactions – Cross reactions and Marcus Hush theory.

Reaction mechanism of coordination compounds – Types of ligand substitution reactions – mechanism; Dissociative mechanism (D), Associative mechanism (A) and interchange mechanism (I).

**UNIT-V: Substitution Reactions 9 hours**

Labile and Inert complexes – Substitution Reaction in octahedral complexes – replacement of coordinated water, mechanism of acid hydrolysis, base hydrolysis – DCB mechanism – direct and indirect evidences in favour of the mechanism – Ligand substitution reactions without cleavage of M-L Bond – Anation Reactions – Substituion in square planar complexes – General mechanism, Trans effect – influences of entering, leaving and other groups. Application of trans effect – synthesis of isomers of Pt(II) complexes – theories of trans effect and cis-trans isomerisation reaction – Application of substitution reactions in the synthesis of Platinum and Cobalt complexes.

**Distribution of hours:** Theory-70%; Problems-30%

**TEXT BOOKS**

| S.No | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| 1. | H. J. Emelius and Sharpe | Modern aspects of Inorganic chemistry | Universal book stall, New Delhi | 1989 |
| 2. | F. Basolo and R.G. Pearson | Mechanism of Inorganic reactions | Wiley Eastern | 1967 |
| 3. | J. E. Huheey, E. A. Keiter and R. L. Keiter | Inorganic chemistry- Principles on structure and reactivity | 4th Ed, Pearson-education | 2002 |
| 4. | F. A. Cotton and G.Wilkinson | Advanced Inorganic Chemistry | Wiley Eastern | 1988 |
| 5. | S. F. A. Kettle | Co-ordination compounds | ELBS | 1973 |
| 6. | K. F. Purcell and J. C. Kotz | Inorganic Chemistry | WB Sanders Co, USA, | 1977 |
| 7. | D. F. Shriver, P. W. Atkins and C. H. Longford | Inorganic Chemistry | ELBS, 2nd Ed | 1994 |
| 8. | R. B. Heslop and K. Jones | Inorganic Chemistry | Elsevier | 1976 |
| 9. | D. Bannerjea | Co-ordination Chemistry | TATA Mcgraw Hill | 1993 |
| 10. | M. L. Tobe | Inorganic Reaction Mechanism | Nelson | 1972 |
| 11 | K.Burjer | Co-ordination Chemistry Experimental Methods, | Butterworths | 1973 |
| 12 | B.N.Figgis, | Introduction to Ligand Fields | Wiley Eastern Ltd, | 1976 |
| 13 | W.E.Addision | Structural Principles of Inorganic Chemistry | Longman | 1961 |

**REFERENCE BOOKS**

| S.No | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| **1.** | S.F.A. Kettle | Coordination Chemistry | EIBS | 1973 |
| **2.** | K. Burger | Coordination Chemistry | Burter Worthy | 1973 |
| **3.** | K.F. Purcell and J.C. Kotz | Inorganic Chemistry | WB Saunders Co., USA | 1977 |

**TEACHING METHODOLOGY:**

- PowerPoint presentation
- Models
- Group discussion
- Seminar and Assignments
- Animated videos
- Board and chalk

**SYLLABUS DESIGNERS:**

1. Dr.P.N.Sudha, Principal, Department of Chemistry
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# PAPER-V: ORGANIC REACTION MECHANISMS AND REARRANGEMENTS

| Semester | Subject Code | Category | Instruction Hours | | | | | | Credits |
|---|---|---|---|---|---|---|---|---|---|
| | | | Lecture | | Theory | | Practical | | |
| | | | Per Week | Per Semester | Per Week | Per Semester | Per Week | Per Semester | |
| II | | Core | 3 | 45 | 3 | 45 | 0 | 0 | 3 |

**COURSE OBJECTIVES:**

- Understanding addition, elimination, rearrangement and naming reactions along with their mechanism and synthetic utility.
- Understanding various types of oxidation and reduction reactions along with their mechanism and synthetic utility.

**COURSE OUTCOMES:**

- On the successful completion of course, students will be able to

| CO Number | CO statement | Knowledge level |
|---|---|---|
| CO1 | Get a clear picture about the addition reactions happening through nucleophilic, electrophilic groups and to learn about the addition reactions between double bonded carbon compounds | **K2 & K3** |
| CO2 | Gain knowledge on the nucleophilic and electrophilic additions to carbonyl compounds and naming reactions | **K2 & K3** |
| CO3 | Obtain an outline about elimination reactions and the rules used to study elimination reactions with some specific examples | **K3** |
| CO4 | Acquire knowledge about the reagents which causes various rearrangement reactions | **K2 & K3** |
| CO5 | Learn about the basic mechanism of oxidation in various organic compounds such as alcohols, aldehydes, ketones, olefins etc and two types of reduction reactions like complete reduction and selective reduction using different reducing agents | **K2 & K4** |

* CO-Course Outcomes

Knowledge level K1-Remember; K2-Understand; K3-Apply; K4-Analyze

**MAPPING WITH PROGRAM OUTCOMES**

| COS | PO1 | PO2 | PO3 | PO4 | PO5 | PO6 |
|---|---|---|---|---|---|---|
| **CO1** | M | M | M | M | S | S |
| **CO2** | M | M | S | S | S | M |
| **CO3** | M | M | M | M | S | M |
| **CO4** | M | S | S | S | S | M |
| **CO5** | M | S | S | S | M | S |

**UNIT-I: Addition to Carbon-Carbon Double Bond** **9 hours**

Electrophilic addition to carbon – carbon double and triple bonds – Nucleophilic addition to carbon–carbon multiple bonds – Generation and addition of carbenes-Michael addition and Robinson annulation.

Hydroxylation of olefinic double bonds ($OsO_4$, $KMnO_4$); Woodward and Prevost oxidation – Epoxidation using peracids including Sharpless epoxidation – Ozonolysis. Hydrogenation (homogenous and heterogeneous) and Transfer hydrogenation – Hydroboration – Hydration of carbon-carbon double and triple bonds.

**UNIT-II: Addition to Carbon-Oxygen Double Bond** **9 hours**

Nucleophilic addition to –C=O bond – A study of Mannich, benzoin, Darzen's glycidic ester, Stobbe and Knovenagel condensation reactions – Wittig, Wittig-Horner olefination reactions; Sulfur and Sulfonium ylides and their reactions – Julia olefination and Peterson alkene synthesis – Asymmetric reduction of carbonyl functions (Corey's procedure).

**UNIT-III: Elimination** **9 hours**

Elimination reactions: E1, E2, E1cb and Ei-elimination – Conformation of mechanism; solvent, substrate, leaving group effects – Typical elimination reactions – dehydration, dehydrohalogenation and dehalogenation – Saytzeff's *Vs* Hoffmann elimination; Stereochemistry of $E_2$ eliminations – Elimination in cyclohexane ring system; Mechanism of pyrolytic eliminations – Examples: Chugaev reactions and Cope elimination – Hoffmann degradation and pyrolysis of esters.

**UNIT-IV: Molecular Rearrangments and Reactions** **9 hours**

A study of mechanism of the following rearrangements: Beckmann, Curtius, Hofmann, Schmidt, Lossen, Pinacol, Wagner – Meerwin, Demjanov, Dienone – Phenol, Favorski, Benzidine, Claisen, Cope, Sommlet – Hauser, Pummerer, Baeyer – Villiger, Wolf, Stevens and Von – Richter rearrangements.

A study of the following name reactions: Dieckmann cyclization, Hofmann – Loffler Freytag reaction, Mitsunobu reaction, Shapiro reaction, Eschenmoser – Tanabe and Ramburg – Backlund reactions.

**UNIT-V: Oxidation and Reduction Reactions** **9 hours**

Oxidation of methylene to carbonyl, oxidation of aryl methenes – allylic oxidation of olefins – Oxidation with Cr (including PCC, PDC, Jones) and Mn (including $MnO_2$ and $BaMnO_4$) reagents; Oxidation with LTA, DDQ, $Hg(OAc)_2$ and $SeO_2$; Oxidation using DMSO either with DCC or $Ac_2O$ or Oxaloyl chloride; Oxidation using IBX and Dess-Martin Periodinane (DMP) reagent.

Clemmenson and Wolf-Kishner reduction – Huang Millon modification – Birch reduction and MPV reduction. Reduction with sodium borohydride, lithium aluminium hydride, tritertiarybutoxyaluminium hydride, sodium Cyanoborohydride, $Zn(BH_4)_2$, DIBAL-H, Red-Al, $Et_3SiH$ and $Bu_3SnH$. Selectrides – Selectivity in reduction 4-t-butylcyclohexanone using selected hydride reductions.

**Distribution of hours:** Theory-90%; Problems-10%

**TEXT BOOKS**

| S.No | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| 1 | Jerry March | Advanced Organic Chemistry | John Wiley & Sons, 5th Ed | 2001 |
| 2 | F. Carey and R. J. Sundberg | Advanced Organic Chemistry-Part A and B | Springer Science 5 th Ed | 2007 |
| 3 | M. B. Smith and Jerry March | Advanced Organic Chemistry | John Wiley & Sons, 5th Ed | 2001 |

| | | | | |
|---|---|---|---|---|
| 4 | J. Clayden, N. Greeves and S. Warren | Organic Chemistry, | Oxford University Press, 2nd Ed | 2012. |
| 5 | M. B. Smith | Organic Synthesis, | Academic Press 3rd Ed | 2011 |
| 6 | R. O. C. Norman and J. M. Coxon, | Principles of Organic Synthesis | Chapman & Hall, 3rd Ed | 1993 |
| 7 | Stuart Warren | Organic Synthesis | Disconnection Approach, Wiley India (P) Ltd | 2007 |
| 8 | V.K.Ahluwalia | Oxidation in Organic Synthesis | CRC Press, 1st Ed | 2012 |
| 9 | V.K.Ahluwalia | ,Reduction in Organic Synthesis | CRC Press, 1st Ed | 2012 |

**TEACHING METHODOLOGY:**

- PowerPoint presentation
- Models
- Group discussion
- Seminar and Assignments
- Animated videos
- Board and chalk

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## PAPER-VI: QUANTUM CHEMISTRY AND ANALYTICAL TECHNIQUES

| Semester | Subject Code | Category | Instruction Hours | | | | | | Credits |
|---|---|---|---|---|---|---|---|---|---|
| | | | Lecture | | Theory | | Practical | | |
| | | | Per Week | Per Semester | Per Week | Per Semester | Per Week | Per Semester | |
| II | | Core | 4 | 60 | 4 | 60 | 0 | 0 | 4 |

## COURSE OBJECTIVES

- To learn the principles of quantum mechanics of simple systems, quantum mechanical treatment of multi electron atoms.
- To learn the principles, instrumentation, interpretation and applications of micro wave, IR, Raman spectroscopy, Polarography, Amperometry, Coulometry, various thermal analysis, various elemental analysis and surface analysis techniques

## COURSE OUTCOMES:

- On the successful completion of course, students will be able to

| CO Number | CO statement | Knowledge level |
|---|---|---|
| CO1 | Revise and update the mathematical concepts of vectors and tensors to chemical systems by solving eigenvalue and eigenvector problems in matrices and first and second order differential equations that are used for solving the time independent Schrodinger equation, particle in a potential-free box, particle on a ring, harmonic oscillator and particle in a Coulomb potential exactly and demonstrate the solutions for hydrogen atom and molecular rotations and vibrations | **K2 & K3** |
| CO2 | Calculate the energy of simple mujltielectron atoms and molecules, solve all the model problems in quantum mechanics for which exact analytical methods and solutions are available and will apply them to analyze the basis behind the postulatory method of quantum mechanics | **K3 & K2** |
| CO3 | Gain knowledge about the basic principles of rotational and vibrational spectroscopic techniques in different researches | **K3 & K4** |
| CO4 | Acquire knowledge about the basic principles of various electroanalytical techniques such as polarography, amperometry and to study the importance of potentiometric, conductometric and complexometric titration | **K2 & K4** |
| CO5 | Get better understanding of principles, instrumentation and applications of various elemental analysis, surface analysis techniques which will be employed in current research nano projects | **K2 & K3** |

* CO-Course Outcomes

Knowledge level K1-Remember; K2-Understand; K3-Apply; K4-Analyze

**MAPPING WITH PROGRAM OUTCOMES**

| COS | PO1 | PO2 | PO3 | PO4 | PO5 | PO6 |
|---|---|---|---|---|---|---|
| **CO1** | M | M | M | M | S | S |
| **CO2** | M | M | S | S | S | M |
| **CO3** | M | M | M | M | S | M |
| **CO4** | M | S | S | S | S | M |
| **CO5** | M | S | S | S | M | S |

**UNIT-I: Quantum Chemistry-I** **12 hours**

Black body radiation – Planck's quantum theory – Wave particle duality – Uncertainty Principle. Operators-linear, commutation, Hermitian and Hamiltonian operators – Eigen functions and Eigen values-Postulates of quantum mechanics – Derivation of Schrodinger's time-independent wave equation and its application to particle in a one dimensional box – particle in a three dimensional box, harmonic oscillator, rigid rotor and hydrogen atom.

**UNIT-II: Quantum Chemistry-II** **12 hours**

Born-Oppenheimer approximation-Hydrogen molecule ion – LCAO-MO and VB treatments of the hydrogen molecule – Antisymmetry and Pauli's exclusion principle. Slater detrimental wave function, term symbols and spectroscopic states – Russell Saunders coupling.

The variation theorem and Perturbation theory. Applications of variation method and perturbation theory to helium atom. Hybridization – determination of bond angles of sp, $sp^2$ and $sp^3$ hybridizations – Huckel pi electron (HMO) theory and its applications to ethylene, butadiene and benzene – A brief idea of Hartree and Hartree-Fock self consistent field theory.

**UNIT III: Rotational and Vibrational Spectroscopy** **12 hours**

Microwave spectroscopy – Theory – selection rules – Instrumentation; Energy levels in atoms and molecules – Fourier transformation Rotational spectra of diatomic and polyatomic molecules – P,Q,R branches – effect of isotopic substitution. Non – rigid rotator – Linear molecules. Theory of Rotational Raman spectra.

Vibrational spectra of diatomic molecules – selection rules – overtones, combination and hot bands - Fermi resonance Energy of diatomic molecule – simple harmonic and unharmonic oscillator, rotational character of vibration spectra – Theory of Vibrational Raman spectroscopy-Coherant – Antistokes Raman Spectroscopy (CARS).

**UNIT-IV: Spectro and Electroanalytical Techniques** **12 hours**

X-ray Photoelectron Spectroscopy **(**XPS), Atomic absorption Spectroscopy (AAS),

Atomic emission spectroscopy (AES) – Principles, theory, instrumentation and applications – interpretation of spectra – Merits and demerits – Coloumetry – Polarography – theory, apparatus, DME – Diffusion, Kinetic and catalytic currents – Current – voltage curves for reversible and irreversible system – qualitative and quantitative applications to inorganic system.

Amperometric titrations – theory, apparatus, types of titration curves, successive titration and indicator electrodes – Applications. Cyclic voltametry – theory, application to inorganic systems. Potentiometric, conductomertric and complexometric titrations – Masking and demasking agents

**UNIT V: Surface and Thermal Analysis Techniques 12 hours**

Principles, theory, instrumentation and applications of Scanning Electron Microscopy (SEM), Scanning Tunneling Microscopy (STM), Transmission Electron Microscopy (TEM), Energy Dispersive X-ray Analysis (EDAX), Atomic Force Microscopy (AFM), Electron Spectroscopy for Chemical Analysis (ESCA)– interpretation of spectra – Merits and demerits.

Principles, theory and applications of Thermo Gravimetric Analysis, DTA, DSC, DTG. Interpretation of various thermal analysis curves.

**Distribution of hours: Theory-70%; Problems-30%**

**TEXT BOOKS**

| S.No | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| 1 | P. W. Atkins | Molecular Quantum Mechanics | Oxford University Press, Oxford | 1983 |
| 2 | M. W. Hanna, Quantum | Mechanics in Chemistry | W. A Benjamin Inc. London | 1965 |
| 3 | I. N. Levine | Quantum Chemistry | Allyn and Bacon,Boston | 1983 |
| 4 | H. Eyring, J. Walter and G. Kimball, | Quantum Chemistry, Quantum Chemistry | John Wiley and Sons, New York, | 1944 |
| 5 | M. W. Hanna | Mechanics in Quantum Chemistry | W.A. Benjamin Inc. London | 1965. |
| 6 | G. M. Barrow | Introduction to Molecular Spectroscopy | McGraw Hill, New York | 1988. |
| 7 | D. A. McQuarrie | Quantum Chemistry | University Science Books, MilValley, | 1998. |

| | | | | |
|---|---|---|---|---|
| | | | California | |
| 8 | B. K. Sen. | Quantum Chemistry | Tata McGraw Hill | 1992 |
| 9 | A. K. Chandra | Introduction to Quantum Chemistry | Tata McGraw Hill | 1997. |
| 10 | W. Levine | Quantum Chemistry | Prentice Hall | 1994 |
| 11 | R. K. Prasad | Quantum Chemistry | Wiley Eastern | 1993 |
| 12 | C. F. Banwell | Fundamentals of Molecular Spectroscopy | McGraw Hill, New York | 1966 |
| 13 | D. A. Skoog and D. M. West | Fundamentals of Analytical Chemistry | Holt Rinehart and Winston Publications, IV Edn | 1982 |
| 14. | D. A. Skoog, D. M. West, F. J. Holler and S. R. Crouch | Fundamentals of Analytical Chemistry | Thomson Asia Pte Ltd., Singapore, 8th Ed | 2004 |
| 15. | D. A. Skoog | Principles of Instrumental Analysis | Saunders College Pub.Co, 3rd Ed | 1985 |
| 16. | Willard, Merit, Dean and Settle | Instrumental Methods of Analysis | CBS Publishers and Distributors, 4th Ed | 1989 |
| 17 | G. D. Christian and J. E. O. Reilly | Instrumental Analysis | Allyn and Bacon Inc, 2nd Ed | 1986 |
| 18 | R. S. Drago | Physical methods in chemistry | Reinhold, New York | 1968 |
| 19 | V. K. Ahluwalia | Reduction in Organic Synthesis | CRC Press, 1st Ed | 2012 |

**REFERENCE BOOKS**

| **S.No** | **Authors** | **Title** | **Publishers** | **Year of publication** |
|---|---|---|---|---|
| 1. | G.D. Christian and J.E.G. Reily, Allegn | Instrumental Analysis | Becon II Edition | 1986 |
| 2. | Wilson alld | Comprehensive Analytical Chemistry | Wilson series. | 1986 |
| 3. | R.C. Kapoor and B.S. Aggarwal | Principles of Polarography | Wiley Easter Limited | 1991 |
| 4. | Kolthoff and Elwing | Treatise on Analytical Chemistry | | |
| 5. | H.A. Strobel, Addison | Chemical Instrumentation | Wesley Publ. Co | 1976 |

**TEACHING METHODOLOGY:**

- PowerPoint presentation
- Group discussion
- Seminar and Assignments
- Animated videos
- Board and chalk

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# ELECTIVE PAPER-A: MODERN SYNTHETIC STRATEGIES AND RENEWABLE ENERGY RESOURCES

| Semester | Subject Code | Category | Instruction Hours | | | | | | Credits |
|---|---|---|---|---|---|---|---|---|---|
| | | | Lecture | | Theory | | Practical | | |
| | | | Per Week | Per Semester | Per Week | Per Semester | Per Week | Per Semester | |
| II | | Elective | 3 | 45 | 3 | 45 | 0 | 0 | 3 |

## COURSE OBJECTIVES:

- To understand the basic aspects of organic reactions in terms of acceptor, donor synthons, retrosynthetic analysis and various types of organic syntheses involved in accessing natural products.
- To understand the mechanism, synthetic utility of transition metal catalyzed organic reactions, concept of asymmetric synthesis, various types of total synthesis involved in natural products, advantages of green reactions and their utility.

## COURSE OUTCOMES:

- On the successful completion of course, students will be able to

| CO Number | CO statement | Knowledge level |
|---|---|---|
| CO1 | Use retrosynthetic method for the logical dissection of complex organic molecules and devise synthetic methods | **K3 & K2** |
| CO2 | Learn various organic reactions and reagents used in them as tools applied in the art of organic synthesis | **K3 & K2** |
| CO3 | Gain knowledge about structural elucidation of steroids, synthesis of various natural products | **K2 & K4** |
| CO4 | Learn the importance of minimizing waste, saving power and doing organic synthesis according to the principles of green chemistry | **K2 & K3** |
| CO5 | Acquire knowledge about the applications of various types of renewable energy sources and biofuel cells | **K3 & K4** |

* CO-Course Outcomes

Knowledge level K1-Remember; K2-Understand; K3-Apply; K4-Analyze

**MAPPING WITH PROGRAM OUTCOMES**

| COS | PO1 | PO2 | PO3 | PO4 | PO5 | PO6 |
|---|---|---|---|---|---|---|
| **CO1** | M | M | M | M | S | S |
| **CO2** | M | M | S | S | S | M |
| **CO3** | M | M | M | M | S | M |
| **CO4** | M | S | S | S | S | M |
| **CO5** | M | S | S | S | M | M |

**UNIT-I: Synthetic Methodolgy 9 hours**

Synthons (acceptor and donor) – Synthetic equivalent – Target molecule – Retrosynthetic analysis –Functional group interconversion – Disconnection approach – One group disconnection – Disconnection of alcohols, olefins and ketones – Logical and illogical disconnections, Two group disconnection – 1,2 – 1,3 – 1,4 – 1,5 – and 1,6 – deoxygenated skeletons and dicarbonyls – Umpolung, antithesis, 1,3 – Dipolar cycloaddition methodologies (Azide, nitrile oxide, azomethine ylides and carbonyl ylides) – Concept of Tandem, cascade and domino reactions in organic synthesis – Various types of cyclization and ring formation reaction – anionic, cationic, radical and transition metal mediated cyclizations.

**UNIT-II: Novel Reagents and Asymmetric Synthesis 9 hours**

Protection and deprotection of functional groups (R-OH, R-CHO, RCOR, R-$NH_2$ and R-COOH – Role of palladium and nickel catalysts in organic reactions including Pd(0), Ni(0), Pd(II) and Ni(II) complexes – Typical reactions involving Heck, Negishi, Suzuki – Miyaura, Kumada, Sonogashira, Stille and Hiyama coupling for carbon-carbon bond formation reactions – Buchwald – Hartwig coupling for the carbon – heteroatom bond formation reactions.

Selectivity – Resolution – Kinetic resolution reactions – Desymmetrization – Asymmetric induction – Chiral auxiliary – Generation of Asymmetric synthesis – Substrate – Auxiliary – Reagent and Catalyst control. Auxiliary controlled alkylation of chiral enolates – Evans oxazolidones, chiral hydrazones and chiral imines – Enders RAMP/SAMP and chiral sulfoxide – Asymmetric oxidation [dihydroxylation, epoxidation Sharpless, Jacobsen, Shi] and Asymmetric reduction (Noyori, Corey, Pfaltz) – Boranes reduction.

**UNIT-III: Steroids and Total Synthesis of Natural Products 9 hours**

Structural elucidation of cholesterol, stigmasterol and ergosterol – synthesis of cholesterol – conversion of cholesterol to progesterone, oestrone and testosterone-Biosynthesis of cholesterol and bile acids.

Classification of Organic Synthesis. Demonstration of various types of total syntheses using alkaloid (Epibatidine and Ibogamine), Prostaglandin ($PGE_1$) and Terpenes (longifolene and cedrene). Total synthesis of quinine, morphine, reserpine, cocaine and papaverine

**UNIT-IV: Essentials of Green Chemsitry 9 hours**

Introduction to green chemistry-definition, origin, history, needs, goals, twelve principles of green chemistry – Usage of Conventional and Green solvents-Advantages, Limitations and drawbacks – Green Synthesis – Designing, Choice of starting materials, choice of reagents, choice of catalysts – biocatalysts, polymer supported catalysts – choice of solvents – Synthesis involving basic principles of green chemistry – Examples: synthesis of adipic acid, methyl methacrylate, paracetamol – Microwave, Ultrasonication and Ultrasound assisted reactions – esterification, reduction and coupling reactions.

**UNIT-V: Renewable Energy Resources 9 hours**

Renewable energy sources – types of renewable energy sources – Solar cells – basic principles, types and their applications – Fuel cells – basic principles, types and their applications. Working principle and applications of Biofuel cells – brief introduction about hydroelectric, biomass, wind power and geothermal power and their applications and limitations – energy from some other natural source.

**Distribution of hours: Theory-100%; Problems-Nil**

**TEXT BOOKS**

| S.No | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| 1 | Jiro Tsuji | Palladium Reagents and Catalysts | Wiley & Sons | 1995 |
| 2 | M. B. Smith and Jerry March | Advanced Organic Chemistry | John Wiley & Sons, $5^{th}$ Ed | 2001 |
| 3 | W. Carruthers | Some Modern Methods of Organic Synthesis | Cambridge University Press, $3^{rd}$ Ed, Reprint | 1998 |

| | | | | |
|---|---|---|---|---|
| 4 | R. O. C. Norman and J. M. Coxon | Principles of Organic Synthesis | Chapman & Hall, 3rd Ed | 1993 |
| 5 | Louis S. Hegedus | Transition Metals in the Synthesis of Complex Organic Molecules | University Science Books, 2nd Ed | 1999 |
| 6 | L. Brandsma, S. F. Vasilevsky and H. D. Verkruijsse | Applications of Transition Metal Catalysts in Organic Synthesis | Springer-Verlag | 1999 |
| 7 | R. E. Gawley & J Aube | Principles of Asymmetric Synthesis | Elsevier, 2nd Ed | 2012 |
| 8 | Noyori, R | Asymmetric Catalysis in Organic synthesis | Wiley | 2001 |
| 9 | I. L. Finar, t | Organic Chemistry Vol 2, Stereochemistry and the Chemistry of Natural Produc | Dorling Kindersley India (P) Ltd | 2009 |
| 10 | Corey and Cheng | The Logics of Chemical Synthesis | John Wiley & Sons | 1989 |
| 11 | K.C. Nicolau and Sorenson | Classics in Total Synthesis | Wiley | 1996 |
| 12 | P. T. Anastas and T. C. Williamson | Frontiers in Benign Chemical Syntheses and Processes, Green Chemistry | Oxford University Press, Oxford | 1998 |
| 13 | V. K. Ahluwalia | Methods and Reagents of Green Chemistry: An Introduction by Green Chemistry | Kluwer Academic Publisher & Anamaya Publishers | 2004 |
| 14. | R. A, Sheldon, I. Arends and Ulf. Hanefeld | Green Chemistry and Catalysis | John Wiley & Sons | 2007 |
| 15. | Gadi Rothenberg | Catalysis: Concepts and Green Applications | John Wiley & Sons | 2015 |

**REFERENCE BOOKS**

| S.No | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| 1 | W. Carruther and Jain Coldham | Modern Methods of organic synthesis | Cambridge University Press, 4th edition | 2015 |
| 2. | Micheal B. Smith | Organic Syntheis | McGraw Hill, 2nd edition | 2002 |
| 3. | Stuart Warren | organic synthesis, the disconnection approach | John Wiley and sons (Asia) Pvt. Ltd. | 2008 |
| 4. | R.E. Ireland | Organic synthesis | Prentice hall of India, Pvt. Ltd New Delhi | 1975 |
| 5. | V.K. Ahluwalia | Green Chemistry: Environmentally Benign Reactions | CRC press | 2008 |

**TEACHING METHODOLOGY:**

- Board and chalk
- PowerPoint presentation
- Group discussion
- Seminar and Assignments
- Animated videos
- Board and chalk

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## ELECTIVE PAPER-B: PHARMACEUTICAL CHEMISTRY

| Semester | Subject Code | Category | Instruction Hours | | | | | | Credits |
|---|---|---|---|---|---|---|---|---|---|
| | | | Lecture | | Theory | | Practical | | |
| | | | Per Week | Per Semester | Per Week | Per Semester | Per Week | Per Semester | |
| II | | Elective | 3 | 45 | 3 | 45 | 0 | 0 | 3 |

**COURSE OBJECTIVES:**

- To study about the drug metabolism and effect of various drugs.
- To enhance the knowledge in the various areas of molecular modelling, molecular docking, drug design techniques with detail concepts of all the mentioned areas.

**COURSE OUTCOME:**

- On completion of the course, the student should be able to:

| CO Number | CO statement | Knowledge level |
|---|---|---|
| **CO1** | Acquire knowledge on the importance of drugs, drug administration, drug metabolism, elimination and discuss the challenges faced in each step of the drug discovery process. | **K2 & K3** |
| **CO2** | Get knowledge about the industrial methods using for drug preparation and formulation. | **K3 & K4** |
| **CO3** | Understand the pharmaceutical industry regulation for manufacturing, packing and marketing. | **K3 & K4** |
| **CO4** | Gain knowledge about important drugs and its adverse effects. | **K2 & K3** |
| **CO5** | Acquire knowledge about anaesthetics, antihistamines and organic pharmaceuticals. | **K3 & K4** |

* CO-Course Outcomes
Knowledge level K1-Remember; K2-Understand; K3-Apply; K4-Analyze

**MAPPING WITH PROGRAM OUTCOMES**

| COS | PO1 | PO2 | PO3 | PO4 | PO5 | PO6 |
|---|---|---|---|---|---|---|
| **CO1** | M | S | S | M | M | M |
| **CO2** | M | S | M | M | S | M |
| **CO3** | M | S | S | S | S | M |
| **CO4** | M | S | S | M | S | M |
| **CO5** | M | M | S | S | M | S |

**UNIT - I: Classification of Drugs** **9 hours**

Classification of drugs based on sources - mode of administration - site of action, absorption of drugs - Drugs distribution and elimination - Role of kidney in elimination.

Drug design- Development of new drugs - procedures followed in drug design, concepts of prodrugs and soft drugs.

**UNIT - II : Industrial Aspects - I** **9 hours**

Unit operation – Principle – extraction - maceration and percolation method – Drying: Tray dryer and drum dryer – Evaporation - Climing film evaporators and calandria – Distillation - Fractional distillation and bubble cap column steam distillation – Centrifugation - Supercentrifugation and non-perforated basket – Filtration: filter press and drum filter – Comminution - mortar and pestle type and Bal mills - types of formulation - Importance of it – factors affecting formulation - finished pharmaceuticals - packing materials - polymers, plastics and metals – closures - repacking.

**UNIT - III : Industrial Aspects –II** **9 hours**

Regulations - pharmacopeia - Good manufacturing practices (GMP) – Material Management- Laboratory controls- Validations- Drug analysis - aspirin, paracetamol and ciprofloxacin.

**UNIT - IV : Effect of Drugs** **9 hours**

Adverse responses and side effects of drugs, allergy - Drugs intolerance - Drug addiction, drug abuses and their biological effects.

Anticancer drugs: Anticancer drugs and their mechanism of action-

Natural and man made radioisotopes and their applications.

Antipsychotic drugs- the neuroleptics, antidepressant, butyrophenones, serendipity and drug development.

**UNIT - V : Anaesthetics, Antihistamines And Organic Pharmaceuticals** **9 hours**

Anaesthetics - General and local - gaseous anaesthetics - ether and vinyl ether - halogenated hydrocarbons like chloroform - intravenous anesthetics - thiopentalsodium and cocaine - Antiseptics and disinfectants – Phenols and related compounds - formaldehyde and ethanol.

Antihistamines – classification H1 and H2 receptor antagonists.

Organic Pharmaceuticals – their role as preservatives and food additives.

**Distribution of Marks**: Theory-100%

## TEXT BOOKS

| S.No | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| 1. | Foye, Williams O | Principles of Medicinal Chemistry, 7th edition | Wolters kluwer, lippincoatt Williams and vikkins | 1996 |
| 2. | G.R Chatwal | Synthetic Drugs | Himalaya Publisher | 2009 |
| 3. | Dr. Jayashree Gosh, S. Chand | A Textbook of Pharmaceutical Chemistry | S. Chand and company limited | 2014 |
| 4. | A. O Bentley | Textbook of Pharmaceutical Chemistry | Oxford Univ., Press. | 1925 |
| 5. | M.N Chatterje and Rana shinde | Text book of Medical Biochemistry, 8th edition | Jaypee Brothers pub | 2012 |
| 6. | A. Berger | Medicinal Chemistry, Vol 1 &2 | Wiley Interscience, New York | 1990 |
| 7. | Asutoshkar | Medicinal Chemistry | Wiley Eastern Ltd., Chennai | 1992 |
| 8. | Bentely and Driver's | Textbook of Pharmaceutical Chemistry | Oxford Univ. Press. | 1985 |

## REFERENCE BOOKS

| S.No | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| 1. | Asuthosh Kar, | Medicinal Chemistry, Revised, 3rd edition | New Age, International Publishers | 2005 |
| 2.. | G.R. Chatwal, Madhu Arrora | Pharmaceutical Chemistry organic | Himalaya Pub | 2008 |
| 3. | H.J Roth, A. Kleemann | Pharmaceutical Chemistry : vol.1 Drug synthesis | Ellis horwood Ltd. | 2001 |

## TEACHING METHODOLOGY:

- Board and chalk
- PowerPoint presentation
- Models
- Group discussion
- Seminar and Assignments
- Animated videos

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## ELECTIVE PAPER-C: HETEROCYCLIC CHEMISTRY

| Semester | Subject Code | Category | Instruction Hours | | | | | | Credits |
|---|---|---|---|---|---|---|---|---|---|
| | | | Lecture | | Theory | | Practical | | |
| | | | Per Week | Per Semester | Per Week | Per Semester | Per Week | Per Semester | |
| II | | Elective | 3 | 45 | 3 | 45 | 0 | 0 | 3 |

**COURSE OBJECTIVES**

- To study about the chemistry of heterocyclic compounds.
- To enhance the knowledge strategies for designing the chemical synthesis for higher heterocycles.

**COURSE OUTCOME**

- On completion of the course, the student should be able to:

| CO Number | CO statement | Knowledge level |
|---|---|---|
| **CO1** | Gain knowledge about aromatic compounds and aromatic heterocyclic compounds. | **K2 & K3** |
| **CO2** | Get knowledge about strain, bond angle strain, torsional strain and their consequences in small ring heterocycles and conformations of six membered heterocycles. | **K3 & K4** |
| **CO3** | Understand about the three membered, four membered and five membered heterocyclics. | **K3 & K4** |
| **CO4** | Acquire knowledge about mesoionic heterocyclics. | **K2 & K3** |
| **CO5** | Gain knowledge about higher heterocyclic compounds | **K3 & K4** |

* CO-Course Outcomes
Knowledge level K1-Remember; K2-Understand; K3-Apply; K4-Analyze

**MAPPING WITH PROGRAM OUTCOMES**

| COS | PO1 | PO2 | PO3 | PO4 | PO5 | PO6 |
|---|---|---|---|---|---|---|
| **CO1** | M | M | S | M | M | M |
| **CO2** | M | S | M | S | S | M |
| **CO3** | M | S | S | S | S | M |
| **CO4** | M | S | S | M | S | M |
| **CO5** | M | M | M | S | S | S |

**UNIT I: Nomenclature of Heterocycles** **9 hours**

Introduction - nomenclature systems - systematic nomenclature system (Hantzsch – Widman system) and replacement nomenclature system for monocyclic, fused, spiro and bridged heterocycles - Aromatic heterocycles – Introduction - chemical behavior of aromatic heterocycles - classification (structural types) - Criteria of aromaticity in heterocycles (bond lengths, dipole moments, empirical resonance energy, delocalization energy, Dewar resonance energy, chemical shits and $^{1}$HNMR spectra).

**UNIT- II: Nonaromatic Heterocycles** **9 hours**

Introduction - strain, bond angle strain - torsional strain and their consequences in small ring heterocycles - conformations of six membered heterocycles – molecular geometry - barriers to ring inversion - pyramidal inversion and 1,3 - diaxial interactions. Stereoelectronic effect in saturated six membered heterocycles- anomeric effect - other related effects and attractive interactions through space.

**UNIT III: Small Ring Heterocycles** **9 hours**

Three membered and four membered heterocycles - Synthesis and reactions of aziridines, oxiranes, thiranes, azetidines, oxetanes and thietanes - Benzo- fused five membered heterocycles: Synthesis and reactions including medicinal applications of benzopyrroles, benzofurans and benzothiophenes.

**UNIT- IV: Meso - Ionic Heterocycles** **9 hours**

General classification - chemistry of some important meso-ionic heterocycles of type A and B and their applications - Six membered heterocycles with one heteroatom - Synthesis and reactions of pyrylium salts and pyrones and their comparisons with pyridinium and thiopyrylium salts and pyridines

**UNIT-V: Higher Heterocycles** **9 hours**

Six membered heterocycles with two or more heteroatoms Synthesis and reactions of diazines. triazines and tetrazines - Seven and large membered heterocycles - Synthesis and reactions of azepines, oxepines, thiepines and diazepines - Synthesis of five and six membered heterocycles with P, As, Sb and Bi.

**Distribution of Marks**: Theory-100%

**TEXT BOOKS:**

| S.No | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| 1. | Gupta, M. Kumar and V.Gupta | Heterocyclic Chemistry | Vol. 1 Spinger Verlag -3, R. R | 1998 |
| 2. | T. Eicher and S. Hauptmann, Thieme | The Chemistry of Heterocycles | First Edition, | 2003 |
| 3. | J. A. Joule, K. Mills and G. F. Smith, Chapman and Hall | Heterocyclic Chemistry | London,New York : Chapman & Hall | 1995 |
| 4. | T. L. Gilchrist | Heterocyclic Chemistry | Longman Scientific Technical | 2017 |
| 5. | G. R. Newkome and W.W. Paudler | Contemporary Heterocyclic Chemistry | Wily –inter Science. | 1982 |

**REFERENCES BOOKS:**

| S.No | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| 1. | R. M. Acheson, John wiely. | An Introduction to the Heterocyclic Compounds | Interscience Publishers | 1960 |
| 2. | A. R. Katrizky and C.W. Rees, eds | Comprehensive Heterocyclic Chemistry | Pergamon press**,**Elsevier Science, Ltd | 1996 |

**TEACHING METHODOLOGY:**

- Board and chalk
- PowerPoint presentation
- Models
- Group discussion
- Seminar and Assignments
- Animated videos

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## II SEMSTER
## ORGANIC CHEMISTRY PRACTICALS –I

| Semester | Subject Code | Category | Instruction Hours | | | | | | Credits |
|---|---|---|---|---|---|---|---|---|---|
| | | | Lecture | | Theory | | Practical | | |
| | | | Per Week | Per Semester | Per Week | Per Semester | Per Week | Per Semester | |
| II | | Core | 0 | 0 | 0 | 0 | 5 | 75 | 5 |

**COURSE OBJECTIVES:**

Students should be able to apply principles of separation and isolation techniques in organic reactions and also to synthesize some important organic molecules.

**COURSE OUTCOME:**

At the end of the course, the students should be able to separate the organic mixtures using separating funnel and purity of components can checked by measuring their melting point/boiling point

Identification of components in a two-component mixture and preparation of their derivatives. Determination of b.p. / m.p. for the components.

Any Six preparation form the following

(i) Preparation of o-benzyl benzoic acid

(ii) p-Nitrobenzoic acid from p-nitrotoluene

(iii) Anthraquinone from anthracene

(iv) Benzhydrol from Benzophenone

(v) m-Nitroaniline from m-dinitrobenzene

(vi) 1,2,3,4 – Tetrahydrocarbazole from phenyl hydrazine

(vii) p-chlorotoluene form p-toluidine

(viii) 2,3 – Dimethylindole from phenyl hydrazine and 2 – butanone (boiling acetic acid)

(ix) Methyl orange from sulphanilic acid

**REFERENCE BOOKS:**

1. Organic Chemistry Laboratory Manual, Dr. M. S. Gnanaprakasam, Visvanathan Pvt.,Ltd.,

2. A text book of Practical Organic Chemistry by Arthur I.Vogel

3. Laboratory Manual of Organic Chemistry Raj K. Bansal, Wiley Eastern limited.

**TEACHING METHODOLOGY:**

- Board and chalk
- Demonstration
- Conducting practicals
- Conducting Viva

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## INORGANIC CHEMISTRY PRACTICALS – I

| Semester | Subject Code | Category | Instruction Hours | | | | | | Credits |
|---|---|---|---|---|---|---|---|---|---|
| | | | Lecture | | Theory | | Practical | | |
| | | | Per Week | Per Semester | Per Week | Per Semester | Per Week | Per Semester | |
| II | | Core | 0 | 0 | 0 | 0 | 5 | 75 | 5 |

**COURSE OBJECTIVES:**

The students should be able to apply the principles of qualitative and quantitative analytical techniques (semi micro) in inorganic chemistry for compound identification by group separation and to prepare different metallic coordination complexes.

**COURSE OUTCOMES:**

At the end of the course, the students should be able to plan and conduct experiments for identifying inorganic compounds and preparing the coordination complexes

**UNIT - I**

Semimicro qualitative analysis of mixture containing two common and two less familiar cations.

The following are the less familiar cations to be included. W, Ti, Te, Se, Ce, Zr, V, Li, Mo.

**UNIT - II**

a) Colorimetric experiments – Estimation of Fe, Ni, Cu and Mn.

b) Preparation of the following (any 5):

(i) Potassium tris(oxalato)aluminate (III) trihydrate

(ii) Tris (thiourea)copper (I) chloride

(iii) Potassium tris(oxalato)chromate (III) trihydrate

(iv) Sodium dithiosulphatocuprate (I)

(v) Tris(thiourea)copper (I) sulphate

(vi) Tetrammine copper(II)sulphate

**REFERENCE BOOKS**

1. Textbook of quantitative Analysis, A. Vogel, CBS Pub.,
2. Quantitative Inorganic Analysis, Upadhyaya, S. Chand & Co., Ltd.,
3. Advanced Practical Chemistry, Chatterjee, Books & Allied (P) Ltd

**TEACHING METHODOLOGY:**

- Board and chalk
- Demonstration
- Conducting practicals
- Conducting Viva

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# PHYSICAL CHEMISTRY PRACTICALS - I

| Semester | Subject Code | Category | Instruction Hours | | | | | | Credits |
|---|---|---|---|---|---|---|---|---|---|
| | | | Lecture | | Theory | | Practical | | |
| | | | Per Week | Per Semester | Per Week | Per Semester | Per Week | Per Semester | |
| II | | Core | 0 | 0 | 0 | 0 | 5 | 75 | 5 |

**COURSE OBJECTIVES:**

The students should be able to validate the conceptual understanding acquired from the theory classes

**COURSE OUTCOMES:**

At the end of the course, the students should be able to explain the principle behind the experiments performed in the laboratory plan and perform experiments and interpret experimental results

**Experiments for Physical Chemistry Practical – I**

1. Study of the kinetics of acid catalysed hydrolysis of ester and determine the relative strength of acids
2. Determination of the temperature coefficient and Arrhenius activation energy and frequency factor for the acid catalysed hydrolysis of ester
3. Study the iodination of acetone cataysed by acids.
4. Study of the kinetics of reaction between potassium iodide and persulphate and determination of the rate constant of primary salt effect
5. Study of the kinetics of reaction between KI and $K_2S_2O_8$ and determination of the order
6. Study of the phase diagram for a simple binary system
7. Study of the adsorption of oxalic acid by charcoal [Fruendlich isotherm]
8. Determination of the distribution coefficient of iodine between $CCl_4$ and water (Demo)
9. Determination of the equilibrium constant for the reaction between potassium iodide and iodine by partition method (Demo).
10. Determination of the concentration of the given unknown potassium iodide solution using partition method (Demo).
11. Study the inversion of cane sugar in the presence of acid using Polarimeter

**TEACHING METHODOLOGY:**

- Board and chalk

- Demonstration
- Conducting Experiments
- Conducting Viva

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# SCHEME OF VALUATION FOR PRACTICAL EXAMINATIONS

# ORGANIC CHEMISTRY PRACTICALS-I

**Organic practicals** **- Max. Marks: 60**

Record - 10

Qualitative organic analysis - 30

Preparation - 10 (Quality – 3 & Quantity- 7)

Viva - 10

---

60

---

**Qualitative Organic Analysis: 30**

Pilot Separation - 4

Aliphatic/Aromatic - 2+2

Saturated/Unsaturated - 2+2

Elements (N, X & S) - 3+3

Functional Group tests - 2+2

Confirmatory - 2+2

Derivative - 2+2

# SCHEME OF VALUATION FOR PRACTICAL EXAMINATIONS

# INORGANIC CHEMISTRY PRACTICALS – I

**Inorganic Practical : Max. Marks :60**

| | | |
|---|---|---|
| Record | - | 10 |
| Colorimetry | - | 10 (Experiment-7+ Procedure-3) |
| Preparation | - | 10 (Quality-3+ Quantity- 7) |
| Qualitative Analysis | - | 20 (Each radical – 5) |
| Viva | - | 10 |
| | | 60 |

**Calorimetry**:

Result: 7 Marks

| **Instrument** | **Marks** |
|---|---|
| % error | |
| 5% | 7 |
| 7% | 5 |
| 10% | 4 |
| 12% | 3 |
| Above 12% | 2 |

# SCHEME OF VALUATION FOR PRACTICAL EXAMINATIONS

# PHYSICAL CHEMISTRY PRACTICALS-I

**Maximum marks :60**

| | | |
|---|---|---|
| Record | - | 10 |
| Manipulation | - | 20 |
| Practical | - | 20 |
| Viva voce | - | 10 |
| | | 60 |

**Practical:**

**For all experiments**

| | |
|---|---|
| Calculation | : 5 marks |
| Graph | : 7 marks |

**Result**

Error up to 5%: 8 marks

6 to 10% : 5 marks

> 10% : 3 marks

## QUESTION PAPER PATTERN

**Section-A (5 Questions x 6 marks = 30 marks)**

- Questions in Section-A will contain 10 questions in “Either Or” pattern drawn from 5 units (two questions from each unit in either or pattern)

**Section-B (3 Questions x 15 Marks = 45 Marks)**

- Questions in Section-B will contain 5 questions of open choice drawn from 5 units (One question from each unit)

## PAPER – VII: NUCLEAR CHEMISTRY AND ORGANOMETALLIC CHEMISTRY

| Semester | Subject Code | Category | Instruction Hours | | | | | | Credits |
|---|---|---|---|---|---|---|---|---|---|
| | | | Lecture | | Theory | | Practical | | |
| | | | Per Week | Per Semester | Per Week | Per Semester | Per Week | Per Semester | |
| III | | Core | 4 | 60 | 4 | 60 | 0 | 0 | 4 |

## COURSE OBJECTIVES:

- To learn basic principles of nuclear chemistry, various nuclear reactions as energy sources, working functions of nuclear reactors and applications of tracers in different fields.
- To gain knowledge about different types of organometallic complexes and their activity as an effective catalyst.

## COURSE OUTCOMES:

- On the successful completion of course, students will be able to

| CO Number | CO statement | Knowledge level |
|---|---|---|
| **CO1** | Understand nuclear properties and its reactions with mechanisms. | K3 & K4 |
| **CO2** | Categorize the radioactive decay and mode of working nature of nuclear reactors. | K2 & K3 |
| **CO3** | Gain knowledge of organometallic chemistry, EAN rule and its applications. | K2 & K3 |
| **CO4** | Get clear knowledge about the carbon donors, metallocenes and various reactions in organometallic chemistry. | K3 & K4 |
| **CO5** | Identify the bonding aspects of simple organometallic compounds, different types of organometallic reactions and to explain different catalytic reactions. | K3 & K4 |

*CO-Course Outcomes

Knowledge level: K1 – Remember; K2 – Understand; K3 – Apply; K4 – Analyze

**MAPPING WITH PROGRAM OUTCOMES**

| COS | PO1 | PO2 | PO3 | PO4 | PO5 | PO6 |
|---|---|---|---|---|---|---|
| **CO1** | M | S | S | M | S | M |
| **CO2** | S | M | S | S | S | M |
| **CO3** | M | S | M | S | M | S |
| **CO4** | M | M | S | M | S | M |
| **CO5** | M | S | S | M | S | S |

**UNIT-I: Nuclear Chemistry – I** **12 hours**

Nuclear Structure : Mass and Charge, nuclear moments, nuclear forces, nuclear stability – magic numbers, binding energy, mass defects (simple problems) and packing fraction. Nuclear isomerism – internal conversion – nucleus models – salient features of liquid drop and shell models of the nucleus.

Nuclear Reaction : Types of reactions, cross section, Q-value and threshold energy – compound nucleus theory – high energy nuclear reactions – types of nuclear fission and fusion reactions, photonuclear and thermonuclear reactions, mechanism of hydrogen burning and carbon burning reactions.

**UNIT-II: Nuclear Chemistry – II** **12 hours**

Radioactive Decay : Mode of radioactive decay, rate, half life and average life. Radioactive equilibrium – transient and secular nuclear reactions. Tracer techniques – isotope dilution analysis and neutron activation analysis – carbon and rock dating – application of tracers in chemical analysis, pharmacology, agriculture and industry.

Nuclear reactors – detection and determination of radioactivity by Wilson's cloud chamber, bubble chamber, Geiger Muller counters, scintillation counters, cherenkov counters, fast breeder reactors, particle accelerators, linear accelerators, cyclotron and synchrotron.

**UNIT-III: Organometallic Chemistry – I** **12 hours**

Introduction to organometallic chemistry – classification of ligands – stability of orgaometallic complexes by 18e- rule and EAN rules – bonding in organometallic compounds –metal-carbon ionic bonding, metal-carbon sigma bonding, metal-carbon multiple bonding and factors providing stability to metal-carbon bond. Metal alkenyl complexes – Zeise's salt, metal allyl complexes and metal acetylene complexes.

Synthesis, structure, bonding in metal carbonyls, metal carbonyl hydrides, metal carbonyl halides and metal nitrosyls. Bonding modes of metal cyanide, metal isocyanide, metal phosphine, cyclopentadiene, cyclobutadiene, benzene, cycloheptatrienyl and cyclooctatetraene (cot) ligands.

**UNIT-IV: Organometallic Chemistry – II** **12 hours**

Metallocenes – synthesis, types of metallocenes, role of η5 Cyclopentadienyl ring, η6 arene metal complexes – half sandwich complexes – structure and bonding of ferrocene, dibenzene chromium – Important types of reactions of organometallic compounds – association, substitution, addition, elimination, ligand protonation, electrophilic and nucleophilic attack on ligands, carbonylation, decarbonylation, oxidative addition and reductive elimination – Template synthesis of macrocyclic ligands – fluxional properties – reactivity of cyclopentane rings of metallocene activity of dioxygen, dinitrogen, dihydrogen.

**UNIT-V: Organometallic Chemistry – III** **12 hours**

General principles of catalysis – conditions for metal to act as catalyst – basic reactions involved in the catalysis by organometallic compounds – Tolman catalytic loops – catalytic mechanism in the following reactions: hydrogenation of olefins (Wilkinson's catalyst) – hydroformylation of olefins using Cobalt or Rhodium catalysts (Oxo process) – oxidation of olefins to aldehydes and ketones (Wacker process) – Cyclooligomerisation of acetylene using Ni catalyst (Reppe's catalyst) – Synthetic gasoline by using ZSM-5 catalyst (Fischer-Tropsch and mobil process) polymerization of olefins (Zeigler – Natta Catalyst) – polymer bound catalyst.

**Distribution of hours:** Theory – 80%; Problems – 20%

**TEXT BOOKS**

| S.No | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| 1. | Vasishta Bhatt | Essentials of Coordination Chemistry | Elsevier | 2016 |
| 2. | R. K. Sharma | Textbook of Coordiantion Chemistry | Discovery Publishing House | 2007 |
| 3. | James E. Huheey, Ellen A. Keiter, Richard A. Keiter, Okhil A. Medhi | Inorganic Chemistry : Principles of Structure and Reactivity | 4th Edition, Dorling Kindersley | 2009 |
| 4. | R. Gopalan, V. Ramalingam | Concise Coordination Chemistry | VIKAS publishing house pvt ltd | 2001 |
| 5. | H. J. Arniker | Essentials of Nuclear Chemistry | New Age International | 2005 |
| 6. | S. F. A. Kettle | Coordination compounds | Nelson & ELBS | 1979 |
| 7. | K. F. Purcell and J. C. Kotz | Inorganic Chemistry | WB Sanders Co, USA | 1977 |
| 8. | D. F. Shriver, P. W. Atkins and C. H. Longford | Inorganic Chemistry | Oxford University Press | 1990 |
| 9. | R. B. Heslop and K. Jones | Inorganic Chemistry | Elsevier | 1976 |
| 10. | G. Friedlander, J. W. Kennedy and J. M. Miller | Nuclear and Radiochemistry | Wiley eastern Co., | 1964 |
| 11 | R. C. Mehrothra, A. Singh | Organometallic Chemistry | Wiley eastern Co., | 1992 |

**REFERENCE BOOKS**

| S.No | Authors | Title | Publishers | Year of |
|---|---|---|---|---|

| | | | | **publication** |
|---|---|---|---|---|
| 1. | Peter A C Mcpherson | Principles of Nuclear Chemistry | World Scientific | 2017 |
| 2. | Maheshwar Sharon and Madhurai Sharon | Nuclear Chemistry | Ane Books | 2009 |
| 3. | Smiljko Asperger | Chemical Kinetics and Inorganic Reactions Mechanisms | 2nd Edition, Springer | 2003 |
| 4 | Shirver and Atkins | Inorganic Chemistry | 5th Edition, Oxford University Press | 2010 |
| 5 | Walter D. loveland, David J, Morrissey, Glen T. Seaborg | Modern Nuclear chemistry | Wiley eastern Co., | 2017 |
| 6 | Gregory Choppin, Jan-Olov Liljenzin, Jan Rydberg, Christian Ekberg | Radiochemistry and Nuclear Chemistry | 4th Edition, Elsevier | 2013 |
| 7 | G. Coates, M. L. Green and K. Wade | Principles of Organometallic Chemistry | Methven co., | 1988 |
| 8 | P. Powell | Principles of Organometallic Chemistry | Chappman and Hall | 1988 |
| 9 | G. S. Manku | Theoretical Principles of Inorganic Chemistry | McGraw-Hill Education | 2006 |
| 10 | F. Basolo and R.G. Pearson | Mechanism of Inorganic Reaction | Wiley eastern Co., | 1967 |
| 11 | M. Satake and Y. Mido | An Introduction to Nuclear Chemistry | Discovery publishing house | 2003 |
| 12 | S. F. A. Kettle | Physical Inorganic Chemistry: A Coordination Chemistry Approach | Oxford University Press | 1998 |
| 13 | R. C.Mehrotra and A. Singh | Organometallic Chemistry : A Unified Approach | 2nd Edition, New Age International Private ltd | 2004 |
| 14 | W. Parkins and R. C. Poller | An Introduction to Organometallic Chemistry | Macmillan | 1986 |

**TEACHING METHODOLOGY:**

- PowerPoint presentation
- Models
- Group discussion
- Seminar and Assignments
- Animated videos
- Board and chalk

**SYLLABUS DESIGNER:**

Mrs. J. Saranya, Assistant Professor, Department of Chemistry

**PAPER – VIII: SPECTROSCOPY AND APPLICATIONS**

| Semester | Subject Code | Category | Instruction Hours | | | | | | Credits |
|---|---|---|---|---|---|---|---|---|---|
| | | | Lecture | | Theory | | Practical | | |
| | | | Per Week | Per Semester | Per Week | Per Semester | Per Week | Per Semester | |
| III | | Core | 4 | 60 | 4 | 60 | 0 | 0 | 4 |

## COURSE OBJECTIVES:

- To learn the principles and applications of UV, IR, NMR and Mass Spectral data in structural elucidation of organic compounds.
- To understand the structure and bonding nature of inorganic compounds using FTIR, NMR, ESR and Mössbauer spectroscopy

## COURSE OUTCOMES:

- On the successful completion of course, the students will be able to

| CO Number | CO statement | Knowledge level |
|---|---|---|
| CO1 | Gain knowledge about the basic principles and structural elucidation of organic and inorganic compounds by UV and IR spectra. | K2 & K4 |
| CO2 | Understand basic principles and applications of NMR spectra to simple organic and inorganic compounds. | K2 & K4 |
| CO3 | Identify the structure of organic and inorganic molecules by understanding the principles and applications of $^{13}C$ NMR, $^{19}F$ NMR and $^{31}P$ NMR spectra. | K3 & K4 |
| CO4 | Understand the basic principles of mass spectrometry and its applications in the molecular mass and structural determination of organic compounds. | K2 &K3 |
| CO5 | Acquire knowledge about the principles and applications off ESR and Mossbauer spectroscopy | K2 & K4 |

*CO-Course Outcomes

Knowledge level: K1 – Remember; K2 – Understand; K3 – Apply; K4 – Analyze

## MAPPING WITH PROGRAM OUTCOMES

| COS | PO1 | PO2 | PO3 | PO4 | PO5 | PO6 |
|---|---|---|---|---|---|---|
| **CO1** | M | S | M | S | S | M |
| **CO2** | M | M | S | M | S | S |
| **CO3** | M | S | S | M | S | M |
| **CO4** | S | S | M | S | M | M |
| **CO5** | M | M | S | S | M | M |

## UNIT – I: UV and IR Spectroscopy 12 hours

**Electronic absorption:** Beer-Lamberts law – Selection rules – Franck-Condon principle – Types of electronic excitation – effect of conjugation and solvent – Chromophore and Auxochrome – Bathochromic and Hypsochromic shift – Types of bands – Applications in organic structural determination – Woodward-Fieser rule for conjugated systems and α, β unsaturated carbonyl compounds – Scott rules for aromatic ketones – Applications of ORD studies – octant rule and axial haloketone rule.

**Infrared Spectra**: Identification of functional groups in Organic Compounds – Finger print region – Inter and Intramolecular hydrogen bonding – Various factors affecting IR stretching frequencies – Interpretation of Infrared spectra.

Inorganic compounds – effect of coordination on the stretching frequency of the following complexes – sulphato, sulphito, carbonato, $NO_3^-$ ion, $NO_2^-$ ion, thiocyanato, cyano, $PR_3$, $AsR_3$, halogen and aqua complexes – M-M bonds – bond angles from relative intensities.

**UNIT – II: Nuclear Magnetic Resonance and their applications 12 hours**

Origin of NMR spectrum – nuclear spin states – NMR active nuclei ($^1$H NMR, $^{13}$C NMR, $^{19}$F NMR and $^{31}$P NMR) – $^1$H NMR – chemical shift, standards in NMR, shielding and deshielding, factors affecting chemical shift – spin-spin coupling – low and high resolution spectra – splitting origin and rules – coupling constant - factors affecting coupling constant – variation of coupling constant with dihedral angle (Karplus curve) – simplification of complex spectra using shift reagents – Two interacting nuclei: AB, AX and AA'BB' – dd – pair of doublet and AB quartet – Three interacting nuclei: AMX, ABX and ABC systems (only pattern is required).

Dynamic NMR of DMF, cyclohexane and iodocyclohexane – double irradiation / spin decoupling – nuclear overhauser effect – proton NMR applications to structural elucidation of simple organic molecules.

**UNIT – III: $^{13}$C NMR, $^{19}$F NMR and $^{31}$P NMR Techniques 12 hours**

$^{13}$C NMR – proton decoupled and off resonance of $^{13}$C NMR spectra – factors affecting $^{13}$C chemical shift – homonuclear and heteronuclear coupling – origin of $^{13}$C satellite peaks – Attached Proton Test (APT) and Distortionless Enhancement by Polarization Transfer (DEPT) spectrum (DEPT-45, DEPT-90 and DEPT-135).

$^{19}$F NMR – Precessional frequency and heteronuclear coupling – Identification of organofluoro compounds – $CF_3CO_2Et$ and $CF_3CH_2OH$ and equimolar mixture of $[TiF_6]^{2-}$ and $TiF_4$ in ethanol, $ClF_3$, $BrF_5$ using NMR.

$^{31}$P NMR – Chemical shift and heteronuclear coupling – Identification of organo phosphorous compounds such as $(Me)_3P$, $(EtO)_3P{=}O$, $P_4S_3$, $H_3PO_3$, $H_3PO_2$, $HPF_2$, $Ph_3P$ and

P-P bond in NMR.

**UNIT – IV: ESR and Mossbauer Spectroscopy 12 hours**

**ESR spectroscopy:** Introduction – presentation of ESR spectra – g and A parameters – spin densities – evaluation of spin – orbit coupling – Mc-Connel relationship – factors affecting the magnitude of g and A – Zero field splitting – Kramer's degeneracy – ESR spectra of V(II), Mn(II), Fe(II), Co(II), Ni(II), Cu(II) complexes, bis(salicylaldimine)copper(II), $[Co_3(CO)_9Se]$, $[(NH_3)_5Co\text{-}O_2\text{-}Co(NH_3)_5]^{5+}$ – $Mn^{2+}$ and vanadyl complexes – Applications of EPR based on number of signals multiplicity, anisotropy and bio-inorganic molecules.

**Mossbauer spectroscopy:** Introduction – principle – instrumentation – recoil energy – Doppler effect – number of MB signals – experimental technique of measuring resonance absorption – isomer shift – quadrupole splitting – magnetic hyperfine splitting – applications to $^{57}Fe$, $^{119}Sn$ and $^{129}I$ compounds – Mossbauer spectra – problems

**UNIT – V: Mass Spectrometry 12 hours**

Origin, basics and block diagram of Mass spectrum – Various types of Ionization techniques (EI, CI, FD, FAB, SIMS) – Stability of molecular ions, metastable ions, base peaks and isotope peaks – Fragmentation patterns of organic molecules – benzenes, phenyl halides, phenols, benzyl alcohols, benzyl halides, aliphatic alcohols, aliphatic and aromatic aldehydes, ketones, acids, esters, amides, aliphatic / aromatic nitro and amine compounds and heterocyclic compounds (furan, pyrrole and pyridine only) – McLafferty rearrangements of organic molecules – Retro Diels – Alder fragmentation – Identification of organic compounds using mass spectrometry – problems.

**Distribution of hours:** Theory – 80%; Problems – 20%

**TEXT BOOKS**

| S. No | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| 1 | William Kemp | Organic Spectroscopy | 3rd Edition, Palgrave | 2017 |
| 2 | P. S. Kalsi | Spectroscopy of Organic Compounds | 6th Edition, New Age International Publishers | 2017 |
| 3 | R. S. Drago | Physical Methods in Inorganic Chemistry | Affiliated East-West Press Pvt. Ltd., New Delhi | 2012 |
| 4 | Y.R. Sharma | Elementary Organic Spectroscopy : Principles and Chemical Applications | S. Chand & Co | 2007 |
| 5 | H. Kaur | Spectroscopy | Pragati Prakasan Publications, Meerut, | 2006 |

**REFERENCE BOOKS**

| S. No | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| **1.** | J. Dyer | Application of Absorption Spectroscopy of Organic Compounds | Prentice and Hall of India, Pvt., New Delhi | |
| **2** | P. J. Wheatley | The Determination of Molecular Structure | 2nd edition, Dover Publications, Mineola | 1981 |
| **3** | E. A. V. Ebsworth, | Structural Methods in Inorganic Chemistry, | 3rd Ed ELBS, Great Britain | 1987 |
| **4** | C. N. Banwell | Fundamentlas of Molecular Spectroscopy | 4th edition, McGraw Hill Education, Noida | 1994 |
| **5** | L. D.S.Yadav | Organic Spectroscopy | Springer | 2005 |
| **6** | Donald L. Pavia, Gary M. Lampman, George S. Kriz , James R Vyvyan | Introduction to Spectroscopy | 4th Edition, Brooks | 2009 |
| **7** | Harald Gunther | NMR Spectroscopy : Basic Principles, Concepts and Applications in Chemistry | Wiley | 2013 |
| **8** | R. M. Silverstein, G. C. Bassler and T. C. Morrill | Spectrometric Identification of Organic Compounds | John Wiley | 1991 |
| **9** | R. S. Macomber | A Complete Introduction to NMR Spectroscopy | John Wiley | 1998 |
| **10** | Jag Mohan | Organic Spectroscopy Principles and Applications | Alpha Science International Ltd | 2004 |

**TEACHING METHODOLOGY:**

- PowerPoint presentation
- Models
- Group discussion
- Seminar and Assignments
- Animated videos
- Board and chalk

**SYLLABUS DESIGNER:**

Dr. T. Gomathi, Assistant Professor, Department of Chemistry

## PAPER – IX: THERMODYNAMICS AND GROUP THEORY

| Semester | Subject Code | Category | Instruction Hours | | | | | | Credits |
|---|---|---|---|---|---|---|---|---|---|
| | | | Lecture | | Theory | | Practical | | |
| | | | Per Week | Per Semester | Per Week | Per Semester | Per Week | Per Semester | |
| III | | Core | 4 | 60 | 4 | 60 | 0 | 0 | 4 |

## COURSE OBJECTIVES

- To learn the principles of activity and fugacity, theories of kinetic activity, various applications of Quantum statistics, techniques of heat capacity.
- To learn the concepts of group theory, determining vibrations, hybrid orbitals, selection rules for spectral transitions.

## COURSE OUTCOMES:

- On the successful completion of course, students will be able to

| CO Number | CO statement | Knowledge level |
|---|---|---|
| CO1 | Acquire knowledge of classical thermodynamics in the evaluation of macroscopic properties and the principles of fugacity and activity. | K2 & K3 |
| CO2 | Gain knowledge on Nernst heat theorem, third law of thermodynamics, theories of kinetic activity and to understand the techniques of heat capacity. | K3 & K2 |
| CO3 | Gain knowledge about the basic principles of statistical thermodynamics and various applications of quantum statistics | K3 &K4 |
| CO4 | Acquire knowledge about the basic concepts of group theory and to construct the character tables | K2 &K4 |
| CO5 | Get better understanding how to apply group theory for determining vibrations and hybrid orbitals and to determine the selection rules for spectral transitions, energies and molecular orbitals. | K3 &K4 |

*CO – Course Outcomes

Knowledge level K1 – Remember; K2 – Understand; K3 – Apply; K4 – Analyze

## MAPPING WITH PROGRAM OUTCOMES

| COS | PO1 | PO2 | PO3 | PO4 | PO5 | PO6 |
|---|---|---|---|---|---|---|
| **CO1** | S | M | S | M | M | S |
| **CO2** | S | M | S | M | S | M |
| **CO3** | M | S | M | S | S | M |
| **CO4** | S | M | S | M | S | S |
| **CO5** | M | S | M | S | M | S |

### UNIT – I: Thermodynamics and Non-Ideal Systems 12 Hours

Concepts of partial molar properties – partial molar free energy – partial molar volume and partial molar heat content – Gibbs-Duhem equation – chemical potential – variation of chemical potential with temperature and pressure – Van't Hoff isotherm – fugacity – determination of fugacity of gases by graphical method – variation of fugacity with temperature

and pressure – Lewis Randall rule – Duhem-Margules equation – Thermodynamics of real solutions – activity and activity coefficient of non-electrolytes and electrolytes – standard states – determination of activity and activity coefficient of non-electrolyte – EMF method and cryoscopic method – Excess functions.

**UNIT – II : Irreversible Thermodynamics 12 Hours**

Nernst heat theorem – Third law of thermodynamics – applications of third law – Entropy change – calculation of absolute entropies – apparent exceptions to third law – Non-equilibrium thermodynamics – basic concepts – forces and fluxes – Entropy of irreversible processes – Entropy production – Clausius inequality – Phenomenological equations – Onsager reciprocity relations – Coupled reaction sm – Principle of microscopic reversibility – Onsager reciprocal relations – Verification – Entropy production – rate of entropy production – entropy production in chemical reactions.

**UNIT – III : Statistical Thermodynamics 12 Hours**

Objectives of statistical thermodynamics – Concept of distributions – Types of ensembles – Thermodynamic probability – Most probable distribution Law – Classical statistics – Maxwell-Boltzmann (MB) statistics – Quantum statistics – Bose-Einstein (BE) and Fermi-Dirac (FD) statistics – Derivation of distribution function – MB, BE and FD statistics – comparison – Partition functions – Separation of partition functions.

Translational, rotational, vibrational and electronic partition function – relation between partition function and thermodynamic quantities – Equipartition theorem – Debye and Einstein heat capacity of solids.

**UNIT – IV: Group Theory – I 12 Hours**

Symmetry elements and operations**,** point groups and Schoenflies symbols – Determination of point group – Groups and classes of symmetry operations – Matrix representation of symmetry operations – Similarity transformations – reducible and irreducible representations – Symbols and rules of irreducible representations – Reduction formula – Direct product representation – Great orthogonality theorem – Group multiplication table for $C_{2v}$, $C_{3v}$ and $C_{2h}$ – character table – construction of character table for $C_{2v}$ and $C_{3v}$ groups.

**UNIT– V: Group Theory– II 12 Hours**

Applications of group theory – Determination of representations of vibrational modes in non-linear molecules ($H_2O$, $NH_3$, $BF_3$ and $CH_4$) – Determination of Hybrid orbitals in non-linear molecules – Examples: $NH_3$, $BF_3$, $CH_4$, $SF_6$ and $XeF_4$ – Symmetry selection rules of infra-red and Raman spectra – application of group theory for the electronic spectra of formaldehyde and ethylene.

**Distribution of hours: Theory – 80%; Problems – 20%**

**TEXT BOOKS**

| S. No. | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| 1. | P. W. Atkins | Physical Chemistry | Oxford University Press, Oxford | 1990 |
| 2. | D. A. McQuarrie | Textbook of Physical Chemistry | University Science Books, Mill Valley | 1983 |
| 3. | R. A. Alberty and R. J. Silbey | Physical Chemistry | John Wiley and Sons, New York | 1992 |
| 4. | V. Ramakrishnan and M. S. Gopinathan | Group Theory in Chemistry | Vishal Publications | 1988 |
| 5. | J. Rajaram and J.C. Kuriacose | Thermodynamics for Students of Chemistry | Lal Nagin Chand, New Delhi | 1971 |
| 6. | F. A . Cotton | Chemical Application of Group Theory | John Wiley and Sons, New York | 1971 |
| 7. | K. V. Raman | Group Theory and its Applications to Chemistry | Tata McGraw-Hill Publishing Company | 1990 |
| 8. | J. Rajaram and J. C. Kuriacose | Irreversible Thermodynamics | Lal Nagin Chand, New Delhi | 1989 |
| 9. | S. Glasstone | Thermodynamics for Chemists | Affiliated East West Press, New Delhi | 1960 |
| 10. | R. P. H. Gasser and W. G. Richards | Introduction to Statistical Thermodynamics | World Scientific, Singapore | 1995 |

**REFERENCE BOOKS**

| S. No. | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| 1. | Philip Reid and Thomas Engel | Thermodynamics, Statistical Thermodynamics & Kinetics | Pearson | 2007 |
| 2. | Yi-Chen Cheng | Macroscopic and Statistical Thermodynamics | World Scientific, Singapore | 2006 |
| 3. | M.C. Gupta | Statistical Thermodynamics | New Age International | 2007 |
| 4. | P. Reid and T. Engel | Physical Chemistry | Pearson | 2013 |
| 5. | B. N. Roy | Fundamentals of Classical and Statistical Thermodynamics | Wiley | 2012 |
| 6. | J. N. Gurtu and A. Gurtu | Advanced Physical Chemistry | Pragathi Prakashan, Meerut | 2014 |
| 7. | G. M. Barrow | Physical Chemistry | Tata McGraw Hill, New York | 2011 |
| 8. | P. K. Bhattacharya | Group Theory and its Applications | Himalaya Publishers | 2010 |
| 9. | A. Salahuddin and | Group Theory and its | PHI learning | 2015 |

| | | | | |
|---|---|---|---|---|
| | G. Krishnan | Applications | | |
| 10. | S. Swarnalakshmi, T. Saroja and R. M. Ezhilarasi, | A Simple Approach to Group Theory in Chemistry | University press (India) private Ltd | 2008 |

**TEACHING METHODOLOGY:**

- PowerPoint presentation
- Group discussion
- Seminar and Assignments
- Animated videos
- Board and chalk

**SYLLABUS DESIGNER:**

Mrs. R. Bharathi Priyadharsini, Assistant Professor, Department of Chemistry

## ELECTIVE PAPER – III A: MATERIAL CHEMISTRY

| Semester | Subject Code | Category | Instruction Hours | | | | | | Credits |
|---|---|---|---|---|---|---|---|---|---|
| | | | Lecture | | Theory | | Practical | | |
| | | | Per Week | Per Semester | Per Week | Per Semester | Per Week | Per Semester | |
| III | | Elective-III | 3 | 45 | 3 | 45 | 0 | 0 | 3 |

**COURSE OBJECTIVES:**

- To provide basic knowledge of materials science, so that the students would be able to understand and distinguish between variety of materials based on their structure and properties
- To develop understanding the characteristics of the biomaterials and to make them aware of the growing applications and possibilities of materials to enhance the quality of life.

**COURSE OUTCOMES:**

- On the successful completion of course, students will be able to

| CO Number | CO statement | Knowledge level |
|---|---|---|
| CO1 | Learn about biomaterials, classifications, their properties, performance specification and biological applications. | K3 & K2 |
| CO2 | Understand and appreciate the importance of the polymers as an important class of material and its characterisation. | K3 & K2 |
| CO3 | Gain knowledge about ceramics and bioceramic, its structural importance for industrial applications. | K2 &K4 |
| CO4 | Impart basic knowledge about the manufacturing techniques of various materials. | K2 &K3 |
| CO5 | Know about the industrially important polymers and their properties. | K3 &K4 |

*CO – Course Outcomes

Knowledge level: K1 – Remember; K2 – Understand; K3 – Apply; K4 – Analyze

**MAPPING WITH PROGRAM OUTCOMES**

| COS | PO1 | PO2 | PO3 | PO4 | PO5 | PO6 |
|---|---|---|---|---|---|---|
| **CO1** | S | S | M | M | S | S |
| **CO2** | S | M | S | S | S | S |
| **CO3** | M | M | S | M | S | M |
| **CO4** | S | S | S | S | S | S |
| **CO5** | M | S | S | S | M | M |

**UNIT – I: Biomaterials** **9 hours**

Definition of biomaterials, requirements and classification of biomaterials – Metals and non-metallic alloys, Polymers, Ceramics, glasses, Bio-resorbable and biodegradable materials, Bio-derived macromolecules and fibers.

Standard and assessments of biomaterials – surface properties of materials, physical properties of materials and mechanical properties.

Biocompatibility – introduction to the biological environment – material response: swelling and leaching – corrosion and dissolution – deformation and failure – friction and wear – host response – the inflammatory process – coagulation and hemolysis approaches to thrombo- resistant materials development.

Metallic biomaterials : titanium and titanium based alloys – stainless steel – Co-Cr alloys.

**UNIT– II: Polymers 9 hours**

Classification of polymers – copolymers, tacticity, geometrical isomerism, molecular weight distribution and averages – measurement of molecular weight – synthesis of polymers – step-growth polymerization, chain-growth polymerization and polymerisation techniques .

Polymer conformation and chain dimensions – Freely oriented perpendicular chains – Gaussian model – amorphous state – glass transition temperature $T_g$ – the crystalline state – ordering of polymer chains – crystalline melting temperature ($T_m$) – techniques to determine crystallinity $T_c$ – Determination of $T_g$ – Relationship between $T_m$ and $T_g$ – Mechanical properties – Introduction to viscoelasticity – dynamic mechanical analysis – mechanical models of viscoelastic behaviour – Boltzmann superposition principle – Introduction to rubber elasticity.

**UNIT – III: Ceramics 9 hours**

**Ceramics** : Introduction to ceramic materials – Classification of ceramics – Crystal structure and bonding of common advanced ceramic materials – Mechanical behaviour of ceramics – Types of ceramics – oxide and non-oxide ceramics – Allotropes of carbon – graphite, diamond and fullerene – preparation and characterisation of ceramics powders.

Classification of bioceramic materials – Alumina and zirconia in surgical implants and their coatings – Bioactive glasses and glass ceramics with their clinical applications – Photochromic and photosensitive glasses – Synthesis and characteristics of dense and porous hydroxyapatite and calcium phosphate ceramics – Resorbable bioceramics – Characterisation of ceramics and bio-ceramics – Applications of ceramics in advanced technologies.

**UNIT – IV: Processing of Materials 9 hours**

**Polymer Processing :** Plastics elastomers and fibres – Compounding processing techniques – calendaring, die casting, rotational casting, film casting, injection moulding, blow moulding, extrusion moulding, thermoforming, foaming, reinforcing and fibre spinning.

**Ceramic processing** : Pressing – CIP – HIP – slurry processing, slip casting, pressure

casting, tape casting, gel casting, rapid prototyping, electrophoretic deposition, electro-spinning – Sol-gel processing – Thermal and plasma spraying – Thick and thin film coatings PVD and CVD techniques.

**UNIT– V: Commercial Important Materials 9 hours**

Polyethylene – polyvinyl chloride – polyamides – polyurethanes – polyesters – polytetrafluoro ethylene (Teflon) – Nafian and ion-exchange resins – Functional polymers – Fire-retarding polymers and electrically conducting polymers – Biopolymers: starch, cellulose and chitosin derivatives.

Carbon nanotubes – Graphene – Fullerenes – Composites: metal matrix, polymer matrix and ceramic matrix – Different biomaterials: Orthopaedic materials, cardiovascular materials, dental materials and ophthalmic materials.

**Distribution of hours: Theory – 100%**

**TEXT BOOKS**

| S. No | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| 1. | K. L. Choy | Process Principles and Applications of Novel and Cost-effective ESAVD Based methods | World Scientific Publishing, Singapore | 2002 |
| 2. | A. Jones and M. Mitchell | Nanotechnology-Commercial Opportunity | Evolution Capital Ltd. London, | 2001 |
| 3. | G. Schmid | Nanoparticles | Wiley-VCH | 2004 |
| 4. | V. R. Gowariker, N. V. Viswanathan and Jayadev Sreedhar | Polymer Chemistry | New Age International (P) Ltd, | 2005 |
| 5. | G. Odian | Principles of Polymerization | Wiley-Inter science | 2004 |
| 6. | L. H. Sperling | Introduction to Physical Polymer Science | Wiley-Inter science | 1986 |
| 7. | Sujata V Bhat | Biomaterials | 2nd ed, Narosa Publishing House, New Delhi | 2010 |
| 8. | J. B. Park, J. D. Bronzino | Biomaterials- Principles and Applications | CRC press | 2002 |

**REFERENCE BOOKS**

| S. No | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| 1 | M. Rubinstein and R. A. Colby | Polymer Physics | Oxford University Press | 2003 |
| 2. | T. Pradeep | Nano: The Essentials | Tata McGraw Hill | 2007 |
| 3. | M. Arumugam | Materials Science | Anuradha Agencies, | 2006 |

| | | | | |
|---|---|---|---|---|
| | | | Kumbakonam | |
| 4 | Fredrick H. Silver | Biomaterials Medical Devices and Tissue Engineering | Chapman and Hall | 2003 |
| 5 | N. Ghista | Biomechanics of Medical Devices | Macel Dekker | 1982 |
| 6 | R. Alcock and F. W. Lamber | Contemporary Polymer Chemistry | Prentice Hall | 1981 |
| 7 | R. J. Young and P. A. Lovell | Introduction to Polymers | Chapman and Hall | 2002 |
| 8 | Larry L Hench, Julian R Jones | Biomaterials, Artificial Organs and Tissue Engineering | Woodhead Publications, Cambridge | 2005 |
| 9 | Joon Park and R. S. Lakes | Biomaterials: An Introduction | 3rd Edition, Springer | 2007 |
| 10 | F. W. Billmeyer | Textbook of Polymer Science | John Wiley & Sons, New York | 1984 |
| 11 | M. Arumugam | Engineering Physics | Anuradha Agencies, Kumbakonam | 2003 |
| 12 | F. W. Billmeyer | Textbook of Polymer Science | John Wiley & Sons, New York | 2003 |

**TEACHING METHODOLOGY:**

- Board and chalk
- PowerPoint presentation
- Group discussion
- Seminar and Assignments
- Animated videos
- Board and chalk

**SYLLABUS DESIGNER:**

Mrs. J. Saranya, Assistant Professor, Department of Chemistry

## ELECTIVE PAPER – III B: BASIC PHARMACOLOGY

| Semester | Subject Code | Category | Instruction Hours | | | | | | Credits |
|---|---|---|---|---|---|---|---|---|---|
| | | | Lecture | | Theory | | Practical | | |
| | | | Per Week | Per Semester | Per Week | Per Semester | Per Week | Per Semester | |
| III | | Elective-III | 3 | 45 | 3 | 45 | 0 | 0 | 3 |

**COURSE OBJECTIVES:**

- To study the basic principles and history of drugs, metabolism and adverse effect of various drugs.
- To learn about anticancer drugs, use of bioassays, screening and manufacturing factors of dugs.

**COURSE OUTCOMES:**

- On the successful completion of course, students will be able to

| CO Number | CO statement | Knowledge level |
|---|---|---|
| CO1 | Understand the types and properties of drugs | K3 & K2 |
| CO2 | Gain knowledge about the adverse effects of drugs | K3 & K2 |
| CO3 | Gain knowledge about the bioassays and anticancer drugs | K2 &K4 |
| CO4 | Acquire knowledge about various methods of screening effects | K2 &K3 |
| CO5 | Understand the Principles of pharmacopeia and manufacturing practices of drugs | K3 &K4 |

*CO – Course Outcomes

Knowledge level K1 – Remember; K2 – Understand; K3 – Apply; K4 – Analyze

**MAPPING WITH PROGRAM OUTCOMES**

| COS | PO1 | PO2 | PO3 | PO4 | PO5 | PO6 |
|---|---|---|---|---|---|---|
| **CO1** | M | S | S | M | S | S |
| **CO2** | M | M | S | M | S | M |
| **CO3** | S | S | M | M | M | S |
| **CO4** | M | S | S | M | S | M |
| **CO5** | M | S | S | S | M | M |

**UNIT – I : Principles and Classification of Drugs 9 hours**

History of development of Pharmacology – introduction – general principles of route of drug administration – pharmacokinetics – absorption – distribution – metabolism – excretion – pharmacodynamics – general mechanism of drug action – Classification of drugs based on sources - mode of administration – site of action – absorption of drugs – Drugs distribution and elimination – Role of kidney in elimination.

**UNIT– II: Adverse effect of Drugs 9 hours**

Elementary introduction to adverse drug reactions – drug interactions – drug allergy – adverse responses and side effects of drugs – drugs intolerance – Drug addiction – drug abuses and their biological effects – toxicity - general concepts – acute – subacute – chronic toxicity tests – teratogenicity – carcinogenicity – iatrogenic diseases – Lethal Dose 50 – Effective Dose 50 – tolerance – habituation.

**UNIT – III: Anticancer drugs and Bioassays 9 hours**

Anticancer drugs: General introduction of anticancer drugs – mechanism of action – Natural and man-made radioisotopes and their applications

Bioassays: General principles – general methods – biological variations – animal ethics – Bioassays of insulin – heparin – d-tubocurarin – digitalis – acetylcholine – adrenaline – histamine.

**UNIT– IV: Screening of Drugs 9 hours**

General principles of screening of drugs – general screening methods – clinical trial – Screening methods for evaluation of anti-inflammatory – analgesics – antipyretics – antiulcer, anticonvulsants – hepatoprotective – antidiabetic – diuretic and drugs acting on CNS.

**UNIT –V: Industrial Aspects 9 hours**

Regulations – pharmacopeia – Good manufacturing practices (GMP) – risk and importance of GMP – Guidelines of GMP – ten Principles of GMP – design and construct the facilities and equipments – procedures and instructions – document work – validate work – monitor facilities and equipment – operating procedure – design develop and demonstrate job competence – protect against contamination – control component and product related processes – conduct planned and periodic audits – current GMP in manufacturing process and its importanctance – drug analysis – aspirin – paracetamol and ciprofloxacin.

**Distribution of hours: Theory – 90%; Problems –10%**

**TEXT BOOKS**

| S.No. | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| 1. | Goodman & Gillman | The Pharmacological Basis of Therapeutics | 13th Edition, McGraw Hill Companies, New York, USA, | 2017 |
| 2. | Jayashree Gosh | A Textbook of Pharmaceutical Chemistry | S. Chand Pub., | 2012 |
| 3. | G. R. Chatwal | Pharmaceutical Chemistry | Himalaya Pub., | 2010 |
| 4. | Bentley | Textbook of Pharmaceutical Chemistry | Oxford Univ., Press. | 2006 |

| | | | | |
|---|---|---|---|---|
| 5. | Chatterje | Textbook of Medical Biochemistry | Jaypee Brothers pub. | 2001 |

**REFERENCE BOOKS**

| S. No | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| 1 | Katzung G. Bertram | Basic and Clinical Pharmacology | McGraw Hill Companies, New York, USA | 2001 |
| 2 | Dipak K. Sarker | Quality System and Control for Pharmaceutics | John wiley & sons Ltd. | 2000 |
| 3 | Donald Cairns | Essentials of Pharmaceutical Chemistry | 4th Edition, Pharmaceutical Press | 2012 |
| 4 | H. Beckett , J. B . Stenlake | Practical Pharmaceutical Chemistry | 4th Edition, The Athlone Press | 1988 |
| 5 | Camille Georges Wermuth, David Aldous, Pierre Raboisson, Didier Rognan | The Practice of Medicinal Chemistry | 4th Edition, Elsiver | 2015 |
| 6 | Charles Dickson | Experiments in Pharmaceutical Chemistry | 2nd Edition, CRC Press | 2014 |
| 7 | Rang H. P., Dale M. M., Ritter J. M. | Pharmacology | Churchill livingstone, New York | 1999 |
| 8 | R. S. Satoskar | Pharmacology and Pharmacotherapeutics | 16th Edition, Mumbai Popular Prakashan | 1999 |
| 9 | Munson L. Paul,. | Principles of Pharmacology, | Chapman & Hill, N. Y. | 1995 |
| 10 | S. K. Kulkarni & P. C. Dandiya | Introduction to Pharmacology | 5th Edition, Vallabh Prakasha, | 1998 |

**TEACHING METHODOLOGY:**

- Board and chalk
- PowerPoint presentation
- Group discussion
- Seminar and Assignments
- Animated videos
- Board and chalk

**SYLLABUS DESIGNER:**

Mrs. J. Saranya, Assistant Professor, Department of Chemistry

## ELECTIVE PAPER – IIIC: INDUSTRIAL CHEMISTRY

| Semester | Subject | Category | Instruction Hours | Credits |
|---|---|---|---|---|

| | Code | | Lecture | | Theory | | Practical | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | Per Week | Per Semester | Per Week | Per Semester | Per Week | Per Semester | |
| III | | Elective-III | 3 | 45 | 3 | 45 | 0 | 0 | 3 |

**COURSE OBJECTIVES:**

- To learn about Fuels, corrosion, Paints and Pigments
- To study the Resins, Plastics and Liquid Fuels.

**COURSE OUTCOMES:**

- On the successful completion of course, students will be able to

| CO Number | CO statement | Knowledge level |
|---|---|---|
| CO1 | Understand the classification of fuels and calorific value | K3 & K2 |
| CO2 | Gain knowledge about the mechanism of electrochemical corrosion, galvanic corrosion. | K3 & K2 |
| CO3 | Gain knowledge about the constituents, manufacture, functions, types of paint and pigments. | K2 &K4 |
| CO4 | Acquire knowledge about thermosetting resins and its types. | K2 &K3 |
| CO5 | Understand the liquid fuels and advantages of catalytic cracking over thermal cracking. | K3 &K4 |

*CO – Course Outcomes

Knowledge level K1 – Remember; K2 – Understand; K3 – Apply; K4 – Analyze

**MAPPING WITH PROGRAM OUTCOMES**

| COS | PO1 | PO2 | PO3 | PO4 | PO5 | PO6 |
|---|---|---|---|---|---|---|
| **CO1** | M | S | M | S | M | S |
| **CO2** | S | M | S | M | S | M |
| **CO3** | S | S | M | S | M | S |
| **CO4** | M | M | S | S | M | M |
| **CO5** | S | S | M | M | S | M |

**UNIT– I: Fuels and Combustion 9 hours**

Introduction – Classification of Fuels – Calorific Value – Theoretical Calculation of Calorific value of a fuel – gross calorific value and net calorific value – Characteristics of a Good fuels – Solid fuels – Wood – Coal – Classification of Coal by Rank – Selection of Coal – Analysis of Coal and its significance.

**UNIT– II: Corrosion and its control 9 hours**

Introduction – Economic aspects of corrosion – Dry or Chemical Corrosion – Wet or electrochemical corrosion – Mechanism of Electrochemical Corrosion – Galvanic Corrosion – Concentration Cell Corrosion – Differential aeration corrosion – Pitting Corrosion – Underground or soil corrosion – Passivity.

**UNIT– III: Paints and Pigments 9 hours**

Paints: Classification of paints – Distempers – constituents of paints – setting of the paint – Requirements of a good paint – Emulsion paints – Latex paints – paint removers – Varnishes – Solvents and thinners.

Pigments – Introduction – Requirements of organic pigments - Types of Pigments – Applications.

**UNIT – IV: Resins and Plastics** **9 hours**

Important thermosetting resins – Phenol Formaldehyde Resin or Phenolic Resin – Amino Resins and Plastics – Epoxy Resins – Acrylic Resins and Plastics – Polyester resins – Silicone Resins – Silicone fluids – Silicone greases – Polyurethanes – Foamed or cellular plastics.

**UNIT–V: Liquid Fuels** **9 hours**

Liquid fuels – Petroleum cracking – Advantages of catalytic cracking over thermal cracking – Synthetic Petrol – Refining of Gasoline – Reforming – Knocking – Octane number of Gasoline – Diesel Engine Fuels – Diesel – Octane number of Diesel Oil – Diesel index.

**Distribution of hours: Theory – 100%**

**TEXT BOOKS**

| S.No. | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| 1. | B. K. Sharma | Industrial Chemistry | Goel publishing house, Meerut | 2003 |
| 2. | S. P. Mahajan | Pollution Control Process in Industries | Tata McGraw - Hill Publishing Company Ltd., New Delhi | 2005 |
| 3. | C. K. Varshney | Water pollution and management | Wiley Eastern Ltd., Chennai - 20. | 1995 |
| 4. | R. K. Das | Industrial Chemistry | Kalyani Publications, New Delhi | 1982 |

**REFERENCE BOOKS**

| S.No | Authors | Title | Publishers | Year of publication |
|---|---|---|---|---|
| 1 | A. Ravikrishnan | Engineering Chemistry | Sri Krishna Publications | 2006 |
| 2. | B. K Sharma | Industrial Chemistry | Goel Publications | 2014 |
| 3. | B. K. Sharma | Fuels And Petroleum Processing | Krishan Prakashan | 2014 |
| 4. | P. C. Jain and Monika Jain | Engineering Chemistry | Dhanpat Rai publishing company | 2013 |
| 5. | N. | Engineering | Prentice Hall India Learning | 2014 |

| | | | | |
|---|---|---|---|---|
| | Krishnamurthy | Chemistry | Private Limited | |

**TEACHING METHODOLOGY:**

- Board and chalk
- PowerPoint presentation
- Group discussion
- Seminar and Assignments
- Animated videos
- Board and chalk

**SYLLABUS DESIGNERS:**

Dr. D. Shakila, Assistant Professor, Department of Chemistry

## PAPER – X: PHOTOCHEMISTRY, HETEROCYCLES AND NATURAL PRODUCTS

| Semester | Subject Code | Category | Instruction Hours | | | | | | Credits |
|---|---|---|---|---|---|---|---|---|---|
| | | | Lecture | | Theory | | Practical | | |
| | | | Per Week | Per Semester | Per Week | Per Semester | Per Week | Per Semester | |
| IV | | Core | 6 | 90 | 6 | 90 | 0 | 0 | 4 |

**COURSE OBJECTIVES:**

- To understand the organic photochemistry and pericyclic reactions, their mechanism and synthetic utility.
- To understand the heterocycles, biosysnthesis and synthesis of natural products

**COURSE OUTCOMES:**

- On the successful completion of course, students will be able to

| CO Number | CO statement | Knowledge level |
|---|---|---|
| **CO1** | Acquire good foundation in reaction mechanisms involved in photochemistry. | K2 & K4 |
| **CO2** | Get knowledge in pericyclic reactions and mechanisms in photochemical reactions. | K2 & K3 |
| **CO3** | Learn the importance of synthesis and reactivity of five member and six membered heterocycles. | K2 & K4 |
| **CO4** | Acquire the knowledge in the synthesis, reactions of higher heterocycles with two hetero atoms | K3 & K4 |
| **CO5** | Get clear idea about the isolation, classification, structural elucidation and synthesis of terpenes and terpenoids. | K2 & K3 |

* CO – Course Outcomes

Knowledge level: K1– Remember; K2 – Understand; K3 – Apply; K4 – Analyze

**MAPPING WITH PROGRAM OUTCOMES**

| COS | PO1 | PO2 | PO3 | PO4 | PO5 | PO6 |
|---|---|---|---|---|---|---|
| **CO1** | M | M | S | M | S | M |
| **CO2** | S | M | S | M | S | M |
| **CO3** | S | S | M | S | M | M |
| **CO4** | M | M | S | M | S | S |
| **CO5** | S | S | M | S | M | M |

**UNIT – I: Organic Photochemistry** **12 hours**

Photochemistry of ketones – Norrish Type-I, Norrish type-II – Photoreduction – photochemistry of olefins – cis-trans isomerisation – Photocycloaddition – Paterno-Buchi reaction – photochemistry of aromatic compounds – photorearrangements – Di-π methane rearrangement – oxa and aza di-π methane rearrangements – Barton reaction and Photo-Fries

reaction – Photochemistry of cyclohexadienones – photochemistry of santonin – synthesis of Vitamin D.

**UNIT–II: Pericyclic Reactions 12 hours**

Classification – orbital symmetry – Woodward Hoffmann rule – FMO analysis of electro cyclic – cycloaddition – sigmatropic reactions – hydrogen shift – carbon shift reactions. Correlation diagram method for cycloaddition reactions ($\pi^{2s}+\pi^{2s}$) – ( $\pi^{4s}+\pi^{2s}$) – electrocyclic reactions – butadiene, cyclobutene system and interconversion of hexatriene to cyclohexadiene – Diels-Alder reaction, Ene reaction and dipolar cycloaddition reactions – Claisen and Cope reactions – degenerate Cope reaction – fluxional isomerism – semibullvalene and bullvalene – Synthetic applications of pericyclic reactions.

**UNIT – III: Heterocycles - I 12 hours**

Nomenclature – Non-aromatic heterocyclic compounds – three – four – five – six member rings with one hetero atom (N, O, S) – structure – synthesis – reactions – physical and chemical properties – Aromatic heterocyclic compounds – five and six membered heterocyclic systems with one heteroatom – Pyrrole – Furan – Thiophene – Pyridine – Two heteroatoms – Pyrazole – Imidazole – Pyrimidine – Pyrazine – Benzo fused heterocyclic systems – Indole – Quinoline – Isoquinoline

**UNIT - IV: Heterocycles - II 12 hours**

Six membered heterocycles with two or more hetero atoms: Synthesis and reactions of diazines, triazines and tetrazines.

Seven and large membered heterocycles: Synthesis and reactions of azepines, oxepines, thiepines and diazepines – Synthesis of five and six membered heterocycles with P, As, Sb and Bi.

**UNIT – V: Chemistry of Terpenes and Terpenoids 12 hours**

Biosynthesis of acyclic and monocyclic terpenes from acetyl CoA – synthesis of *trans* chrysanthemic acid – biosynthesis of loganin and seco-loganin – asymmetric synthesis using limonene and menthol – chemical degradation – structure and synthesis of alpha-pinene and camphor – biosynthesis of sesquiterpenes – structure of transannular cyclisation and synthesis of caryophyllene

**Terpenoids:** Isolation and classification – general methods to elucidate the structure of terpenoids – structural elucidation of zingiberine, eudesmol, caryophyllene, abietic acid and santonin.

**Distribution of hours: Theory – 90%; Problems – 10%**

**TEXTBOOKS**

| S. No | Authors | Title | Publishers | Year of Publication |
|---|---|---|---|---|
| 1. | J. A. Joule and K. Mills | Heterocyclic Chemistry | John Wiley, 5th Ed | 2010 |
| 2. | T. L. Gilchrist | Heterocyclic Chemistry | Dorling Kindersley India (P) Ltd, Third Impression | 2008 |
| 3. | R. K. Bansal | Heterocyclic Chemistry | New Age International (P) Ltd, 5th Ed | 2014 |
| 4. | Charles A. Depuy and Orville L. Chapman, Englewood Cliffs | Molecular Reactions and Photochemistry | New Jersey: Prentice-Hall | 1972 |
| 5. | Nicholas J Turro, V. Ramamurthy and J. C. Scaiano | Modern Molecular Photochemistry for Organic Molecules | University Science Books, 1st Ed | 2010 |
| 6. | Jagdamba Singh and Jaya Singh | Photochemistry and Pericyclic Reactions | New Age International (P) Ltd, 3rd Ed | 2012 |
| 7. | P. L. Gilchrist and R. C. Storr | Organic Reactions & Orbital Symmetry | Cambridge [Eng.] University Press | 1972 |
| 8. | Sunil Kumar, Vinod Kumar and S. P. Singh | Pericyclic Reactions:A Mechanistic and Problem Solving Approach | Academic Press (Elsevier | 2016 |
| 9. | S. Sankararaman | Pericyclic Reactions: A Textbook: Reactions, Applications | Wiley-VCH | 2005 |
| 10. | Woodward and Hoffman | The Conservation of Orbital Symmetry Theory | Academic Press | 1971 |

**REFERENCE BOOKS**

| S. No | Authors | Title | Publishers | Year of Publication |
|---|---|---|---|---|
| 1. | K. K. Rohatgi Mukherjee | Fundamentals of Photochemistry | New Age International Publishers | 2017 |
| 2. | V. Ramamurthy | Organic Photochemistry | CRC Press | 2019 |
| 3. | J. M. Coxon, B. Halton | Organic Photochemistry | Cambridge India | 2015 |
| 4. | K. C. Majumdar | Textbook of Pericyclic Reactions | Medtech Publishers | 2015 |
| 5. | Satyajit Dey | Pericyclic Reactions and Organic Photochemistry Through Solved Problems | Techno World | 2019 |
| 6. | O.P. Agarwal | Chemistry of Natural Products | GOEL Publishing House | 2015 |

| | | | | |
|---|---|---|---|---|
| 7. | I.L. Finar, | Organic Chemistry, Stereochemistry and Chemistry of Natural Products | Volume II, Pearson Education | 2002 |
| 8. | T. L. Gilchrist | Heterocyclic Chemistry | Longman Scientific Technical | 2017 |
| 9. | I. L. Finar | Organic Chemistry Vol 1 & 2 | Dorling Kindersley India (P) Ltd | 2009 |
| 10. | Gurdeep Charwal | Chemistry of Natural Products | Himalaya Publishing House | 2018 |

**TEACHING METHODOLOGY:**

- Board and chalk
- PowerPoint presentation
- Group discussion
- Seminar and Assignments
- Animated videos
- Board and chalk

**SYLLABUS DESIGNERS:**

Dr. D. Shakila, Assistant Professor, Department of Chemistry

## PAPER– IV:ELECTIVE PAPER A: SCIENTIFIC RESEARCH METHODOLOGY

| Semester | Subject Code | Category | Instruction Hours | | | | | | Credits |
|---|---|---|---|---|---|---|---|---|---|
| | | | Lecture | | Theory | | Practical | | |
| | | | Per Week | Per Semester | Per Week | Per Semester | Per Week | Per Semester | |
| IV | | Elective | 3 | 45 | 3 | 45 | 0 | 0 | 3 |

**COURSE OBJECTIVES:**

- To study about the importance of research, literature survey, search engines and evaluation of analytical datas.
- To learn the scientific writing and publication of research articles.

**COURSE OUTCOMES:**

- On the successful completion of course, students will be able to

| CO Number | CO statement | Knowledge level |
|---|---|---|
| **CO1** | Acquire good knowledge about the nature and importance of research | K2 & K4 |
| **CO2** | Gain clear concepts of separation techniques | K2 & K3 |
| **CO3** | Analyse the various error analysis and to evaluate the data | K3 & K4 |
| **CO4** | Apply the statistical treatment of various tests | K3 & K4 |
| **CO5** | Understand the conventions of thesis writing and paper publication | K3 & K4 |

* CO – Course Outcomes

Knowledge level K1 – Remember; K2 – Understand; K3 – Apply; K4 – Analyze

**MAPPING WITH PROGRAM OUTCOMES**

| COS | PO1 | PO2 | PO3 | PO4 | PO5 | PO6 |
|---|---|---|---|---|---|---|
| **CO1** | S | M | S | M | S | S |
| **CO2** | M | S | S | S | M | S |
| **CO3** | S | M | M | S | S | M |
| **CO4** | M | S | S | M | M | S |
| **CO5** | M | S | M | S | M | S |

**UNIT– I : Meaning of Research, Literature and Search Engines 9 hours**

Nature and importance of research – aims, objective, principles and problems – selection of research problem – purpose of research – scientific methods – role of theory – characteristics of research – Types of research: fundamental or pure research – applied research – action research – historical research – experimental research.

Survey of scientific literature – primary and secondary sources – citation index for scientific papers and journals – patents.

ASAP Alerts, CA Alerts, SciFinder, Chem Port, Science Direct, Web of Science,

Scopus, STN International.

**UNIT – II : Conduct of Research work** **9 hours**

Physical properties useful in analysis and methods of separation prior to analysis – Isolation techniques – extraction – Soxhlet extraction, crystallization, sublimation – methods for vacuum sublimation and distillation under reduced pressure.

Chemistry of working with hazardous materials – acid / water sensitive – corrosive – toxic – explosive and radioactive materials.

**UNIT – III : Evaluation of Analytical Data** **9 hours**

Evaluation of analytical data – Precision and accuracy – Mean, Median, Range, Deviation – Arithmetic – Relative arithmetic – Standard – Relative standard – Variance – Error in chemical analysis – Absolute, Relative, determinate, random – Systematic – Instrumental, Methodic, Personal, Proportional, Constant errors – Histogram – statistical methods – Gaussian Curve – normal distribution curve – Poisson curve – Characterizing measurements and results – Detection limits.

**UNIT – IV : Statistical Treatment of Analytical Data** **9 hours**

Statistical treatment of finite samples – the students 't' test and F test – Criteria for rejection of an observation – Q test – significant figures and computation rules – data plotting – Correlation diagram – least square analysis – correlation and regression analysis – correlation coefficient – bar diagram.

**UNIT – V: Scientific Writing** **9 hours**

**Scientific writings**: Research reports – theses – journal articles and books.

**Steps to publish a scientific article in a journal**: Types of publications – communications – articles – reviews – when to publish – where to publish – specific format required for submission – organization of the material – Documenting: abstracts – indicative or descriptive abstract – informative abstract – footnotes – endnotes – referencing styles – bibliography – journal abbreviations.

Conventions of writing – the general format – page and chapter format – use of quotations and footnotes – preparation of tables and figures – referencing – appendices.

**Distribution of hours: Theory – 80%; Problems – 20%**

**TEXT BOOKS**

| S. No | Authors | Title | Publishers | Year of Publication |
|---|---|---|---|---|
| 1. | John W. Creswell | Research Design | International Student 4th Edition | 2013 |
| 2. | Arthur Vogel | Textbook of | ELBS Edition | 1978 |

| | | | | |
|---|---|---|---|---|
| | | Quantitative Chemical Analysis | | |
| 3. | J. Anderson, H. M. Durston and M. Poole | Thesis and Assignment writing | Wiley Eastern Ltd | 1970 |
| 4. | Kothari | Research Methodology | Willey Eastern Pub | 1985 |
| 5. | Donglas A. Skoog and Donald, M. West | Fundamental of Analytical Chemistry | Halt Saundersons International Edition. | 1963 |
| 6. | Y. K. Singh | Fundamental of Research Methodology and Statistics | New Age International Pvt.Ltd | 2006 |

**REFERENCE BOOKS**

| S.No | Authors | Title | Publishers | Year of Publication |
|---|---|---|---|---|
| 1. | C. R. Kothari | Research Methodology | New Age International Publisher | 2020 |
| 2. | Ranjit Kumar | Research Methodology | Pearson India | 2005 |
| 3. | R. Panneerselvam | Research Methodology | Prentice Hall India Learning Pvt. Ltd. | 2011 |
| 4. | Deepak Chawla | Research Methodology concept and Cases | S. Chand & Company | 2011 |
| 5. | Bhanwar Lal Garg | An Introduction to Research Methodology | RBSA Publisher | 2015 |
| 6. | Y.K.Singh | Fundamentals of Research Methodology and Statistics | New Age International Pvt.Ltd | 2006 |

**TEACHING METHODOLOGY:**

- Board and chalk
- PowerPoint presentation
- Group discussion
- Seminar and Assignments
- Animated videos
- Board and chalk

**SYLLABUS DESIGNER:**

Dr. T. Gomathi, Assistant Professor, Department of Chemistry

## PAPER – IV: ELECTIVE PAPER – B: SUPRAMOLECULAR CHEMISTRY

| Semester | Subject Code | Category | Instruction Hours | | | | | | Credits |
|---|---|---|---|---|---|---|---|---|---|
| | | | Lecture | | Theory | | Practical | | |
| | | | Per Week | Per Semester | Per Week | Per Semester | Per Week | Per Semester | |
| IV | | Elective | 3 | 45 | 3 | 45 | 0 | 0 | 3 |

**COURSE OBJECTIVES:**

- Understanding the basic concepts and terminologies in Supramolecular Chemistry.
- To understand about the importance and applications of Supramolecular Chemistry.

**COURSE OUTCOMES:**

- On the successful completion of course, students will be able to

| CO Number | CO statement | Knowledge level |
|---|---|---|
| **CO1** | Gain better knowledge about the concepts and terminologies used in supramolecular chemistry | K2 & K4 |
| **CO2** | Apply principles and synthesis of molecular recognition | K2 & K3 |
| **CO3** | Analyse the various error analysis and to evaluate the datas | K3 & K4 |
| **CO4** | Gain clear ideas of supramolecules in nanoscience | K2 & K3 |
| **CO5** | Learn the applications of supramolecular chemistry in various aspects | K2 & K3 |

* CO – Course Outcomes

Knowledge level K1– Remember; K2 – Understand; K3 – Apply; K4 –Analyze

**MAPPING WITH PROGRAM OUTCOMES**

| COS | PO1 | PO2 | PO3 | PO4 | PO5 | PO6 |
|---|---|---|---|---|---|---|
| **CO1** | M | M | S | M | S | M |
| **CO2** | S | M | S | S | M | M |
| **CO3** | S | S | M | S | M | S |
| **CO4** | M | M | S | S | M | S |
| **CO5** | M | S | M | M | S | M |

**UNIT – I : Concepts of Supramolecular Chemistry 9 hours**

Terminology and definitions in supramolecular chemistry – Intermolecular forces **–** Ion pairing **–** ion-dipole and dipole-dipole interactions **–** hydrogen bonding **–** cation-pi **–** anion-pi **–** pi-pi interactions and Van-der-Waal forces – Solvent and solution properties **–** solvation and hydrophobic effect.

**UNIT – II: Molecular Recognition 9 hours**

Principle of molecular recognition **–** host-guest complementarity **–** preorganisation **–** chelate effect **–** cooperativity – Synthesis and applications of supramolecular host (crown ethers, lariat ethers, podands, cryptands, spherands, calix[n]arenes, cyclodextrin) as cation and anion binding receptors and receptors for ion-pair recognition.

**UNIT – III: Supramolecular Reactivity and Catalysis 9 hours**

Organocatalysis mediated through hydrogen bonding – preconcentration – self-assembly of catalysts and preorganisation of catalyst – substrate systems – Influence of organisation (effective molarity) on catalysis, Catalytic acyl transfer – acid-base catalysis – catalysed hydrolysis of ATPase mimic.

**UNIT – IV: Supramolecules in Nanoscience 9 hours**

Nano-capsules and containers – main synthetic strategies for their preparation ( Examples of each type) – Potential uses of such assemblies as nano-reactors and for transport (e.g. drug-delivery) – Self-assembly of metal nanoparticles (via H-bonding and electrostatic forces) – Using the coordination bond to prepare large supramolecular assemblies – Cages, macrocycles and catenanes – Polymeric materials and grids

**UNIT – V: Applications of Supramolecular Chemistry 9 hours**

Rational Design – Molecular Paneling – Supramolecular reactivity and catalysis – Supramolecular devices – Nanoscience applications – Supramolecular Chemistry in Biology: Membranes – Macrocyclic systems – Photosynthesis – Oxygen transport – Biological mimics – Enzymes – Metallobiosites – Heame analogues.

**Distribution of hours: Theory – 100%**

**TEXT BOOKS**

| S. No | Authors | Title | Publishers | Year of Publication |
|---|---|---|---|---|
| 1. | P. A. Gale and J. W. Steed | Supramolecular Chemistry: From Molecules to Nanomaterials | John Wiley & Sons | 2012 |
| 2. | F. Diederich, P. J. Stang, R. T. Tykwinski | Modern Supramolecular Chemistry | John Wiley & Sons | 2008 |
| 3. | J. W. Steed, D. R. Turner, K. J. Wallace | Core Concepts in Supramolecular Chemistry and Nanochemistry | John Wiley & Sons | 2007 |
| 4. | J. W. Steed and J. L. Atwood | Supramolecular Chemistry | John Wiley & Sons 2nd edition | 2011 |
| 5. | J. M. Lehn, Wiley VCH, Weinheim | Supramolecular Chemistry: Concepts and Perspectives | John Wiley & Sons | 1995 |

| | | | | |
|---|---|---|---|---|
| 6. | V. Balzani (Editor), L. De Cola, Kluwer, Dordrecht | Supramolecular Chemistry | John Wiley & Sons | 1992 |

**REFERENCE BOOKS**

| S. No | Authors | Title | Publishers | Year of Publication |
|---|---|---|---|---|
| 1. | H. Dodziuk | Introduction to Supramolecular Chemistry | Kluwer Academic Publishers, The Netherlands | 2002 |
| 2. | Asim K. Das and Mahua Das | Introduction to Supramolecular Chemistry | CBS Publisher | 2017 |
| 3. | J. Lehn | Supramolecular Chemistry: Concepts and Perspectives | John Wiley | 2014 |
| 4. | T. Kunitake, K Ariga, Berlin | Supramolecular Chemistry – Fundamentals and Applications. | Springer-Verlag Heidelberg | 2006 |
| 5. | P. S. Kalsi | Bioorganic, Bioinorganic and Supramolecular Chemistry | New Age International Publshers | 2017 |
| 6. | D. John | Supramolecular and Cluster Chemistry | Sarup Book | 2019 |

**TEACHING METHODOLOGY:**

- Board and chalk
- PowerPoint presentation
- Group discussion
- Seminar and Assignments
- Animated videos
- Board and chalk

**SYLLABUS DESIGNER:**

Mrs. R. Bharathi Priyadharsini, Assistant Professor, Department of Chemistry

## PAPERIV: ELECTIVE PAPER- C: NANOSCIENCE AND TECHNOLOGY

| Semester | Subject Code | Category | Instruction Hours | | | | | | Credits |
|---|---|---|---|---|---|---|---|---|---|
| | | | Lecture | | Theory | | Practical | | |
| | | | Per Week | Per Semester | Per Week | Per Semester | Per Week | Per Semester | |
| IV | | Elective | 3 | 45 | 3 | 45 | 0 | 0 | 3 |

**COURSE OBJECTIVES:**

- To understand preparation, characterization and synthesis of nanomaterials.
- To understand about the importance and applications of nanotechnology in various fields.

**COURSE OUTCOMES:**

- On the successful completion of course, students will be able to

| CO Number | CO statement | Knowledge level |
|---|---|---|
| **CO1** | Learn about the synthesis and chemical process of nanoscience | K2 & K3 |
| **CO2** | Apply principles and characterization of nanoscience by XRD, SEM, EDAX, TEM, | K3 & K4 |
| **CO3** | Analyse the various application of nanotechnology in remediation of pollution | K3 & K4 |
| **CO4** | Get knowledge about the tissue engineering and degradation of cell culture | K2 & K3 |
| **CO5** | Gain clear knowledge about drug delivery and gene delivery systems | K2 & K3 |

* CO – Course Outcomes

Knowledge level K1 – Remember; K2 – Understand; K3 – Apply; K4 – Analyze

**MAPPING WITH PROGRAM OUTCOMES**

| COS | PO1 | PO2 | PO3 | PO4 | PO5 | PO6 |
|---|---|---|---|---|---|---|
| **CO1** | S | M | S | M | M | S |
| **CO2** | M | S | M | S | S | M |
| **CO3** | S | M | M | M | S | S |
| **CO4** | M | S | M | S | M | M |
| **CO5** | M | S | M | S | M | S |

**UNIT– I : Synthesis of Nanomaterials Chemical Processes 9 hours**

Chemical precipitation and co-precipitation, polyol – borohydride reduction methods – Sol-Gel synthesis; Microemulsions synthesis – Hydrothermal – Solvothermal synthesis methods – Microwave assisted synthesis – Sonochemical assisted synthesis – Core-Shell nanostructure – Organic – Inorganic hybrid nanocomposites – Quantum dot (QDs) synthesis.

**UNIT – II: Nanostructured Materials Characterization Techniques 9 hours**

X-ray diffraction (XRD) – SEM – EDAX – TEM – Elemental mapping – FTIR – UV-Visible spectrophotometer – Laser Raman Spectroscopy – Nanomechanical – Characterization using Nanoindentation – Differential Scanning Calorimeter (DSC) – Differential Thermal Analyzer (DTA) – Thermo gravimetric Analysis (TGA) – TEM – X-ray Photoelectron Spectroscopy (XPS) – Electrochemical Characterisation measurements.

**UNIT – III: Nanotechnology - Environmental and Health Effects 9 hours**

Environmental pollutants in air, water, soil, hazardous and toxic wastes – application of nanotechnology in remediation of pollution – The challenge to occupational health and hygiene – toxicity of nanoparticles – effects of inhaled nanosized particles – skin exposure to nanoparticles – impact of CNTs on respiratory systems – hazards and risks of exposure to nanoparticles – monitoring nanoparticles in workplace and sensors.

**UNIT – IV: Tissue Engineering 9 hours**

Introduction – Stem cells – Morphogenesis – Generation of tissue in the embryo – Tissue homeostasis – Cellular signaling – Extracellular matrix as a biologic scaffold for tissue engineering – Natural polymers in tissue engineering applications – Degradable polymers for tissue engineering – Degradation of bioceramics – Cell source – Cell culture: harvest – selection, expansion and differentiation – Cell nutrition – Cryobiology.

**UNIT – V: Drug Delivery Systems and Fundamentals of Drug Nanoparticles 9 hours**

Production – Size – Surface area – Suspension and Settling, Magnetic and Optical Properties, Biological Transport – Manufacturing of Nanoparticles: Ball-Milling – High-Pressure Homogenization – Spray-Drying Production in Nonaqueous Liquids – Hot-Melted Matrices – Pelletisation Techniques – Direct Compress – Delivery of Nanoparticles – Brain Delivery – Ocular Drug Delivery – Gene Delivery Systems – Carriers in Cancer Therapy – Cardiovascular System – Vascular Delivery to the Lungs – Targeting Lymphatics.

**Distribution of hours: Theory – 100%**

**TEXT BOOKS**

| S. No | Authors | Title | Publishers | Year of Publication |
|---|---|---|---|---|
| 1. | Sanjay Mathur and Mrityunjay Singh | Nanostructured Materials and Nanotechnology– II, | Willey | 2008 |

| | | | | |
|---|---|---|---|---|
| | | Eds. | | |
| 2. | Carl C. Koch | Nanostructured Materials | Noyes Publications, New York | 2002 |
| 3. | G. A. Nazri and G. Pistoia | Science and Technology | Kulwer Acdemic Publishers, Dordrecht, Netherlands | 2004 |
| 4. | P. Brown and K. Stevens | Nanofibers and Nanotechnology in Textiles | Woodhead publication London | 2006 |
| 5. | J. Altmann, Routledge | Military Nanotechnology: Potential Applications and Preventive Arms Control | Taylor and Francis Group | 2006 |
| 6. | Jennifer Kuzma and Peter VerHage | Nanotechnology in Agriculture and Food Production | Woodrow Wilson International Center | 2006 |
| 7. | D. Shi, B. Aktas, L. Pust, F. Mikailov | Nanostructured Magnetic Materials and their Applications, Ed. | Springer | 2002 |

**REFERENCE BOOKS**

| S. No | Authors | Title | Publishers | Year of Publication |
|---|---|---|---|---|
| 1. | K. K. Chattopadhyay | An Introduction to Nanoscience and Nanotechnology | Prentice Hall Learning Pvt. Ltd. | 2009 |
| 2. | Charles P. Poole | An Introduction to Nanotechnology | Wiley-Interscience | 2008 |
| 3. | Victor E. Borisenko | A Handbook on Nanoscience and Nanotechnology | Wiley VCH | 2008 |
| 4. | T. Pradeep | A Textbook of Nanoscience and Nanotechnology | McGraw Hill Education | 2017 |
| 5. | B. K. Parthasarathy | Nanoscience and Nanotechnology | Isha books | 2017 |
| 6. | B. S. Murthy | Textbook of Nanoscience and Nanotechnology | Springer | 2013 |
| 7. | Hari Singh Nalwa | Encyclopedia of Nanoscience and Nanotechnology | American Scientific Publishers | 2004 |

**TEACHING METHODOLOGY:**

- Board and chalk
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**SYLLABUS DESIGNER:**

Mrs. R. Bharathi Priyadharsini, Assistant Professor, Department of Chemistry

## IV SEMESTER
## ORGANIC CHEMISTRY PRACTICAL - II (60 HOURS)

**Any Six Preparations From The Following Involving Two Stages**

1. sym-Tribromobenzene from aniline.
2. Benzanilide from benzophenone
3. m-Nitrobenzoic acid from methyl benzoate
4. 2,4 - Dinitrobenzoic acid from p-nitrotoluene
5. m-Nitrobenzoic acid from methylbenzoate
6. Benzil from benzaldehyde
7. Anthraquinone from phthalic anhydride
8. Phthalide from phthalic anhydride
9. 2 - Phenylindole from phenylhydrazine
10. 2, 4 - dinitrophenyl hydrazine from p-nitrochlorobenzene

**Any Two Exercises in the Extraction of Natural Products**
(Need not to be given for examination)

1. Caffeine from tea leaves
2. Lactose from milk
3. Citric acid from lemon
4. Piperine from black pepper

**Chromatographic Separations** (Need not be given for examination)
1. Column chromatography - separation of anthracene and picric acid from anthracene picrate.
2. Thin layer chromatography separation of green leaf pigments.
3. Paper chromatography-Identification of amino acids.

**Any Five Estimation**
1. Estimation of aniline
2. Estimation of phenol
3. Estimation of glucose
4. Estimation of amino group
5. Estimation of amide group
6. Saponification of fat or an oil
7. Iodine value of an oil
8. Estimation of sulphur in an organic compound
9. Estimation of methyl ketone

**IV Special Interpretation of Organic Compounds UV, IR, PMR And Mass Spectra Of 12 Compounds**
1. 1,3,5- Trimethyl benzene
2. Pinacolone

3. p-Methoxybenzylalcohol
4. Benzyl bromide
5. Phenylacetone
6. Acetone
7. Isoopropyl alcohol
8. 2-N,N-Dimethylaminoethanol
9. Pyridine
10. 4-Picoline
11. 1,3-dibromo - 1, 1- dicholoropropene
12. Cinnamaldehyde

**Organic Practical : Max.Marks :60**

| | |
|---|---|
| Preparation | 10 Marks |
| Estimation | 20 Marks |
| Record | 10 Marks |
| Interpretation of spectra | 10 Marks |
| Practical Viva | 10 Marks |
| Total | 60 Marks |

**RECOMMENDED BOOKS**


1. A text book of Practical Organic Chemistry by Arthur I.Vogel, CBS Pub.,
2. Laboratory Manual of Organic Chemistry Raj K. Bansal, Wiley Eastern limited.
3. Laboratory manual of Organic Chemistry by Mann and Saunders.
4. Advanced Practical Chemistry, Chatterjee, Books & Allied (P) Ltd.,

## IV SEMESTER
## INORGANIC CHEMISTRY PRACTICAL – II (60 HRS)

**Quantitative Analysis Of Complex Materials**

**A. Estimation of mixture containing two metal ions**

a. Copper and Nickel
b. Copper and Zinc
c. Iron and Nickel
d. Iron and Magnesium

**B. Analysis of alloys (Need not be given for examination)**

1. Estimation of tin and lead in solder.
2. Estimation of copper and zinc in brass.
3. Estimation of chromium and nickel in stainless steel.

**C. Analysis of inorganic complex compounds (Need not be given for examination)**

1. Preparation of cis and trans potassium bis(Oxalato)diaquochromate and analysis of each of these for Chromium.
2. Preparation of potassium tris(Oxalato)ferrate(III) and analysis for iron and oxalate.

**D. Preparation of the following :**

1. Sodium hexanitrocobaltate (III)
2. Tris (ethylene diamine) cobalt (III) chloride
3. Chloropentammine cobalt (III) chloride
4. Bis (acetylacetanto) copper (II)
5. Hexamminenickel (II) chloride
6. Sodium bis(thiosulphato) cuprate (I)
7. Hexamminecobalt (III) chloride
8. Ammonium hexachloro stanate(IV).
9. potassium trioxalato ferrate(III),

**E. List of spectra to be given for interpretation**

1. $^{31}P$ NMR Spectra of methylphosphate
2. $^{31}P$ NMR Spectra of $HPF_2$
3. $^{19}F$ NMR Spectra of $CIF_3$
4. $^{1}H$ NMR Spectra of Tris (ethythioacctoacetanato) cobalt (III)
5. High resolution $^{I}$ H NMR spectra of (N-propylisonitrosoacetylacetoneiminato) (acetylacetoneiminato) Nickel (II)
6. ESR Spectra of the aqueous $ON(SO_3)^{2}$- ion.
7. ESR Spectra of the H atoms in $CaF_2$.
8. ESR Spectra of the $(Mn\ (H_2O)_6)^{2+}$.
9. ESR Spectra of the bis (salicylaldiminato) copper (II)
10. IR Spectra of the sulphato ligand.
11. IR Spectra of the dimethylglyoxime ligand and its Nickel (11) complex.

12. IR Spectra of carbonyls
13. Mossbauer spectra of $FeSO_4$ $7H_2O$
14. Mossbauer spectra of $FeCl_3$.
15. Mossbauer spectra of $(Fe(CN)_6)^{3-}$
16. Mossbauer spectra of $(Fe\ (CN)_6)^{4-}$

| **Inorganic Practical** | **: Max.Marks :60** |
|---|---|
| Preparation | 10 Marks |
| Estimation : | |
| Volumetric | 10 Marks |
| Gravimetry | 10 Marks |
| Record | 10 Marks |
| Interpretation of spectra | 10 Marks |
| Practical Viva | 10 Marks |
| Total | 60 Marks |

**Recommended books**

1. Textbook of quantitative Analysis, A. Vogel, CBS Pub.,
2. Quantitative Inorganic Analysis, Upadhyaya, S. Chand & Co., Ltd.,
3. Handbook of Methods in Environmental Studies VOL.l Water and Wastewater Analysis, S.K.Maiti, ABD Publisher 2005.
4. Mars G. Fontana, Corrosion Engineering, Mc Graw Hill series in Materials Science and Engineering,1987.

## IV SEMESTER

## PHYSICAL CHEMISTRY PRACTICAL II (60 HOURS)

### Experiments in electrochemistry, conductometry and potentiometry

Experiments given to familiarise only the interpretation of spectra provided. Interpretation of simple UV-visible spectra of simple molecules for the calculation of molecular data and identification of functional groups (5 typical spectra will be provided).

IR and NMR spectral calculations of force constant –identification and interpretation of a spectra (5 each in IR and NMR will be provided).

**List of experiments for physical chemistry practical - II**

**Conductometric experiments:**

1. Determination of cell Constant.
2. Determination of the equivalent conductance of a weak acid at different concentrations and verification of Ostwald's dilution law and calculation of the dissociation constant of the acid.
3. Determination of equivalent conductance of a strong electrolyte at different concentrations and examination of the validity of the Onsager's theory as limiting law at high dilutions.
4. Conductometric titrations of a mixture of HCl, $CH_3COOH$ and NaOH.
5. Determination of the dissociation constant of formic acid at different dilution.
6. Determination of the strength of strong acid using strong base.
7. Determination of strength of weak acid using strong base.
8. Determination of the strength of strong acid using weak base.
9. Determination of the strength of Barium chloride using Magnesium sulphate.

**Potentiometric experiments**

10. Determination of strength of strong acid using strong base and weak acid against strong base
11. Determination of dissociation constant of a weak acid.
12. Determination of the strength of $FeSO_4$ using $KMnO_4$

13. Determination of strength of KI using $KMnO_4$
14. Determination of pH of a given buffer solution
15. Determination of strength of a mixture of halides using $AgNO_3$ - Precipitation titration.

| **PHYSICAL PRACTICAL** | **Max. Marks 60** |
|---|---|
| Experiment | 30 Marks |
| Interpretation of spectra | 10 Marks |
| Record | 10 Marks |
| Viva-voce | 10 Marks |
| Total | 60 Marks |

**REFERENCE**

1. Advanced Practical Chemistry, Chatterjee, Books & Allied (P) Ltd.,