# HAJEE KARUTHA ROWTHER HOWDIA COLLEGE

(An Autonomous Institution Affiliated to Madurai Kamaraj University, Madurai.)

**Uthamapalayam, Theni District. Pin Code: 625 533.**

# DEPARTMENT OF CHEMISTRY

## MASTER OF SCIENCE – CHEMISTRY

## SYLLABUS

## Choice Based Credit System – CBCS

**(As per TANSCHE/MKU Guidelines)**

with

## Outcome Based Education (OBE)

(Academic Year 2020 -2021 onwards)

# HAJEE KARUTHA ROWTHER HOWDIA COLLEGE

(An Autonomous Institution Affiliated to Madurai Kamaraj University, Madurai.)

**Uthamapalayam, Theni District. Pin Code: 625 533.**

## Name of the Programme: M.Sc. Chemistry

## Choice Based Credit System (CBCS)
## (As per TANSCHE/MKU Guidelines)

## with
## Outcome Based Education (OBE)

(with effect from the Academic Year 2020 – 2021)

### College Vision and Mission

**Vision**

Our vision is to provide the best type of higher education to all, especially to students hailing from minority Muslim community, rural agricultural families and other deprived, under privileged sections of the society, inculcating the sense of social responsibility in them. Our college is committed to produce talented, duty-bound citizens to take up the challenges of the changing times.

**Mission**

Our mission is to impart and inculcate social values, spirit of service and religious tolerance as envisioned by our beloved Founder President Hajee Karutha Rowther.

The Vision beckons ..... the Mission continues forever.

## Programme Educational Objectives (PEO)

Our graduates will be progressive, efficient, value based, academically excellent, creative, collaborative, empowered and globally competent literates with the skills required for societal change.

They will demonstrate

| | |
|---|---|
| **PEO1** | Comprehensive knowledge and expertise, employability, the acumen of creative and critical thinking, the spirit of enquiry and professional attitude required for a successful career |
| **PEO2** | Accountability, linguistic competence and communication skills in the work environment and beyond |
| **PEO3** | Perseverance, effective collaboration, team spirit, leadership and problem solving skills |
| **PEO4** | Keen sense of civility, professional ethics, receptivity and moral righteousness |
| **PEO5** | Commitment to address social and environmental threats and to act as responsible service-minded, duty-bound global citizens |

## Department Vision and Mission

### Vision

- Generate knowledgeable Chemists and scientists to enhance services to the society.

### Mission

- Enable the students to excel in the subject, research and services.
- Elevate students to international standards.
- Encourage the students to take up competitive examinations.

**Programme Outcomes (PO)**

On the successful completion of M. Sc., Chemistry programme, the students will be able to

| | |
|---|---|
| **PO1** | Understand the essential parts of organic, inorganic and physical chemistry. |
| **PO2** | Categorize and apply the concepts of medicinal, environmental, nano, industrial, polymer, supramolecular and Computer Chemistry in real life situations. |
| **PO3** | Utilize basic analytical and technical skills in the various fields of chemistry to become as academically sound researchers and intellectuals. |
| **PO4** | Formulate novel research ideas in different areas of chemistry to solve various challenges of the society. |
| **PO5** | Formulate novel research ideas in different areas of chemistry to solve various challenges of the society. |

**Program Specific Outcomes (PSO)**

A graduate of M. Sc. Chemistry after two years will

| | |
|---|---|
| **PSO1** | Outline the essential parts of advanced fields of chemistry and pursue higher studies. |
| **PSO2** | Perform as employers in private/government institutions rising up to top positions by applying the learned concepts of chemical science. |
| **PSO3** | Utilize modern research and technological skills amongst the master students in order to become professionals and leaders in the various sectors of Chemical science. |
| **PSO4** | Recognize the importance of utilizing their research knowledge, skills and initiative for the benefit of society. |
| **PSO5** | Participate and succeed in various state, national and international level competitive examinations to get suitable employment in government and global research sectors. |

**Programme Scheme**

**Eligibility**

A candidate who has passed B.Sc., Chemistry as the major subject with physics as one ancillary. The other ancillary subject may be Mathematics or Botany or Zoology is eligible for the Master of Science – Chemistry Degree.

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

Medium of instruction: English.

**For Programme Completion**

A Candidate shall complete:

- Part III - Core papers in semesters I, II, III and IV respectively
- Part III - Elective papers in semesters I, II and IV respectively
- Part IV - Non- Major Elective papers in semester III

**Scheme of Examinations under Choice Based Credit System**

| | |
|---|---|
| Term End Examinations (TEE) | - 75 Marks |
| Continuous Internal Assessment Examinations (CIAE) | - 25 Marks |
| Total | - 100 Marks |

**Pattern of Continuous Internal Assessment Examinations (CIAE)**

| | |
|---|---|
| Average of Two Internal Tests (each 20 marks) | - 20 Marks |
| Seminar / Quiz / Assignment | - 05 Marks |
| Total | - 25 Marks |

**Pattern of Term End Examinations**

**(Max. Marks: 75 / Time: 3 Hours)**

**External Examinations Question Paper Pattern**

Section – A (10 X 1 = 10 Marks)

Answer ALL questions.

- Questions 1 - 10
- Two questions from each unit
- Multiple choice questions and each question carries Four choices

Section – B (5 X 7 = 35 Marks)

Answer ALL questions choosing either A or B.

- Questions 11 - 15
- Two questions from each unit (either…. or…. type)
- Descriptive Type

Section – C (3 X 10 = 30 Marks)

Answer any THREE out of five questions.

- Questions 16 - 20
- One question from each unit
- Descriptive Type

**Passing Marks**

Minimum 34 for External Exam

Eligibility for the degree – passing minimum is **50%**

**Practical Examination**

Internal – 40 marks

External – 60 marks

Total – 100 marks

Passing minimum is **40%**

**Weightage**

| Weightage for Bloom's Taxonomy | Percentage | Marks | |
|---|---|---|---|
| | | CIAE | TEE |
| Knowledge (Remembering) – K1 | 10 | 2 | 7 |
| Understanding – K2 | 10 | 3 | 8 |
| Applying – K3 | 20 | 5 | 15 |
| Analyzing – K4 | 20 | 5 | 15 |
| Evaluating – K5 | 40 | 10 | 30 |
| **Gross Total** | **100** | **25** | **75** |

**Assessment**

**Distribution of questions and marks for Continuous Internal Assessment Examinations**

| Bloom's Taxonomy | Section A | Section B | Section C | Total |
|---|---|---|---|---|
| Knowledge(K1) | 3 (3) | 1 (a or b) (4) | ----- | **40 Marks** |
| Understanding(K2) | 3 (3) | 1 (a or b) (4) | ----- | |
| Apply(K3) | 1 (1) | 1 (a or b) (4) | 1 (8) | |
| Analyzing (K4) | 1 (1) | 1 (a or b) (4) | 1 (8) | |
| CIA Examinations conducted for 40 marks and converted to 20 marks | | | | **40/2 = 20** |
| Evaluating (K5) | Seminar, Quiz/Assignments | | | **10/2 = 5** |

**Distribution of questions and marks for Term End Examinations**

| Bloom's Taxonomy | Section A | Section B | Section C | Total |
|---|---|---|---|---|
| Knowledge(K1) | 7<br>(7) | ------- | ------- | **Total**<br>**75 Marks** |
| Understanding(K2) | 1<br>(1) | 1<br>(a or b)<br>(7) | ------- | |
| Apply(K3) | 1<br>(1) | 2<br>(a or b)<br>(14) | ------- | |
| Analyzing (K4) | 1<br>(1) | 2<br>(a or b)<br>(14) | ------- | |
| Evaluating (K5) | ------- | ------- | 3 out of 5<br>(30) | |

**Note: Figures in parenthesis are Marks**

## Details of Course Category, Code, Credits & Title

| Course Category | Course Code | Course Title | Hrs | CIAE | TEE | Max. Marks | Credits |
|---|---|---|---|---|---|---|---|
| **Semester – I** | | | | | | | |
| **Part – III (OBE)** | | | | | | | |
| Core – I | 20PCHC11 | Organic Chemistry- I | 5 | 25 | 75 | 100 | 5 |
| Core – II | 20PCHC12 | Inorganic Chemistry- I | 5 | 25 | 75 | 100 | 4 |
| Core – III | 20PCHC13 | Physical Chemistry – I | 5 | 25 | 75 | 100 | 4 |
| Core – IV | 20PCHC1P | Organic Chemistry Practical | 10 | 40 | 60 | 100 | 5 |
| Elective - I | 20PCHE11 | Medicinal and Pharmaceutical Chemistry | 5 | 25 | 75 | 100 | 5 |
| | 20PCHE12 | C-Programming: Fundamentals and Applications in Chemistry | | | | | |
| | | **Total** | **30** | | | **500** | **23** |
| **Semester – II** | | | | | | | |
| **Part – III (OBE)** | | | | | | | |
| Core – V | 20PCHC21 | Organic Chemistry- II | 5 | 25 | 75 | 100 | 4 |
| Core – VI | 20PCHC22 | Inorganic Chemistry- II | 5 | 25 | 75 | 100 | 5 |
| Core – VII | 20PCHC23 | Physical Chemistry – II | 5 | 25 | 75 | 100 | 4 |
| Core – VIII | 20PCHC2P | Physical Chemistry Practical | 10 | 40 | 60 | 100 | 5 |
| Elective - II | 20PCHE21 | Analytical Chemistry | 5 | 25 | 75 | 100 | 5 |
| | 20PCHE22 | Computer Applications in Chemistry | | | | | |
| | | **Total** | **30** | | | **500** | **23** |

| Course Category | Course Code | Course Title | Hrs | CIAE | TEE | Max. Marks | Credits |
|---|---|---|---|---|---|---|---|
| **Semester – III** | | | | | | | |
| **Part – III (OBE)** | | | | | | | |
| Core – IX | 20PCHC31 | Organic Chemistry- III | 6 | 25 | 75 | 100 | 5 |
| Core – X | 20PCHC32 | Inorganic Chemistry - III | 6 | 25 | 75 | 100 | 5 |
| Core – XI | 20PCHC33 | Physical Chemistry- III | 5 | 25 | 75 | 100 | 5 |
| Core – XII | 20PCHC3P | Inorganic Chemistry Practical | 10 | 40 | 60 | 100 | 5 |
| **Part – IV** | | | | | | | |
| NME | 20PCHN31 | Applications in Chemistry | 3 | 25 | 75 | 100 | 3 |
| | | **Total** | **30** | | | **500** | **23** |
| **Semester – IV** | | | | | | | |
| **Part – III (OBE)** | | | | | | | |
| Core – XIII | 20PCHC41 | Organic Chemistry- IV | 5 | 25 | 75 | 100 | 4 |
| Core – XIV | 20PCHC42 | Inorganic Chemistry- IV | 5 | 25 | 75 | 100 | 4 |
| Core – XV | 20PCHC43 | Physical Chemistry – IV | 5 | 25 | 75 | 100 | 5 |
| Core – XVI | 20PCHC4P | Project | 10 | 40 | 75 | 100 | 4 |
| Elective - III | 20PCHE41 | Polymer Chemistry | 5 | 25 | 75 | 100 | 4 |
| | 20PCHE42 | Conducting Polymers | | | | | |
| | | **Total** | **30** | | | **500** | **21** |
| | | **Grand Total** | **120** | | | **2000** | **90** |

| Course Code | Course Title | Category | Total Hours | Credits |
|---|---|---|---|---|
| 20PCHC11 | Organic Chemistry - I | Core -I | 75 | 5 |

| Nature of Course | |
|---|---|
| Knowledge Oriented | ✓ |
| Skill Oriented | |
| Employability Oriented | |
| Entrepreneurship Oriented | |

| Course Relevance | |
|---|---|
| Local | |
| Regional | |
| National | |
| Global | ✓ |

**Preamble**

The course has been framed with an objective of instilling maximum knowledge on various chemical reaction mechanism viz. substitution, elimination and addition.

**Course Outcomes (CO)**

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

| No. | Course Outcome | Knowledge Level |
|---|---|---|
| **CO1** | Understand the concept of chemical delocalization, aromaticity and intermediates in the chemical reaction | **K1, K2, K3** |
| **CO2** | Classify and explain the types of intermediates and methods of determining organic reaction mechanism. | **K1, K2, K3 K4, K5** |
| **CO3** | Analyze the reaction mechanism in relation to nucleophilic substitution reactions. | **K1, K2, K3,K4** |
| **CO4** | Determine the mechanism for elimination reactions. | **K1, K2, K3,K4, K5** |
| **CO5** | Interpret and distinguish reaction mechanism of various addition reactions. | **K1, K2, K3,K4, K5** |

**K1-Knowledge K2-Understand K3-Apply K4- Analyse K5- Evaluate**

**Mapping of CO with PO**

| | PO1 | PO2 | PO3 | PO4 | PO5 |
|---|---|---|---|---|---|
| **CO1** | **3** | **1** | **2** | **3** | **3** |
| **CO2** | **3** | **1** | **1** | **3** | **3** |
| **CO3** | **3** | **1** | **3** | **3** | **3** |
| **CO4** | **2** | **3** | **2** | **2** | **3** |
| **CO5** | **3** | **3** | **2** | **3** | **2** |

**1-Low 2-Medium 3-Strong**

**Mapping of CO with PSO**

| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|---|---|---|---|---|---|
| **CO 1** | **3** | **3** | **2** | **2** | **3** |
| **CO 2** | **3** | **3** | **2** | **2** | **3** |
| **CO 3** | **3** | **3** | **3** | **1** | **3** |
| **CO 4** | **3** | **3** | **3** | **1** | **3** |
| **CO 5** | **3** | **3** | **3** | **1** | **2** |

**1-Low** **2-Medium** **3-Strong**

**Syllabus**

**Unit I** 15 Hours

**Delocalized chemical bonding, Aromaticity and Reaction intermediate:** Electron displacement – Steric effect – Tautomerism- Concept of aromaticity – Benzenoid and non-benzenoid compounds – Huckel's rule – Non aromatic and anti aromaticity - Alternant and non-alternant hydrocarbons - aromaticity of cyclopentadienyl anion and Tropylium cation – Azulenes and annulenes. Generation , structure, stability, reactivity and reactions of carbocations, carbanions, free radicals (reactions include Pinacol coupling, McMurray reactions, acyloin reaction, selective radical bromination). Carbenes: Stability - Structure – Generation – Types – Reactions. Nitrenes: Generation and reactions.

**UNIT - II** 15 Hours

**Reaction mechanism-I:** Guidelines for proposing reasonable mechanism – Energetics and energy profile diagrams – transition state – Intermediate – Hammond's postulate – principle of microscopic reversibility - kinetic and thermodynamic controls – kinetic and non-kinetic methods of determining organic reaction mechanism – primary and secondary kinetic isotope effects – Effect of structure on reactivity: Resonance and field effects – Quantitative treatments – Hammett and Taft equation.

**UNIT - III** 18 Hours

**Reaction mechanism-II:** Aliphatic Nucleophilic Substitution Reactions - Mechanism – $S_N1$ and $S_N2$, - Effect of substrate structure, attacking nucleophile, leaving group and reaction medium on reactivity - $S_Ni$, $S_Ei$, Neighboring group participation by n, π and σ bonds – Reactivity at an allylic, aliphatic trigonal and vinylic carbon – Ambident nuleophiles. Aromatic Nucleophilic Substitution Reactions: Unimolecular, Bimolecular and Benzyne mechanism – Effect of substrate, leaving group and attacking nucleophile. Electrophilic substitution reactions: Aliphatic: Bimolecular mechanism $S_E2$ and $S_E1$. Aromatic: Arenium ion mechanism – Orientation and reactivity: Ortho and Para ratio, partial rate factor.

**UNIT-IV** 15 Hours

**Reaction Mechanism III:** $E_1$, $E_2$ and $E_1CB$ mechanism- Competition between substitution and elimination – orientation of double bonds (Bredt's rule and Hofmann and saytzeff rules) – Effect of substrate structure, attacking nucleophile, leaving group and nature of reaction medium on reactivity – Mechanism and orientation in pyrolytic eliminations - Cope and Chugaev reaction (cis-elimination)

**UNIT-V** 15 Hours

**Reaction Mechanism IV:** Electrophilic, Nucleophilic & free radical addition – Mechanism, Orientation and reactivity and reactions - addition to conjugated systems- addition to α, β-unsaturated carbonyl and nitrile systems- Michael addition – addition of Grignard reagents-Diels Alder reaction Enamine reaction - Mechanism of Reformatsky reaction- Darzen reaction- Mannich reaction - Wittig reaction - Stobbe and Dieckman condensation.

**Text Books**:


Jerry March., ***Advanced Organic Chemistry, Reaction mechanism and structure***, John Wiley and sons, New York, 1992, 4th Edition.

R.O.C. Norman., ***Principles of organic synthesis***, Nelson Thornes, Hong Kong 2001, 3rd Edition.

P.J. Garrat., ***Aromaticity***, Mc Graw Hill, India,1991.

F.A. Carey and R.J. Sundberg,. ***Advanced Organic Chemistry***, ***Part A and B***, Plenum Press, 1990, 3rd Edition.

G.M. Badger., ***Aromatic character and Aromaticity***, Cambridge, USA, 2001.


**Reference Books:**


Clayden, Greeves, Warren and Wothers., ***Organic Chemistry***, Oxford Uni Press, UK, 2007.

E.S. Gould., ***Mechanism and structure in Organic Chemistry***, Holtoo INC, 1960.

G. Solomon., ***Organic Chemistry***, John Wiley and sons INC, 1992, 5th Edition.

R.K. Mackie and D.M. Smith, ***Guide Book to Organic synthesis***, Longman, UK, 1993.

Peter Sykes, A Guidebook to ***Mechanism in Organic Chemistry***, Longman, 2003, 6th Edition.


**Pedagogy**

Chalk & Talk, E-Resources, Group Discussion

**Teaching aids**

Black Board, LCD Projector

**Course Contents and Lecture Schedule**

| Module No. | Topic | No. of Lectures | Content Delivery Methods |
|---|---|---|---|
| | **UNIT – I** | | |
| 1.1 | Electron displacement – Steric effect – Tautomerism- Concept of aromaticity – Benzenoid and non-benzenoid compounds – | 3 | Chalk & Talk |
| 1.2 | Huckel's rule - Non aromatic and anti aromaticity- Alternant and non-alternant hydrocarbons - aromaticity of cyclopentadienyl anion and Tropylium cation – | 3 | E-Resources |
| 1.3 | Azulenes and annulenes- Synthesis, structure, stability, reactivity and reactions of carbocations, carbanions | 3 | Chalk & Talk |
| 1.4 | Synthesis, structure, stability, reactivity and reactions of free radicals (reactions include Pinacol coupling, McMurray reactions, acyloin reaction, selective radical bromination). | 3 | E-Resources |
| 1.5 | Carbenes: Stability - Structure – Generation – Types –Reactions. Nitrenes: Generation and reactions. | 3 | Discussion |
| | **UNIT – II** | | |
| 2.1 | Guidelines for proposing reasonable mechanism –Energetics and energy profile diagrams – transition state– Intermediate | 3 | E-Resources |
| 2.2 | Hammond's postulate – principle of microscopic reversibility - kinetic and thermodynamic controls | 3 | Chalk & Talk |
| 2.3 | Kinetic and non-kinetic methods of determining organic reaction mechanism | 3 | E-Resources |
| 2.4 | Primary and secondary kinetic isotope effects – Effect of structure on reactivity: Resonance and field effects | 3 | Discussion |
| 2.5 | Quantitative treatments – Hammett and Taft equation. | 3 | Chalk & Talk |

| | | | |
|---|---|---|---|
| **UNIT – III** | | | |
| 3.1 | Aliphatic Nucleophilic Substitution Reactions - Mechanism – $S_N1$ and $S_N2$, - Effect of substrate structure, attacking nucleophile, leaving group and reaction medium on reactivity - $S_Ni$, $S_Ei$. | 6 | E-Resources |
| 3.2 | Neighboring group participation by n, π and σ bonds – Reactivity at an allylic, aliphatic trigonal and vinylic carbon – Ambident nuleophiles. | 5 | Chalk & Talk |
| 3.3 | Aromatic Nucleophilic Substitution Reactions: Unimolecular, Bimolecular and Benzyne mechanism – Effect of substrate, leaving group and attacking nucleophile. | 3 | Discussion |
| 3.4 | Electrophilic substitution reactions: Aliphatic: Bimolecular mechanism $S_E2$ and $S_E1$. | 2 | E-Resources |
| 3.5 | Aromatic: Arenium ion mechanism – Orientation and reactivity: Ortho and Para ratio, partial rate factor. | 2 | E-Resources |
| **UNIT – IV** | | | |
| 4.1 | Elimination reactions$E_1$, $E_2$ and $E_1CB$ mechanism | 3 | Discussion |
| 4.2 | Competition between substitution and elimination – orientation of double bonds (Bredt‘s rule and Hofmann and saytzeff rules) | 3 | E-Resources |
| 4.3 | Effect of substrate structure, attacking nucleophile, leaving group and nature of reaction medium on reactivity. | 3 | Chalk & Talk |
| 4.4 | Mechanism and orientation in pyrolytic eliminations - Cope and Chugaev reaction (cis-elimination) | 3 | Chalk & Talk |

| UNIT –V | | | |
|---|---|---|---|
| 5.1 | Addition to carbon – carbon multiple bonds: Electrophilic, Nucleophilic & free radical addition/ | 3 | E-Resources |
| 5.2 | Mechanism, Orientation and reactivity and reactions - addition to conjugated systems. | 3 | E-Resources |
| 5.3 | Addition to α, β-unsaturated carbonyl and nitrile systems-Michael addition. | 3 | Discussion |
| 5.4 | Addition of Grignard reagents-Diels Alder reaction Enamine reaction | 3 | Chalk & Talk |
| 5.5 | Mechanism of Reformatsky reaction- Darzen reaction- Mannich reaction - Wittig reaction - Stobbe and Dieckman condensation | 3 | E-Resources |
| | **Total** | **75** | |

**Course Designer**
**Mr. G. Arivalagan**
Assistant Professor of Chemistry

| Course Code | Course Title | Category | Total Hours | Credits |
|---|---|---|---|---|
| 20PCHC12 | Inorganic Chemistry -I | Core -II | 75 | 4 |

| Nature of Course | |
|---|---|
| Knowledge Oriented | ✓ |
| Skill Oriented | |
| Employability Oriented | |
| Entrepreneurship Oriented | |

| Course Relevance | |
|---|---|
| Local | |
| Regional | ✓ |
| National | |
| Global | ✓ |

**Preamble**

The course gives in-depth knowledge on electronic structure of atom, bonding and its applications, acid-base concepts and nuclear chemistry. .

**Course Outcomes (CO)**

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

| No. | Course Outcome | Knowledge Level |
|---|---|---|
| **CO1** | Comprehend the electronic structure of atom and periodic properties of elements. | **K1, K2** |
| **CO2** | Explain and compare the concepts of chemical bonding. | **K1, K2,K3,K4** |
| **CO3** | Apply the concepts of VB, MO and VSEPR theory to determine the structure of molecules. | **K1, K2,K3,K4 K5** |
| **CO4** | Illustrate acid-base concepts, its measures and to evaluate various effects on acid base strength. | **K1, K2,K3,K4,K5** |
| **CO5** | Experiment with different types of nuclear reactions, nuclear reactors and to list various nuclear waste disposal and safety measures. | **K1, K2,K3** |

**K1-Knowledge K2-Understand K3-Apply K4- Analyse K5- Evaluate**

**Mapping of CO with PO**

| | PO1 | PO2 | PO3 | PO4 | PO5 |
|---|---|---|---|---|---|
| **CO1** | **3** | **1** | **1** | **3** | **3** |
| **CO2** | **3** | **1** | **3** | **3** | **3** |
| **CO3** | **2** | **1** | **3** | **2** | **3** |
| **CO4** | **3** | **1** | **3** | **2** | **2** |
| **CO5** | **3** | **3** | **2** | **3** | **2** |

**1-Low 2-Medium 3-Strong**

**Mapping of CO with PSO**

| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|---|---|---|---|---|---|
| CO1 | 3 | 3 | 2 | 1 | 3 |
| CO2 | 3 | 1 | 2 | 1 | 3 |
| CO3 | 3 | 1 | 2 | 1 | 3 |
| CO4 | 3 | 1 | 2 | 3 | 3 |
| CO5 | 3 | 3 | 3 | 3 | 3 |

**1-Low** **2-Medium** **3-Strong**

**Syllabus**

**UNIT – I** 15 Hours

**Electronic structure of atom:** Modern views on atomic structure: Wave mechanical description of electron and orbitals, radial density functions and orbital energies, angular functions and orbital shapes-term symbol. Modern periodic table: Periodic properties-Ionisation potential, Ionic radii and covalent radii, Electron affinity, Electronegativity and their trend in the periodic table- Comparison of transition metals of 3d, 4d and 5d series

**UNIT II** 15 Hours

**Nature of the chemical bond:** Ionic bond – Lattice energy and its determination by Born-Haber cycle and Born-Lande Equation – Hardness, electrical conductivity and solubility of ionic compounds – ionic radii. Goldschmidths radius ratio - packing of atoms and ions in solids. Calculation of ionic radius –Pauling‘s method and Linde‘s method. Effective nuclear charge - Slater‘s rule. Covalent bond – qualitative treatment of valence bond theory – Heitler - London theory – Pauling theory and Molecular orbital theory LCAO theory – Hybridisation and resonance.

**UNIT III** 15 Hours

**Bonding application:** Application of VB and MO theories to the structure of homonuclear ($H_2$, $B_2$, $C_2$, $N_2$ and$O_2$) and heteronuclear (CO, NO, HCl, HF) diatomic and selective polyatomic molecules ($CO_3^{2-}$, $NO_2$, $BeH_2$, $CO_2$) comparison of VB and MO theories. Bond properties, bond order, bond energy, bond length and bond polarity. Partial ionic character of covalent bonds - Fajan‘s Rule – Effects of polarization. VSEPR theory and its applications to $H_2O$, $NH_3$, $ICl^{2-}$, $IF_5$, $IF_7$, $ClO^{4-}$ ions. VSEPR applied to Xenon compounds like Xenon halides and xenon oxides.

**UNIT IV** 15 Hours

**Acid-base systems and non-aqueous solvents:** A generalized acid base concepts – steric effects and solvation effects – Measures of Acid Base strength –Factors affecting the strength of acids and bases- Common ion effect and Henderson's equation- Hard and Soft acids and bases – symbiosis – theoretical basis of hardness and softness. Classification of solvents – properties of ionizing solvents. Typical reactions in non–aqueous solvents- liquid HF, liquid $SO_2$, liquid $NH_3$, and sulphuric acid.

**UNIT V** 15 Hours

**Nuclear chemistry:** Radioactive decay and equilibrium- Different types of nuclear reaction – spallation – fission and fusion. Theories of fission. Fissile and Fertile isotopes. Nuclear fusion – stellar energy-Nuclear forces: Liquid drop model, shell model-Calculation of Q-values – Cross section. Detectors: Scintillation counter, Gas Ionisation chamber. Proportional Counter, Cerenkov Counter-Accelerators: Cyclotron, Synchrocyclotron, Betatron. Radio isotopes and their Applications: Activation analysis, Isotopic dilution technique-radiometric titration. Nuclear reactors: Types (Thermo nuclear and breeder reactors) feed materials production. Reprocessing of nuclear materials waste disposal. Atomic power projects in India. Hazardous of radioactive materials and Safety measures.

**Text Books**


Clyde Day, M. Jr & Joel Selbin, ***Theoretical Inorganic Chemistry***, Chapman & Hall Ltd., London, 1967, 5th Reprint.

Chandra, A. K. ***Introductory Quantum Chemistry***, Tata McGraw Hill, New Delhi, 1988,3rd Edition.

Lee, J. D. Concise ***Inorganic Chemistry***, Blackwell Science Ltd., London. 2002, V Edition.

Durrant P. J. and Durrant. B, ***Introduction to advanced inorganic chemistry***, Longman Group Ltd, 1970, London.

Glasstone, S. ***Source Book of Atomic Energy***, Van Nostrand, East West Press (P) Ltd., New Delhi.1967, 3rd Edition.

Friedlander, G. Kennedy J.S and Millodr, M. M. ***Nuclear and radiochemistry***, John Wiley & Sons, New York.1984.


**Reference Books**


Huheey, J. E. Ellen A. Keiter, Richard L. Keiter, ***Inorganic Chemistry***, Pearson Education (Singapore) Pvt. Ltd., New Delhi, 2004, IV Edn.

Madan R. D. Modern ***Inorganic Chemistry***, S. Chand & Company Ltd., New Delhi, 2004.

Wahid U. Malik, G. D. Tuli and R. D. Madan, ***Selected Topics in Inorganic Chemistry***, S. Chand & Co. Ltd., New Delhi, 2006.
Gary L. Miessler and Donald A. Tarr, ***Inorganic Chemistry***, Pearson Education, Inc., New Delhi, 2004,3rd Edn.
William W. Porterfield, ***Inorganic Chemistry***, Elsevier, New Delhi, 2005, II Edn.
Sharpe, A.G. ***Inorganic Chemistry***, Addition – Wesley Longman, UK, 2004, III Edn.
Shriver D. F. and Atkins, P.W. ***Inorganic Chemistry***, Oxford University Press, London, 1999.
Arnikar, H. J. Essentials of ***Nuclear Chemistry***, New Age international (P) Ltd., New Delhi. 2005, IV Edn.

**Pedagogy**

Chalk & Talk, E-Resources, Group Discussion

**Teaching aids**

Black Board, LCD Projector

**Course Contents and Lecture Schedule**

| Module No. | Topic | No. of Lectures | Content Delivery Methods |
|---|---|---|---|
| | **UNIT – I** | | |
| 1.1 | Modern views on atomic structure: Wave mechanical description of electron. | 3 | Chalk & Talk |
| 1.2 | Radial density functions- Orbitals, and orbital energies- Angular functions and orbital shapes - Radii of atoms and ions. | 5 | E-Resources |
| 1.3 | Modern periodic table: Periodic properties- Ionisation potential, Ionic radii and covalent radii. | 4 | Chalk & Talk |
| 1.4 | Electron affinity. Electro negativity- their trend in the periodic table. | 3 | E-Resources |
| | **UNIT – II** | | |
| 2.1 | Ionic bond – Lattice energy and its determination by Born-Haber cycle and Born-Lande Equation. | 3 | E-Resources |
| 2.2 | Hardness, electrical conductivity and solubility of ionic compounds – ionic radii. | 2 | Chalk & Talk |

| | | | |
|---|---|---|---|
| 2.3 | Goldschmidths radius ratio- packing of atoms and ions in solids. Calculation of ionic radius –Pauling's method and Linde's method. Effective nuclear charge Slater's rule. | 4 | E-Resources |
| 2.4 | Covalent bond – qualitative treatment of valence bond theory – Heitler-London theory. | 3 | Discussion |
| 2.5 | Pauling theory and Molecular orbital theory LCAO theory – Hybridisation and resonance. | 3 | Chalk & Talk |
| **UNIT – III** | | | |
| 3.1 | Application of VB and MO theories to the structure of homonuclear ($H_2$, $B_2$, $C_2$, $N_2$). | 3 | E-Resources |
| 3.2 | Heteronuclear (CO, NO, HCl, HF) diatomic and selective polyatomic molecules ($CO_3^{2-}$, $NO_2$, $BeH_2$, $CO_2$). | 3 | Chalk & Talk |
| 3.3 | comparison of VB and MO theories- Bond properties, bond order, bond energy, bond length and bond polarity. | 3 | Discussion |
| 3.4 | Partial ionic character of covalent bonds- Fajan's Rule- VSEPR theory and its applications to $H_2O$, $NH_3$, $IF_5$, $IF_7$, $ClO^{4-}$ ions. | 3 | E-Resources |
| 3.5 | VSEPR applied to Xenon compounds like Xenon halides and xenon oxides. | 3 | E-Resources |
| **UNIT – IV** | | | |
| 4.1 | A generalized acid base concepts- Steric effects and solvation effects. | 3 | Discussion |
| 4.2 | Measures of Acid-Base strength –Factors affecting the strength of acids and bases. | 4 | E-Resources |
| 4.3 | Common ion effect and Henderson's equation- Hard and Soft acids and bases – symbiosis -theoretical basis of hardness and softness. | 4 | Chalk & Talk |
| 4.4 | Classification of solvents – properties of ionizing solvents. Typical reactions in non–aqueous solvents liquid HF, Hydrogen cyanide. Sulphuric acid and acetic acid. | 4 | Chalk & Talk |

| UNIT –V | | | |
|---|---|---|---|
| 5.1 | Radioactive decay and equilibrium- Different types of nuclear reaction – spallation – fission and fusion- Theories of fission. Fissile and Fertile isotopes - Radio isotopes and their applications | 4 | E-Resources |
| 5.2 | Nuclear fusion – stellar energy- Nuclear forces: Liquid drop model, shell model - Detectors: Scintillation counter, Gas Ionisation chamber. | 3 | E-Resources |
| 5.3 | Proportional Counter, Cerenkov Counter Accelerators: Cyclotron, Synchrocyclotron, Betatron. | 2 | Discussion |
| 5.4 | Calculation of Q-values – Cross section - Applications: Activation analysis, Isotopic dilution technique-radiometric titration | 2 | Chalk & Talk |
| 5.5 | Nuclear reactors: Types (Thermo nuclear and breeder reactors) feed materials production. Reprocessing of nuclear materials waste disposal-Atomic power projects in India. Hazardous of radioactive materials and Safety measures. | 4 | E-Resources |
| | **Total** | **75** | |

**Course Designer**
**Ms. A. Nihath Nazleen**
Assistant Professor of Chemistry

| Course Code | Course Title | Category | Total Hours | Credits |
|---|---|---|---|---|
| 20PCHC13 | Physical Chemistry-I | Core -III | 75 | 4 |

| Nature of Course | |
|---|---|
| Knowledge Oriented | ✓ |
| Skill Oriented | |
| Employability Oriented | |
| Entrepreneurship Oriented | |

| Course Relevance | |
|---|---|
| Local | |
| Regional | ✓ |
| National | |
| Global | ✓ |

**Preamble**

The course enables the students to gain knowledge on properties of gases, Thermodynamic equilibrium and bio-physicochemical behavior of molecules.

**Course Outcomes (CO)**

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

| No. | Course Outcome | Knowledge Level |
|---|---|---|
| **CO1** | Explain the properties of gases, liquid crystals, theory of thermodynamic equilibrium and non-equilibrium. | **K1,K2** |
| **CO2** | Compare the thermodynamic equilibrium and non-equilibrium studies. | **K1,K2,K3,K4** |
| **CO3** | Apply the concepts and fundamentals of quantum chemistry. | **K1,K2,K3** |
| **CO4** | Evaluate the quantum chemistry concepts and their applications. | **K1,K2,K3,K4,K5** |
| **CO5** | Develop their knowledge in application of SWE to many electron systems | **K1,K2,K3** |

**K1-Knowledge K2-Understand K3-Apply K4- Analyse K5- Evaluate**

**Mapping of CO with PO**

| | PO1 | PO2 | PO3 | PO4 | PO5 |
|---|---|---|---|---|---|
| **CO1** | **3** | **1** | **1** | **1** | **3** |
| **CO2** | **3** | **1** | **1** | **2** | **3** |
| **CO3** | **2** | **1** | **1** | **1** | **3** |
| **CO4** | **2** | **1** | **1** | **3** | **3** |
| **CO5** | **2** | **1** | **1** | **3** | **3** |

**1-Low 2-Medium 3-Strong**

**Mapping of CO with PSO**

| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|---|---|---|---|---|---|
| CO1 | 3 | 3 | 3 | 3 | 2 |
| CO2 | 3 | 1 | 2 | 2 | 3 |
| CO3 | 3 | 2 | 1 | 1 | 2 |
| CO4 | 3 | 2 | 2 | 1 | 2 |
| CO5 | 3 | 3 | 3 | 1 | 3 |

**1-Low** **2-Medium** **3-Strong**

**Syllabus**

**UNIT I** 15 Hours

**Properties of gases and liquid crystal:** Equations of states - molecular speeds - Maxwell distribution of molecular velocities - one, two and three dimensions; Energy distribution-Maxwell – Boltzmann distribution law Rotation, vibrations and translational degree of freedom- principle of equipartition of energy and heat capacity; Molecular collisions- collision diameter, cross-section, number, frequency, mean free path (definition only); Transport phenomena in gases - Viscosity of gases – viscosity in terms of momentum transfer, thermal conductivity, and diffusion. Liquid crystals- Nematic (p-methoxycinnamic acid), cholesteric (cholestryl benzoate), smectic (ethyl-p-azoxybenzoate)- Theory and its application in liquid crystals display.

**UNIT II** 15 Hours

**Thermodynamics – equilibrium and non-equilibrium:** A general review of enthalpy, entropy and free energy concepts: Nernst heat theorem Genesis of third law and its limitations - derivation of third law and their application to real gases- calculation of $(\delta H/dP)T$, $(\delta E/dV)T$ and $\mu j$. T for gases - Thermodynamics of open systems - partial molar properties- internal energy, molar enthalpy, molar entropy, molar volume, free energy (chemical potential) – determination of partial molar properties; Chemical potential- relationship between partial molal quantities - Gibbs - Duhem equation- Duhem Margules equation; thermodynamic properties of real gases- Fugacity concept- Determination of Fugacity of real gases.

**UNIT III** 15 Hours

**Quantum chemistry-I:** Black Body radiation- Heisenberg's uncertainty principle - de Broglie wave particle duality-Experimental verification of matter waves- Compton effect - The Schrodinger equation and the postulates of quantum mechanics - operators –linear and non-linear operators- commutative and non -commutative operators - Hermitian operators- Eigen function, Eigen values and degeneracy.

**UNIT IV** 15 Hours

**Quantum chemistry-II:** Application of quantum mechanics to simple system-Application of SWE to free particle moving in one dimension-particle moving in a one dimension box - particle moving in 3D cubical and rectangular box- Quantum Mechanical tunneling - particle in a ring- rigid rotor- Simple Harmonic oscillator - hydrogen atom- angular momentum spin momentum ladder operator.

**UNIT V** 15 Hours

**Approximation methods, application of SWE to many electron systems:** Necessity for approximation methods - Variation methods for the Hydrogen atom – Perturbation (first order) method to Helium atom - Slater determinant wave function secular determinant – Hartree – Fock self consistent field method to Helium atom – HMO bielectron theory of Ethylene and Butadiene.

**Text Books**


Glasstone S. A., ***Text book of Physical Chemistry***, McMillan India Ltd., 1999.

Alberty R. A. and Daniels F., ***Physical Chemistry***, John Wiley & Sons, New York, 1978.

Castellan G. W., ***Physical chemistry***, , Wesley Publishing Company, UK,1986,3rd edition.

Glasstone S., ***Thermodynamics for Chemists***, Eastern Wiley publications, 2002.

Atkins P, ***Physical Chemistry***, Oxford University Press, UK, 2002. 7th Edition.

Atkins P. W., ***Molecular Quantum Mechanics***, Oxford University Press, UK, 1986, 2nd Edition.

Hanna H. W., ***Quantum Mechanics in Chemistry***, Benjamin- Cummiza London Publishing Company, UK, 1983.

Chandra A.K., ***Introductory quantum chemistry***, Tata McGrow - Hill Publishing Co Ltd., New Delhi, India. 1988, 3rd edition.

Prasad R.K., ***Quantum Chemistry***, 2004, 4th revised edition.


**Reference Books**


Glasstone S., ***A text book of Physical Chemistry***, McMillan India Ltd., Alasca, 1999.

Walter J. Moore, ***Physical Chemistry***, Orient Longman, New York, 2006, 6th edition.

Klotz. M., Rosenberg, R. M., ***Chemical thermodynamics***, Benjamin, New York, 1996, 4th edition.

Glasstone, S., ***Thermodynamics for Chemists***, Eastern Wiley publications 2002, 5th edition.

Rajaram J., Kuriakose J. C., ***Thermodynamics***, S. N. Chand, New Delhi,1999, 3rd edition.
Levine, ***Quantum Chemistry***, Prentice-Hall, New Delhi, 2006, 6th edition.
Mcquarrie D. A., ***Quantum Chemistry***, Viva Books Pvt. Ltd., New Delhi, 2003.
Levine, ***Quantum Chemistry***, Prentice-Hall, UK, 2003, 5th edition.
Raymond Chang, ***Physical Chemistry with application to biochemical system***, Mc Millan Publishing Company. Inc., New Delhi. 2002.

**Pedagogy**

Chalk & Talk, E-Resources, Group Discussion

**Teaching aids**

Black Board, LCD Projector

**Course Contents and Lecture Schedule**

| Module No. | Topic | No. of Lectures | Content Delivery Methods |
|---|---|---|---|
| | **UNIT – I** | | |
| 1.1 | Equations of states - molecular speeds- Maxwell distribution of molecular velocities - one, two and three dimensions. | 3 | Chalk & Talk |
| 1.2 | Energy distribution-Maxwell – Boltzmann distribution law- Rotation, vibrations and translational degree of freedom- principle of equipartition of energy and heat capacity. | 3 | E-Resources |
| 1.3 | Molecular collisions- collision diameter, cross-section, number, frequency, mean free path (definition only). | 3 | Chalk & Talk |
| 1.4 | Transport phenomena in gases - Viscosity of gases – viscosity in terms of momentum transfer, thermal conductivity, and diffusion. | 3 | E-Resources |
| 1.5 | Liquid crystals- Nematic (p methoxycinnamic acid), cholesteric (cholestryl benzoate), smectic (ethyl-p -azoxybenzoate)-Liquid crystals theory and its application in liquid crystals display. | 3 | Discussion |
| | **UNIT – II** | | |
| 2.1 | A general review of enthalpy, entropy and free energy concepts: Nernst heat theorem- Genesis of third law and its limitations. | 3 | E-Resources |

| | | | |
|---|---|---|---|
| 2.2 | Derivation of third law and their application to real gases- calculation of (δH/dP)T, (δE/dV)T and μj.T for gases. | 3 | Chalk & Talk |
| 2.3 | Thermodynamics of open systems - partial molar properties- internal energy, molar enthalpy, molar entropy, molar volume, free energy (chemical potential). | 3 | E-Resources |
| 2.4 | Determination of partial molar properties; Chemical potential- relationship between partial molal quantities - Gibbs - Duhem equation- Duhem Margules equation. | 3 | Discussion |
| 2.5 | Thermodynamic properties of real gases- Fugacity concept- Determination of Fugacity of real gases. | 3 | Chalk & Talk |
| **UNIT – III** | | | |
| 3.1 | Black Body radiation- de Broglie wave particle duality- Heisenberg's uncertainty principle. | 3 | E-Resources |
| 3.2 | Experimental verification of matter waves- Compton effect - The Schrodinger equation and the postulates of quantum mechanics. | 3 | Chalk & Talk |
| 3.3 | Operators –linear and non-linear operators commutative and non-commutative operators Hermitian operators. | 4 | Discussion |
| 3.4 | Eigen function, Eigen values and degeneracy; Orthogonality and Normalization of wave functions. | 3 | E-Resources |
| 3.5 | Derivation of Schrodingers wave equation. | 2 | E-Resources |
| **UNIT – IV** | | | |
| 4.1 | Application of quantum mechanics to simple system. | 3 | Discussion |
| 4.2 | Application of Schrodinger wave equation (SWE) to free particle moving in one dimension | 3 | Chalk & Talk |
| 4.3 | Particle moving in a one dimension box- Particle moving in 3D cubical and rectangle. | 3 | Discussion |
| 4.4 | Quantum Mechanical tunneling - particle in a ring rigid rotor- Simple Harmonic oscillator | 3 | E-Resources |
| 4.5 | Hydrogen atom- angular momentum spin momentum ladder operator | 3 | Chalk & Talk |

| UNIT –V | | | |
|---|---|---|---|
| 5.1 | Necessity for approximation methods – Variation methods for the Hydrogen atom | 4 | E-Resources |
| 5.2 | Perturbation (first order) method to Helium atom | 2 | E-Resources |
| 5.3 | Slater determinant wave function- secular determinant | 4 | Discussion |
| 5.4 | Hartree – Fock self consistent field method to Helium atom | 2 | Chalk & Talk |
| 5.5 | HMO bielectron theory of Ethylene and Butadiene. | 3 | E-Resources |
| | **Total** | **75** | |

**Course Designer**
**Ms. A. Mumthaj**
Assistant Professor of Chemistry

| Course Code | Course Title | Category | Total Hours | Credits |
|---|---|---|---|---|
| 20PCHC1P | Organic Chemistry Practical | Core -IV | 150 | 5 |

| Nature of Course | |
|---|---|
| Knowledge Oriented | ✓ |
| Skill Oriented | ✓ |
| Employability Oriented | |
| Entrepreneurship Oriented | |

| Course Relevance | |
|---|---|
| Local | |
| Regional | |
| National | |
| Global | ✓ |

**Preamble**

This lab course enhances the laboratory skill of analyzing the functional groups present in a mixture of organic compounds qualitatively, preparing organic compounds, estimation of simple organic compounds.

**Course Outcomes (CO)**

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

| No. | Course Outcome | Knowledge Level |
|---|---|---|
| **CO1** | Identify the organic molecules. | **K1,K2,K3** |
| **CO2** | Separate the organic mixture by chemical methods. | **K1,K2,K3,K4** |
| **CO3** | Estimate the amount of glucose and amino acid viz., glycine and formaldehyde | **K1,K2,K3** |
| **CO4** | Interpret the iodometric method to estimate Ketonic compound. | **K1,K2,K3,K4,K5** |
| **CO5** | Predict the derivatives for the given organic compound. | **K1,K2,K3,K4,K5** |

**K1-Knowledge K2-Understand K3-Apply K4- Analyse K5- Evaluate**

**Mapping of CO with PO**

| | PO1 | PO2 | PO3 | PO4 | PO5 |
|---|---|---|---|---|---|
| **CO1** | **3** | **1** | **3** | **3** | **2** |
| **CO2** | **3** | **1** | **3** | **3** | **2** |
| **CO3** | **3** | **1** | **3** | **2** | **2** |
| **CO4** | **3** | **1** | **2** | **2** | **2** |
| **CO5** | **3** | **2** | **3** | **3** | **1** |

**1-Low 2-Medium 3-Strong**

**Mapping of CO with PSO**

| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|---|---|---|---|---|---|
| **CO1** | **3** | **3** | **3** | **3** | **2** |
| **CO2** | **3** | **3** | **2** | **1** | **2** |
| **CO3** | **3** | **3** | **3** | **3** | **3** |
| **CO4** | **3** | **3** | **2** | **1** | **2** |
| **CO5** | **3** | **3** | **3** | **3** | **2** |

**1-Low** **2-Medium** **3-Strong**

**Syllabus**

**I. Qualitative analysis:**

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

**II. Quantitative analysis:**

a. Estimation of glucose by lane and Eynon method and Bertrand method
b. Estimation of glycine
c. Estimation of formalin
d. Estimation of methyl ketone

**III. Organic preparations**:

(Only for class work) About 3 (five) two-stage preparation:

a. P-Nitro aniline from acetanilide benzophenone
b. P-Bromo aniline from acetanilide Aniline
c. m-Nitro benzoic acid from methyl benzoate.

**Text Books**

Dr. N. S. Gnanpragasam, ***Organic Chemistry: Lab Manual***, Viswanathan**,** S., Printers & Publishers Pvt Ltd, 2009.

**Reference Books**

Brian S. Furniss, ***Vogel's Textbook of Practical Organic Chemistry,*** Pearson India, 2003, 5th edition.

**Course Designer**

**Mr. G. Arivalagan**

Assistant Professor of Chemistry

| Course Code | Course Title | Category | Total Hours | Credits |
|---|---|---|---|---|
| 20PCHE11 | Medicinal and Pharmaceutical Chemistry | Elective -I | 75 | 5 |

| Nature of Course | |
|---|---|
| Knowledge Oriented | ✓ |
| Skill Oriented | |
| Employability Oriented | |
| Entrepreneurship Oriented | |

| Course Relevance | |
|---|---|
| Local | |
| Regional | ✓ |
| National | |
| Global | ✓ |

**Preamble**

Construe the drugs and their interactions with various organs of humans, synthesis of new drugs and their biological activities, therapeutic uses of steroids, alkaloids and antibiotics.

**Course Outcomes (CO)**

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

| No. | Course Outcome | Knowledge Level |
|---|---|---|
| CO1 | Tell the fundamentals of medicinal chemistry, QSAR, bio-isoterism, receptor and enzyme inhibitors as drugs. | K1,K2 |
| CO2 | Discover and evaluate Medicinally useful antibiotics and steroids | K1,K2,K3,K4,K5 |
| CO3 | Classify the drugs such as Antineoplastic Agents, Anti-tubercular drugs, Antimalarial drugs and Diuretics. | K1,K2,K3,K4 |
| CO4 | Plan the synthesis drugs such as Antihypertensive drugs and Antihistamines. | K1,K2,K3 |
| CO5 | Justify the basic concepts of Anti-inflammatory drugs, CNS stimulant drugs and CNS depresents drugs. | K1,K2,K3,K4,K5 |

**K1-Knowledge K2-Understand K3-Apply K4- Analyse K5- Evaluate**

**Mapping of CO with PO**

| | PO1 | PO2 | PO3 | PO4 | PO5 |
|---|---|---|---|---|---|
| CO1 | 1 | 3 | 1 | 3 | 1 |
| CO2 | 1 | 3 | 1 | 3 | 2 |
| CO3 | 1 | 3 | 2 | 2 | 2 |
| CO4 | 1 | 3 | 2 | 2 | 1 |
| CO5 | 1 | 3 | 1 | 2 | 2 |

**1-Low 2-Medium 3-Strong**

**Mapping of CO with PSO**

| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|---|---|---|---|---|---|
| **CO1** | **3** | **3** | **3** | **2** | **3** |
| **CO2** | **3** | **1** | **1** | **3** | **2** |
| **CO3** | **2** | **2** | **1** | **3** | **2** |
| **CO4** | **3** | **2** | **3** | **3** | **2** |
| **CO5** | **2** | **3** | **1** | **3** | **2** |

**1-Low** **2-Medium** **3-Strong**

**Syllabus**

**UNIT I** 15 Hours

**Fundamentals of Medicinal Chemistry:** Definitions of Medicinal Chemistry, Pharmacology and Molecular Pharmacology - Major process involved in drug action - Pharmacokinetics phase – Quantitative Structure Activity Relationship (QSAR) - Hansch approach – Concept of bio-isoterism – Receptors and classification of membrane bound receptors - Enzyme inhibitors as drugs (illustrated with one example).

**UNIT II** 15 Hours

**Medicinally useful antibiotics and steroids:** Structural features and mode of action of the following antibiotics –penicillin G, Cephalosporin and their semi synthetic analogs (β-lactum), Streptomycin (Aminogylcoside), Terramycin (Tetracyclin), Erythorymycin (Macrolide) and Chloramphenicol. Steroids; Oral contraceptives, anabolic steroids, anti - inflammatory steroids.

**UNIT III** 15 Hours

**Chemotheraopeutic *Agents*: *Antineoplastic Agents*:** Classification, synthesis e.g., Cyclophosphamide, Ifofamide, Chlorambucil, Busulfan, Decarbazine, Methotrexate, 6-Mercaptopurine. ***Anti-tubercular drugs*:** Classification, synthesis, e.g., Isoniazid, Pyrazinamine, Ethambutol, Thiacetoazone and Ethionamide. ***Antimalarial drugs:*** Classification, synthesis, e.g., Chloroquine, Primaguine, Amaodiaquine, Proguanil and Pyrimethamine. ***Diuretics:*** Classification, Synthesis, e.g., Furesemide, Acetazolamide, Chlorothiazide

**UNIT IV** 15 Hours

**Synthesis and Therapeutic action and SAR of certain drugs:** ***Antihypertensive drugs****:* Nifedipine, Captopril, Hydralazine, Sodium nitroprusside and Clonidine. ***Antihistamines***: H1-Antagonists: Pheniramine, Chlorpheniramine, Diphenylhydramine, Mepyramine, Promethazine, $H_2$-Antogonist: Cimetidine, Ranitidine and Fomotidine.

**UNIT V** 15 Hours

**Anti-inflammatory drugs:** Antipyretics & Non-narcotic analgesics; Aspirin, sodium salicylate, Paracetamol, phenylbuttazone, Oxypheylbutazone, Ibuprofen, Mefenamic acid and Dichlofenac sodium.

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

**CNS depresent Drugs:** Phenelazine, Isocarboxazide, Imipramine, Nortiptyline, Amitriptyline and Desipramine.

**Text Books**

G.L. Patrick, ***An introduction to Medicinal chemistry***, Oxford University Press, 2001,2nd Edn.

Ashutoshkar, ***Medicinal Chemistry***, New Age International Pvt. Ltd., 2010, 5th edition.

G.R. Chatwal, ***Medicinal Chemistry***, Himalaya Publishing House, 2010,2nd edition.

J. Dharuman, ***Pharmaceutical Organic Chemistry***, AITBS Publishers, 2007,1st edition.

**Reference Books**

T. Nagradi, ***Medicinal Chemistry*** – A Biochemical Approach, Oxford University, 2004.

J. B. Taylor and P.D. Kennewall, ***Introductory Medicinal Chemistry***, Ellisworth Publishers, 1985.

**Pedagogy**

Chalk & Talk, E-Resources, Group Discussion

**Teaching aids**

Black Board, LCD Projector

**Course Contents and Lecture Schedule**

| Module No. | Topic | No. of Lectures | Content Delivery Methods |
|---|---|---|---|
| **UNIT – I** | | | |
| 1.1 | Definitions of Medicinal Chemistry, Pharmacology and Molecular Pharmacology. | 3 | Chalk & Talk |
| 1.2 | Major process involved in drug action - Pharmacokinetics phase. | 3 | E-Resources |
| 1.3 | Quantitative structure Activity relationship (QSAR) | 3 | Chalk & Talk |
| 1.4 | Hansch approach – Concept of bio-isoterism. | 3 | E-Resources |
| 1.5 | Receptors and classification of membrane bound receptors-enzyme inhibitors as drugs. | 3 | Discussion |
| **UNIT – II** | | | |
| 2.1 | Structural features and mode of action of the following antibiotics: penicillin G, Cephalosporin and their semi synthetic analogs (β-lactum). | 6 | E-Resources |
| 2.2 | Streptomycin (aminogylcoside), Terramycin (tetracyclin). | 3 | Chalk & Talk |
| 2.3 | Erythorymycin (macrolide) and Chloramphenicol. | 2 | E-Resources |
| 2.4 | Steroids; Oral contraceptives, anabolic steroids. | 2 | Discussion |
| 2.5 | Anti -inflammatory steroids. | 2 | Chalk & Talk |
| **UNIT – III** | | | |
| 3.1 | Antineoplastic agents: Classification and synthesis of Cyclophosphamide, Ifofamide, Chlorambucil, | 3 | E-Resources |
| 3.2 | Classification and synthesis of Busulfan, Decarbazine, Methotrexate, 6 Mercaptopurine. | 3 | Chalk & Talk |
| 3.3 | Anti-tubercular drugs: Classification, synthesis of Isoniazid, Pyrazinamine, Ethambutol, Thiacetoazone and Ethionamide. | 3 | Discussion |
| 3.4 | Antimalarial drugs: Classification, synthesis of Chloroquine, Primaguine, Amaodiaquine, Proguanil and Pyrimethamine. | 3 | E-Resources |
| 3.5 | Diuretics: Classification, Synthesis of Furesemide, Acetazolamide, Chlorothiazide. | 3 | Discussion |

| | | | |
|---|---|---|---|
| **UNIT – IV** | | | |
| 4.1 | Antihypertensive drugs: Nifedipine, Captopril, Hydralazine. | 3 | Discussion |
| 4.2 | Sodium nitroprusside and Clonidine. | 3 | Chalk & Talk |
| 4.3 | Antihistamines: H1-Antagonists: Pheniramine, Chlorpheniramine. | 3 | Discussion |
| 4.4 | Diphenylhydramine, Mepyramine, Promethazine, H2-Antogonist. | 3 | E-Resources |
| 4.5 | Cimetidine, Ranitidine and Fomotidine. | 3 | E-Resources |
| **UNIT –V** | | | |
| 5.1 | Anti-inflammatory drugs: Antipyretics & Non-narcotic analgesics; Aspirin, sodium salicylate, Paracetamol. | 4 | E-Resources |
| 5.2 | phenylbuttazone, Oxypheylbutazone, Ibuprofen, Mefenamic acid, Dichlofenac sodium. | 3 | Chalk & Talk |
| 5.3 | CNS stimulant Drugs: Amphetamine, Caffeine, Theobromine, Theophylline. | 3 | Discussion |
| 5.4 | Bemegride, Nikethamide,MethyPhenidate. | 2 | Chalk & Talk |
| 5.5 | CNS depresent Drugs: Phenelazine, Isocarboxazide, Imipramine, Nortiptyline, Amitriptyline, Desipramine. | 3 | E-Resources |
| | **Total** | **75** | |

**Course Designer**
**Dr. M. P. Kesavan**
Assistant Professor of Chemistry

| Course Code | Course Title | Category | Total Hours | Credits |
|---|---|---|---|---|
| **20PCHE12** | **C-Programming: Fundamentals & Applications in Chemistry** | **Elective -II** | **75** | **5** |

| Nature of Course | |
|---|---|
| Knowledge Oriented | ✓ |
| Skill Oriented | ✓ |
| Employability Oriented | ✓ |
| Entrepreneurship Oriented | |

| Course Relevance | |
|---|---|
| Local | |
| Regional | |
| National | |
| Global | ✓ |

**Preamble**

The course explains the importance of C-programming and various terms used in C. It also explains the applications of C in solving problems in chemistry.

**Course Outcomes (CO)**

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

| No. | Course Outcome | Knowledge Level |
|---|---|---|
| **CO1** | Recall and explain the basics of C Programming; especially the operators, functions and expressions | **K1,K2** |
| **CO2** | Build a program using proper data input and output logics. | **K1,K2,K3** |
| **CO3** | Develop a program using the decision making looping logics. | **K1,K2,K3** |
| **CO4** | Construct the C Programs for solving the problems by chemical formula translation. | **K1,K2,K3,K4** |
| **CO5** | Evaluate C programs to compute the output for chemical formula in organic, inorganic and physical chemistry. | **K1,K2,K3,K4,K5** |

**K1-Knowledge K2-Understand K3-Apply K4- Analyse K5- Evaluate**

**Mapping of CO with PO**

| | PO1 | PO2 | PO3 | PO4 | PO5 |
|---|---|---|---|---|---|
| **CO1** | **2** | **3** | **1** | **2** | **2** |
| **CO2** | **2** | **3** | **1** | **2** | **1** |
| **CO3** | **1** | **3** | **2** | **1** | **1** |
| **CO4** | **3** | **3** | **3** | **3** | **1** |
| **CO5** | **3** | **3** | **3** | **3** | **3** |

**1-Low 2-Medium 3-Strong**

**Mapping of CO with PSO**

| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|---|---|---|---|---|---|
| CO1 | 2 | 1 | 1 | 2 | 2 |
| CO2 | 3 | 3 | 3 | 3 | 2 |
| CO3 | 3 | 2 | 2 | 3 | 2 |
| CO4 | 3 | 3 | 3 | 2 | 2 |
| CO5 | 3 | 3 | 3 | 3 | 2 |

**1-Low** **2-Medium** **3-Strong**

**Syllabus**

**UNIT I** 15 Hours

**Introduction and overview of C:** Introduction – Importance of C-structure of C-programs - Simple programs-style of the language. Characters – Keywords, Variables and parameters - Data types – Constants - Declaration of and assignments of values to variables. Operators - Arithmetic, Relational, Logical, assignment, Increment and Decrement, Conditional and bitwise operators-Special operators. Expressions - Arithmetic - Evaluation of expression- Procedure of arithmetic operators- Library functions.

**UNIT II** 15 Hours

**Data input and Output:** Character input- The get char function – Character output- The putchar function – Entering input data- the Scan function- Writing output data- The print function- Formatted input and output data- the gets and puts functions-preparing and running a complete program. Decision making and branching: Decision making with IF statement – simple IF statementthe IF…ELSE statement- Nesting of IF…Else statements – The ELSE IF ladder –The Switch statement – The? Operator – the GOTO statement.

**UNIT III** 15 Hours

**Decision making and Looping:** The WHILE statement – The DO statement-The FOR statement – Jumps in loops. **Arrays:** One dimensional array –Two dimensional arrays –Initializing two dimensional arrays- Multidimensional arrays. **User defined functions:** Need for user–defined functions – A multifunction program – The form of C functions -Return values and their types- Calling a function –Category of function- No arguments and no return values –Nesting functions- Recursions- The scope and life time of variables in function.

**UNIT IV** 15 Hours

**Applications of C in Chemistry-I**

Explanation of the formulae, equations and programs to solve the following problems in chemistry:

1. Calculation of Molecular weight of Organic Compounds.
2. Calculation of pH.
3. Determination on First Order rate constant for the given reaction
4. Evaluation of lattice energy using
   i) Born- Haber Cycle
   ii) Born –Lande equation
5. Computing ionic radii- Lande's method and Paulings method
6. Calculation of Normality, Molarity and Molality of a given solution
7. Converting Kelvin to Celsius temperature and vice versa.
8. Determination of enthalpy of a given solution
9. Evaluation of Cell constant
10. Calculation of energy of Hydrogen atom spectral lines.

**UNIT V** 15 Hours

**Applications of C in Chemistry-II**

Explanation of the formulae, equations and programs to solve the following problems in chemistry:

**Organic Chemistry:**

1. Use of Recursive functions to calculate the number of π Resonance structures for an organic conjugated system using res - str = n! / ((n/2)!* ((n/2) + 1)!)
2. Empirical formula of Hydrocarbons and other Organic compounds

**Inorganic Chemistry:**

1. Array manipulation to balance the chemical equations.
2. Half-life and average life periods of radioactive nuclei.
3. Binding energy of nucleus.
4. Program to get output as first ten elements of Periodic Table with their Name, Symbol, Atomic number and Atomic Weight.

**Physical chemistry:**

1. Calculation of RMS, average and MPV of gases.
2. Solving Quadratic equation to evaluate the Equilibrium constant for the reaction $H_2 + I_2 \longrightarrow 2HI$
3. Illustrate use of Loop to calculate the NMR frequency for a nucleus with Spin ½
4. Mean activity coefficient of an Electrolyte (KCl)

**Text Books**

E. Balagurusamy, ***Programming in ANSI C***, Tata McGraw- Hill Publishing Company Ltd., New Delhi, 2005, 3rd edition., 10th Reprint.

**Reference Books**

Brian W. Kernighan & Dennis M. Ritchie, ***The C Programming Language***, Prentice Hall of India Private Limited, New Delhi, 2001 2nd edition.

Byron S. Gottfried, ***Programming with C***, Tata McGraw- Hill Publishing Company Ltd., New Delhi, 2001, 2nd edition.

R. Rajaram, ***C Programming Made Easy***, Scitech Publications, Chennai 1999.

Yeshavant Kanitkar, ***Let Us C***,BPB Publications, New Delhi, 1999, 3rd edition.

Yeshavant Kanitkar, ***C Projects***, BPB Publications, New Delhi, 1998.

K. V. Raman, ***Computers in Chemistry***, Tata McGraw- Hill Publishing Company Ltd., New Delhi, 1993, 3rd edition.

**Pedagogy**

Chalk & Talk, E-Resources, Group Discussion

**Teaching aids**

Black Board, LCD Projector

**Course Contents and Lecture Schedule**

| Module No. | Topic | No. of Lectures | Content Delivery Methods |
|---|---|---|---|
| | **UNIT - I** | | |
| 1.1 | Introduction – Importance of C-structure of C- programs- Simple programs-style of the language. | 4 | E-Resources |
| 1.2 | Characters–Keywords, Variables and parameters- Data types-Constants - Declaration of and assignments of values to variables. | 4 | E-Resources |
| 1.3 | Operators-Arithmetic, Relational, Logical, assignment, Increment and Decrement, Conditional and bitwise operators-Special operators. | 4 | E-Resources |
| 1.4 | Expressions- Arithmetic - Evaluation of expression- Procedure of arithmetic operators- Library functions. | 3 | E-Resources |

| | | | |
|---|---|---|---|
| **UNIT - II** | | | |
| 2.1 | Character input- The getchar function – Character output- The putchar function – Entering input data- the Scanf function- Writing output data- The printf function- Formatted input and output data-the gets and puts functions-preparing and running a complete program. | 7 | E-Resources |
| 2.2 | Decision making and branching: Decision making with IF statement –simple IF statement-the IF…ELSE statement- Nesting of IF…Else statements – The ELSE IF ladder –The Switch statement – The ?: operator – the GOTO statement. | 8 | E-Resources |
| **UNIT - III** | | | |
| 3.1 | Decision making and Looping: The WHILE statement – The DO statement-The FOR statement – Jumps in loops. | 5 | E-Resources |
| 3.2 | Arrays: One dimensional array –Two dimensional arrays –Initializing two dimensional arrays- Multidimensional arrays. | 5 | E-Resources |
| 3.3 | User defined functions: Need for user–defined functions – A multifunction program – The form of C functions - Return values and their types- Calling a function –Category of function- No arguments and no return values –Nesting functions- Recursions- The scope and life time of variables in function. | 5 | E-Resources |
| **UNIT - IV** | | | |
| 4.1 | Calculation of Molecular weight of Organic Compounds. Calculation of pH. Determination on First Order rate constant for the given reaction | 5 | E-Resources |

| | | | |
|---|---|---|---|
| 4.2 | Evaluation of lattice energy using i). Born-Haber Cycle ii). Born –Lande equation. Computing ionic radii- Lande's method and Paulings method. Calculation of Normality, Molarity and Molality of a given solution. | 5 | E-Resources |
| 4.3 | Converting Kelvin to Celsius temperature and vice versa. Determination of enthalpy of a given solution. Evaluation of Cell constant. Calculation of energy of Hydrogen atom spectral lines. | 5 | E-Resources |
| **UNIT - V** | | | |
| 5.1 | Organic Chemistry: Use of Recursive functions to calculate the number of π Resonance structures for an organic conjugated system using res - str = n! / ((n/2)! * ((n/2) + 1)!). Empirical formula of Hydrocarbons and other Organic compounds. | 5 | E-Resources |
| 5.2 | Inorganic Chemistry: Array manipulation to balance the chemical equations. Half-life and average life periods of radioactive nuclei. Binding energy of nucleus. Program to get output as First ten elements of Periodic Table with their Name, Symbol, Atomic number and Atomic Weight. | 5 | E-Resources |
| 5.3 | Physical chemistry: Calculation of RMS, average and MPV of gases. Solving Quadratic equation to evaluate the Equilibrium constant for the reaction $H_2 + I_2 \rightarrow 2HI$. Illustrate use of Loop to calculate the NMR frequency for a nucleus with Spin ½. Mean activity coefficient of an Electrolyte (KCl). | 5 | E-Resources |
| | **Total** | **75** | |

**Course Designer**
**Ms. M. Rekha**
Assistant Professor of Chemistry

| Course Code | Course Title | Category | Total Hours | Credits |
|---|---|---|---|---|
| 20PCHC21 | Organic Chemistry –II | Core -V | 75 | 4 |

| Nature of Course | |
|---|---|
| Knowledge Oriented | ✓ |
| Skill Oriented | ✓ |
| Employability Oriented | |
| Entrepreneurship Oriented | |

| Course Relevance | |
|---|---|
| Local | |
| Regional | |
| National | |
| Global | ✓ |

**Preamble**

The research in chemistry does require the knowledge on various spectroscopic techniques. This course fulfills the said requirements.

**Course Outcomes (CO)**

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

| No. | Course Outcome | Knowledge Level |
|---|---|---|
| **CO1** | Explain the fundamentals of UV-Vis and IR Spectroscopy. | **K1,K2** |
| **CO2** | Make use of the basic principles underlying NMR Spectroscopy and its application in structural elucidation. | **K1,K2,K3** |
| **CO3** | Apply the concept of mass spectroscopy, ORD and CD in analyzing and determining the structure of organic molecules. | **K1,K2,K3** |
| **CO4** | Examine organic stereochemistry vis-à-vis optical and geometrical isomerism. | **K1,K2,K3,K4** |
| **CO5** | Determine the conformational analysis of cyclic, acyclic and heterocyclic system. | **K1,K2,K3,K4,K5** |

**K1-Knowledge K2-Understand K3-Apply K4- Analyse K5- Evaluate**

**Mapping of CO with PO**

| | PO1 | PO2 | PO3 | PO4 | PO5 |
|---|---|---|---|---|---|
| **CO1** | **3** | **1** | **2** | **3** | **3** |
| **CO2** | **3** | **1** | **2** | **3** | **2** |
| **CO3** | **3** | **1** | **2** | **3** | **2** |
| **CO4** | **3** | **1** | **2** | **2** | **3** |
| **CO5** | **3** | **1** | **1** | **3** | **3** |

**1-Low 2-Medium 3-Strong**

**Mapping of CO with PSO**

| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|---|---|---|---|---|---|
| CO1 | 3 | 2 | 1 | 1 | 2 |
| CO2 | 3 | 3 | 3 | 3 | 3 |
| CO3 | 3 | 3 | 3 | 3 | 3 |
| CO4 | 3 | 1 | 2 | 2 | 2 |
| CO5 | 3 | 1 | 1 | 1 | 3 |

**1-Low** **2-Medium** **3-Strong**

**Syllabus**

**UNIT I** 12 Hours

**Ultraviolet spectroscopy:** Basic principle – instrumentation – the absorption laws, types of electronic transitions – Effect of solvent and hydrogen bonding on λmax values - Woodward rules to calculate λmax values of conjugated dienes, conjugated polyenes, and carbonyl compounds.

**Infrared spectroscopy:** Basic principle – Molecular Vibrations – instrumentation – characteristic IR absorption of different functional groups – factors influencing the vibrational frequencies

**UNIT II** 15 Hours

**$^{1}$H NMR spectroscopy:** Basic principles – number of signals – chemical shift –factors influencing chemical shift – spin-spin coupling – coupling constant and factors influencing coupling constant. Simplification of complex spectra – shift reagents, deuterium substitution and spin decoupling.

**$^{13}$C NMR spectroscopy**: Basic principle – comparison with $^{1}$H NMR – noise decoupling – off resonance decoupling – factors affecting the C-13 chemical shifts.

**Advanced NMR Spectroscopy:** Introduction to 2D-NMR - Classification of 2D experiments – HOMO and HETERO nuclear correlation – J resolved correlation. Correlation Spectroscopy (COSY): Pulse sequence – HOMO-COSY, HETERO-COSY, 1D- and 2D- INADEQUATE and NOESY.

**UNIT III** 18 Hours

**Mass Spectroscopy:** Basic instrumentation of Mass spectrometer - types of ions – molecular, isotopic, metastable and fragmentation ions – Tests for molecular ion peak – General fragmentation modes - Retro Diels - Alder reactions – McLafferty rearrangement – Fragmentation pattern of simple organic molecules. Application – Accurate Molecular weight, Molecular formula (Nitrogen rule) – Determination of structures of organic molecules. Introduction to ESI, MALDI and FAB mass spectrometer.

**Optical rotatory dispersion (ORD) and Circular Dichroism (CD):** Circularly polarized light – Circular birefringence and CD – plain curves and their applications – Cotton effects curves. Structural applications – axial haloketone rule, octant rule and their applications. Solving problems based on UV, IR, NMR and Mass data.

**UNIT IV** 15 Hours

**Organic Stereochemistry: Optical isomerism:** Symmetry elements – the concept of chirality – chirality about a center – specification by Cahn - Ingold-Prelog notations – compounds with more than one chiral center – erythro, threo and meso nomenclature – concept of prochirality – homotopic, enantiotopic and diastereotopic ligands and faces – Asymmetric synthesis – Cram's rule and Prelog's rule. Optical activity in allenes and spiranes – StereoChemistry of nitrogen compounds.

**Geometrical isomerism:** E and Z notation – Determination of configuration of geometrical isomers by simple techniques like hydroxylation, hydroboration and methods based on physical properties – Stereoisomerism in cyclic compounds – 3, 4 and 5 membered ring systems.

**UNIT V** 15 Hours

**Configuration and conformation:** Definition – conformational free energy- atropisomers - conformational analysis of acyclic, cyclic, heterocyclic systems – conformational analysis of cyclohexane system - stability and isomerism in mono and disubstituted cyclohexanes – conformation and reactivity of cyclohexane derivatives - conformational analysis of fused ring system - decalins, and perhydrophenanthrene.

## Text Books


D. Nasipuri, ***Stereochemistry of Organic compounds***, New Age International, New Delhi 2004, 2nd edition.

William Kemp, ***Organic Spectroscopy***, ELBS, UK, 1994, 4th Edition.

R.M. Silverstein, G.C. Bassler and T.C. Morrill, ***Spectrometric Identification of organic compounds,*** John Wiley, New York, 2005, 6th Edition.


## Reference Books


E. L. Eliel and S. H. Wiley, ***Stereochemistry of carbon compounds***, John Wiley & Son, Inc, 2003.

V. M. Potapov, ***Stereochemistry***, MIR Publisher, Moscow, 1999.

H. Kagan, ***Organic Stereochemistry***, Edward Arnold, London, 2001.

E.L. Eliel, N.L. Allinger, S.J. Angyal and G.A. Morrison, ***Conformational Analysis,*** Interscience, New York, 2004.

P. Wetirli Marchand, ***Interpretation of $^{13}C$ NMR*** Spectra, VCH Weinheim, UK, 1987.

**Pedagogy**

Chalk & Talk, E-Resources, Group Discussion

**Teaching aids**

Black Board, LCD Projector

**Course Contents and Lecture Schedule**

| Module No. | Topic | No. of Lectures | Content Delivery Methods |
|---|---|---|---|
| **UNIT - I** | | | |
| 1.1 | Ultraviolet spectroscopy – basic principle – instrumentation – the absorption laws, types of electronic transitions – Effect of solvent and hydrogen bonding on λmax values. Effect of solvent and hydrogen bonding on λmaxvalues. | 3 | E-Resources |
| 1.2 | Woodward rules to calculate λmax values of conjugated dienes, conjugated polyenes and carbonyl compounds. | 3 | Chalk & Talk |
| 1.3 | Infrared spectroscopy – basic principle – Molecular Vibrations – instrumentation. | 3 | E-Resources |
| 1.4 | Characteristic IR absorption of different functional groups. Factors influencing the vibrational frequencies. | 3 | Group Discussion |
| **UNIT - II** | | | |
| 2.1 | $^{1}$H NMR spectroscopy: Basic principles – number of signals – chemical shift - factors influencing chemical shift – spin-spin coupling – coupling constant and factors influencing coupling constant. | 3 | E-Resources |
| 2.2 | Simplification of complex spectra – shift reagents, deuterium substitution and spin decoupling. | 3 | E-Resources |
| 2.3 | $^{13}$C NMR spectroscopy: Basic principle – comparison with 1H NMR – noise decoupling – off resonance decoupling – factors affecting the C-13 chemical shifts. | 3 | Chalk & Talk |

| | | | |
|---|---|---|---|
| 2.4 | Advanced NMR Spectroscopy: Introduction to 2D- NMR -Classification of 2D experiments – HOMO and HETERO nuclear correlation – J resolved correlation. | 3 | E-Resources |
| 2.5 | Correlation Spectroscopy (COSY): Pulse sequence – HOMO-COSY, HETERO-COSY, 1D- and 2D- INADEQUATE and NOESY. | 3 | Group Discussion |
| **UNIT - III** | | | |
| 3.1 | Basic instrumentation of Mass spectrometer - types of ions – molecular, isotopic, metastable and fragmentation ions – Tests for molecular ion peak. | 3 | E-Resources |
| 3.2 | General fragmentation modes- Retro Diels - Alder reactions – McLafferty rearrangement – Fragmentation pattern of simple organic molecules. | 5 | E-Resources |
| 3.3 | Application – Accurate Molecular weight, Molecular formula (Nitrogen rule) – Determination of structures of organic molecules. Introduction to ESI, MALDI and FAB mass spectrometer. | 4 | Group Discussion |
| 3.4 | Optical rotatory dispersion (ORD) and Circular Dichroism (CD): Circularly polarized light – Circular birefringence and CD – plain curves and their applications – Cotton effects curves – structural applications – | 3 | E-Resources |
| 3.5 | Axial haloketone rule, octant rule andtheir applications. Solving problems based on UV, IR, NMR and Mass data. | 3 | Chalk & Talk |
| **UNIT - IV** | | | |
| 4.1 | Optical isomerism: Symmetry elements – the concept of chirality – chirality about a center – specification by Cahn -Ingold-Prelog notations – compounds with more than one chiral center – erythro, threo and meso nomenclature. | 5 | E-Resources |

| | | | |
|---|---|---|---|
| 4.2 | Concept of prochirality – homotopic, enantiotopic and diastereotopic ligands and faces – Asymmetric synthesis – Cram's rule and Prelog's rule. Optical activity in allenes and spiranes – StereoChemistry of nitrogen compounds. | 5 | E-Resources |
| 4.3 | Geometrical isomerism: E and Z notation – Determination of configuration of geometrical isomers by simple techniques like hydroxylation, hydroboration and methods based on physical properties – Stereoisomerism in cyclic compounds – 3, 4 and 5 membered ring systems. | 5 | Chalk & Talk |
| **UNIT - V** | | | |
| 5.1 | Configuration and conformation – definition – conformational free energy- atropisomers- conformational analysis of acyclic, cyclic, heterocyclic systems | 5 | E-Resources |
| 5.2 | Conformational analysis of cyclohexane system: stability and isomerism in mono and disubstitutedcyclohexanes. | 5 | Chalk & Talk |
| 5.3 | Conformation and reactivity of cyclohexane derivatives - conformational analysis of fused ring system - decalins, and perhydrophenanthrene. | 5 | E-Resources |
| | **Total** | **75** | |

**Course Designer**
**Mr. G. Arivalagan**
Assistant Professor of Chemistry

| Course Code | Course Title | Category | Total Hours | Credits |
|---|---|---|---|---|
| 20PCHC22 | Inorganic Chemistry –II | Core -VI | 75 | 5 |

| Nature of Course | |
|---|---|
| Knowledge Oriented | ✓ |
| Skill Oriented | |
| Employability Oriented | |
| Entrepreneurship Oriented | |

| Course Relevance | |
|---|---|
| Local | |
| Regional | |
| National | |
| Global | ✓ |

**Preamble**

The course gives detailed information about supramolecular chemistry, solid state chemistry, inorganic rings, cages clusters and polymers, It also explains the chemistry of lanthanides and actinides.

**Course Outcomes (CO)**

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

| No. | Course Outcome | Knowledge Level |
|---|---|---|
| **CO1** | Describe supramolecular chemistry of transition metal compounds, structure and their application in various fields. | **K1,K2,K3** |
| **CO2** | Analyze the structure and defects of solids. | **K1,K2,K3,K4** |
| **CO3** | Compare and solve the structures of Borone, S-N, P-N of inorganic rings, cages, clusters and polymers. | **K1,K2,K3,K4,K5** |
| **CO4** | Categorize the given S-N, P-N, silicone, P-O compounds and deduce their structure. | **K1,K2,K3,K4,K5** |
| **CO5** | Make use of the occurance, extraction, spectral and magnetic properties of lanthanides andactinides. | **K1,K2,K3** |

**K1-Knowledge K2-Understand K3-Apply K4- Analyse K5- Evaluate**

**Mapping of CO with PO**

| | PO1 | PO2 | PO3 | PO4 | PO5 |
|---|---|---|---|---|---|
| **CO1** | **2** | **3** | **1** | **3** | **1** |
| **CO2** | **3** | **1** | **1** | **3** | **2** |
| **CO3** | **3** | **1** | **1** | **3** | **3** |
| **CO4** | **3** | **1** | **1** | **3** | **2** |
| **CO5** | **2** | **1** | **1** | **3** | **2** |

**1-Low 2-Medium 3-Strong**

**Mapping of CO with PSO**

| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|---|---|---|---|---|---|
| CO1 | 3 | 3 | 3 | 3 | 3 |
| CO2 | 3 | 1 | 1 | 1 | 3 |
| CO3 | 3 | 2 | 2 | 2 | 3 |
| CO4 | 3 | 2 | 2 | 3 | 3 |
| CO5 | 3 | 1 | 2 | 1 | 2 |

**1-Low** **2-Medium** **3-Strong**

**Syllabus**

**UNIT I** 15 Hours

**Supramolecular chemistry**: Definition, Nature of supramolecular interactions - Non-Covalent interactions, Host - guest interaction, complexing involving crowns and cryptands – cyclodextrine - Inclusion compounds- Clatharates - intercalation compounds – Molecular recognition, Types of recognition, Self - assembly. General properties of Supra molecular complexes- Molecular Library - Transition metal mediated supramolecules - Directional bond approach - Molecular triangles ( Pd & Pt ) - Molecular squares ( Pd, Pt & Re )- Molecular rectangles - (Pd, Pt, Cu & Re) Molecular Cages ( Pd, Pt & Re) and their applications.

**UNIT II** 18 Hours

**Solid-state chemistry:** Packing of atoms and ions- close packing arrangements-HCP, CCP and BCC lattice. Radius ratio rules- Limiting radius ratio. Structure of typical lattices such as calcite, cesium chloride, Nickel arsenide, Fluorite, Antifluorite, Cadmium iodide, Perovskite, Spinels (normal and inverse). Bragg‘s equation- problems involving Bragg‘s equation. Crystal structure determination- X-ray diffraction study, Electron and Neutron diffractions. Crystal defects- point – Schotky and Frenkel defect - line and plane defects- colour centers- non- stoichiometric Compounds- experimental methods of study of non- stoichiometry- effect of imperfections and non- stoichiometry on physical properties-types of solids-electronic structure of solids- free electron and band theories.

**UNIT III** 15 Hours

**Inorganic Rings, Cages, Clusters and Polymers-I**: Electron deficient compounds: Borane and carboranes - Synthesis, structure and bonding (VBT and MO approach) – topological treatment-wades rule – styx numbers - structural studies by NMR – metallocarboranes - other heteroatom boron derivatives, borates – boroxines - B-P and B-As heterocycles. Synthesis, structure and bonding in Binary sulphur nitrils, S-N cations and anions, cyclic S-N compounds, S-N halogen compounds-Bonds and electron counting in S-N heterocycles-polythiazyls. Structure of aluminosilicates - mica, clay, zeolites,fullers earth. Manufacture, Types and Uses of glasses.

**UNIT IV** 15 Hours

**Inorganic Rings, Cages, Clusters and Polymers - II:** P-N Heterocyclics - Phosphonitrilic compounds: Synthesis, Structure and bonding - phosphazene oligomers-high polymers - polymeric phosphorus nitrides - hydrolysis of phosphazenes - reactions of halo phosphazenes - aminolysis - metathetical reactions - reaction with organometallic reagents - Friedel-Crafts substitutions –rearrangements - theories of bonding - electronic structure and aromaticity - posphazene oligomers - high polymers - polymeric phosphorus nitrides. High, low nuclearcity carbonyl clusters - halide clusters. Isolobal analogy - Synthesis, structure and bonding in Poly anions and isopoly anions of phosphorous, vanadium, chromium, Nolybdenum and tugston. Hetero poly anions of molybdenum and tungsten. Structural prediction by Wade‘s rule - Cappit rule.

**UNIT V** 12 Hours

**a) Lanthanides:** Occurrence - differences between 4f and 5f orbitals - Separation techniques (Fractional crystallization, precipitation, ion-exchange, solvent-extraction and thermal decomposition - Selective reduction and oxidation) - Electronic configurationOxidation states, Lanthanide contraction - Spectral and Magnetic properties - Ln chelatesorganometallic compounds of Ln. Uses of lanthanides (shift reagents, Pu bomb) and their compounds - aqueous chemistry of uranyl compounds - position in the periodic table.

**b) Actinides:** Synthesis of elements - Extraction of Th, U and Pu - electronic configuration and oxidation states, spectral and magnetic properties-position in the periodic table.

**Text Books**


Bradley J. Holliday & Chad A. Mirkin, ***Strategies for the Construction of Supramolecular Compounds through Coordination Chemistry***- Reviews, Angew. Chem. Int. Ltd., 2001.

Katsuhiko Ariga, Toyoki Kunitaka, ***Supramolecular Chemistry-Fundamentals and Applications: Advanced Textbook***, Springer Science & Business Media, 2006.

W. Jones, C. N. R. Rao, ***Supramolecular Organization and Materials Design***, Cambridge University Press, Landon, 2001.

Lee, J. D. Concise ***Inorganic Chemistry***, Blackwell Science Ltd., London. 2002, 5th Edition.

Keer, H.V. Principles of the ***Solid State***, Wiley Eastern Ltd., 1993.

H. G. Heal, ***the Inorganic Heterocyclic Chemistry of Sulphur, Nitrogen and Phosphorus,*** Academic press, New York, 1980.

J. D. Woolings, ***Non Metal Rings, Cages and Clusters***, John Wiley and sons, New York, 1989.

P.J. Durrant and B. Durrant, ***Introduction to advanced inorganic chemistry***, Longman Group Ltd, London,1970.

Purcell K.F. and Kotz J.C., Saunders, ***Inorganic Chemistry***, Philadelphia, 1977.

D. A. Skoog and D. M. West, ***Fundamentals of Analytical Chemistry***, Holler Saunders college publishing, USA, 1998, 6th Edition.

F.A. Cotton and G. Wilkinson, ***Advanced Inorganic Chemistry***, Wiley-Interscience publications, John Wiley & Sons, New Delhi, 1988, 5th Edition.


**Reference Books**


J. E. Huheey, Ellen A. Keiter, Richard L. Keiter, ***Inorganic Chemistry***, Pearson Education (Singapore) Pte. Ltd., Delhi, 2004, 4th Edition.

I. Azaroff, ***Introduction to Solids***, Tata McGraw hill, New Delhi, 2004.

K. Chakrabarthy, ***Solid State Chemistry***, New Age International Publishers, (P) Ltd., 2005.

D. F. Shriver and P.W. Atkins, ***Inorganic Chemistry***, Oxford University Press, London, 1999.

Wahid U. Malik, G.D. Tuli and R. D. Madan, ***Selected Topics in Inorganic Chemistry***, S. Chand & Co. Ltd., New Delhi, 2006.

William W. Porterfield, ***Inorganic Chemistry***, Elsevier, New Delhi, 2005, 2th Edition.


**Pedagogy**

Chalk & Talk, E-Resources, Group Discussion

**Teaching aids**

Black Board, LCD Projector

**Course Contents and Lecture Schedule**

| Module No. | Topic | No. of Lectures | Content Delivery Methods |
|---|---|---|---|
| | **UNIT - I** | | |
| 1.1 | Definition, Nature of supramolecular interactionsNon- Covalent interactions. Host - guest interaction. Complexing involving crowns and cryptandscyclodextrine. | 5 | E-Resources |
| 1.2 | Molecular recognition, Types of recognition. Self- assembly. General properties of Supra molecular complexes- Molecular Library- Transition metal mediated supramolecules - Directional bond approach. | 5 | Chalk & Talk |
| 1.3 | Molecular triangles ( Pd & Pt )- Molecular squares (Pd, Pt & Re)- Molecular rectangles-(Pd, Pt, Cu & Re) Molecular Cages ( Pd, Pt & Re) and their applications-Inclusion compounds- Clatharates - intercalation compounds. | 5 | E-Resources |
| | **UNIT - II** | | |
| 2.1 | Packing of atoms and ions- close packing arrangements-HCP,CCP and BCC lattice - Radius ratio rules- Limiting radius ratio. | 4 | E-Resources |
| 2.2 | Structure of typical lattices such as calcite, cesium chloride, Nickel arsenide, Fluorite, Antifluorite, Cadmium iodide, Perovskite, Spinels ( normal and inverse) - Bragg‘s equation- problems involving Bragg‘s equation. | 5 | E-Resources |
| 2.3 | Crystal structure determination- X-ray diffraction study, Electron and Neutron diffractions - Crystal defects- point – Schotky and Frenkel defect - line and planedefects-colour centers. | 5 | Chalk & Talk |
| 2.4 | Nonstoichiometric Compounds - experimental methods of study of non-stoichiometry - Effect of imperfections and non- stoichiometry on physical properties. | 4 | Discussion |

| | | | |
|---|---|---|---|
| **UNIT - III** | | | |
| 3.1 | Electron deficient compounds: Borane and carboranes - Electron deficient compounds: Borane and carboranes - topological treatment-wades rule – styx numbers. | 3 | E-Resources |
| 3.2 | Structural studies by NMR-metallocarboranes - other heteroatom boron derivatives-borates-boroxines-B-P and B-As heterocycles. | 5 | E-Resources |
| 3.3 | P-N HETEROCYCLICS - Phosphonitrilic compounds: Synthesis, Structure and bonding - Phosphazene oligomers - high polymers- Polymeric phosphorus nitride. | 4 | Group Discussion |
| 3.4 | S-N HETEROCYCLICS: Synthesis, structure and bonding in Binary sulphur nitrils, S-N cations and anions, cyclic S-N compounds, S-N halogen compounds - bonds and electron counting in S-N heterocyclespolythiazyls. | 3 | E-Resources |
| **UNIT - IV** | | | |
| 4.1 | Synthesis of P-N-skeleton - Hydrolysis of phosphazenes- reactions of halo phosphazenes-aminolysis-metathetical reactions. | 5 | Chalk & Talk |
| 4.2 | Reaction with organometallic reagents - Friedel-Crafts substitutions - rearrangements - Theories of bonding-electronic structure and aromaticity - Phosphazene oligomers-high polymers-polymeric phosphorus nitrides. | 5 | E-Resources |
| 4.3 | Metal Clusters: Synthesis, structure and bonding in Poly anions and isopoly anions of phosphorous, vanadium, chromium, Nolybdenum and tugston. Hetero poly anions of molybdenum and tungsten | 5 | Chalk & Talk |

| UNIT - V | | | |
|---|---|---|---|
| 5.1 | Lanthanides: Occurrence - differences between 4f and 5f orbitals - Separation techniques (Fractional crystallization, precipitation, ion-exchange, solvent-extraction and thermal decomposition-Selective reduction and oxidation) | 3 | E-Resources |
| 5.2 | Electronic configuration- Oxidation states, Lanthanide contraction- Spectral and Magnetic properties- Ln chelates-organometallic compounds of Ln. | 3 | Chalk & Talk |
| 5.3 | Lanthanides as shift reagents in NMR-uses of lanthanides and their compounds - Aqueous chemistry of uranyl compounds- position in the periodic table. | 3 | E-Resources |
| 5.4 | Actinides: Synthesis of elements-Extraction of Th and U and Pu. Electronic configuration and oxidation states, spectral and magnetic properties-position in the periodic table | 3 | Chalk & Talk |
| | **Total** | **75** | |

**Course Designer**
**Ms. A. Nihath Nazleen**
Assistant Professor of Chemistry

| Course code | Course Title | Category | Total Hours | Credits |
|---|---|---|---|---|
| 20PCHC23 | Physical Chemistry –II | Core -VII | 75 | 4 |

| Nature of Course | |
|---|---|
| Knowledge Oriented | ✓ |
| Skill Oriented | |
| Employability Oriented | |
| Entrepreneurship Oriented | |

| Course Relevance | |
|---|---|
| Local | |
| Regional | |
| National | |
| Global | ✓ |

**Preamble**

The course enables the students to gain knowledge on electrochemistry, statistical thermodynamics and principles of conventional spectroscopic methods.

**Course Outcomes (CO)**

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

| No. | Course Outcome | Knowledge Level |
|---|---|---|
| **CO1** | Summarise the fundamental concepts and theories of electrochemistry | **K1, K2** |
| **CO2** | Make use of the applications of electrochemistry. | **K1, K2,K3** |
| **CO3** | Identify the need and fundamental derivation of statistical thermodynamics. | **K1, K2,K3** |
| **CO4** | Examine the applications of statistical thermodynamics | **K1, K2,K3,K4** |
| **CO5** | Apply the concepts of spectroscopic techniques such as IR, Raman and microwave. | **K1, K2,K3** |

**K1-Knowledge K2-Understand K3-Apply K4- Analyse K5- Evaluate**

**Mapping of CO with PO**

| | PO1 | PO2 | PO3 | PO4 | PO5 |
|---|---|---|---|---|---|
| **CO1** | **3** | **1** | **3** | **3** | **2** |
| **CO2** | **2** | **2** | **3** | **3** | **3** |
| **CO3** | **2** | **1** | **1** | **2** | **3** |
| **CO4** | **2** | **1** | **1** | **2** | **3** |
| **CO5** | **3** | **3** | **2** | **3** | **3** |

**1-Low 2-Medium 3-Strong**

**Mapping of CO with PSO**

| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|---|---|---|---|---|---|
| CO1 | 3 | 2 | 2 | 1 | 2 |
| CO2 | 3 | 3 | 3 | 2 | 3 |
| CO3 | 3 | 3 | 1 | 1 | 2 |
| CO4 | 3 | 3 | 2 | 2 | 3 |
| CO5 | 3 | 3 | 3 | 3 | 3 |

**1-Low** **2-Medium** **3-Strong**

**Syllabus**

**UNIT I** 15 Hours

**Electrochemistry – I:** Theory of strong electrolytes – Interionic attraction theory – Debye-Huckel theory of strong electrolytes - Debye- Huckel model of ionic atmosphere–Debye-Huckel Onsager equation- derivation, verification and modifications- Debye – Falkenhagen effect and Wien effect; Electrical double layers – formation – Structure of electrified interfaces – Stern model. Debye-Huckel limiting law- extension- Huckel-Bronsted equation - Determination of activity coefficients using Bronsted equation – Applications of conductivity measurements; Nernst equation and its significance – reversible and irreversible cells - electrodes – SHE – Calomel – Glass electrode – Platinum electrode – Glassy carbon electrode – ion selective electrode and measurement of pH.

**UNIT II** 15 Hours

**Electrochemistry-II:** Over voltage – Theories of over voltage - applications of over voltage-hydrogen and oxygen overvoltage; Butler-Volmer equation - Tafel equation; Corrosion - principles of electrochemical corrosion – dry and wet corrosion and its mechanism – Pilling - Bedworth rule. Types of corrosion- galvanic, aeration, stress, pitting corrosion and passivity – factor influencing corrosion – corrosion control - cathodic production - corrosion inhibitors. Principles of Polorography - Cyclic Voltametry – quasi – reversible –irreversible voltamogram; electrochemical energy conversions- Nickel Cadmium, lead acid battery; Fuel cells – H2 - O2 Fuel cell – methyl alcohol fuel cell.

**UNIT III** 15 Hours

**Statistical thermodynamics-I:** Need for statistical mechanics or thermodynamics-Ensemble- types of ensemble – micro canonical - canonical and grand canonical ensemble; Phase space- microstates-probability and distribution- Maxwell Boltzmann classical distribution law-derivation in term of degeneracy; Partition function (Q) – relation between partition function and the following thermodynamic functions – internal energy (E), Helmholtz free energy (A), Pressure (P), Enthalpy (H), Gibbs free energy (G), chemical potential (μi), heat capacity (Cv) and entropy (S);Derivation of Sackur-Tetrode equation – thermodynamic properties of monoatomic gases.

**UNIT IV** 15 Hours

**Statistical thermodynamics-I:** Quantum statistics - Bose-Einstein Statistics derivation- application of Bose-Einstein statistics for a photon gas – Planck's radiation formula - Derivation of Rayleigh - Jeans law-Stefan Boltzman equation. Fermi-Dirac statistics derivation - Application of Fermi-Dirac statistics to electron gas in metals; Population inversion-negative absolute temperature - heat capacity of diatomic gases-Einstein's theory and Debye's theory of heat capacities of solids- third law of thermodynamics and statistical entropy - hydrogen ortho and para nuclear states.

**UNIT V** 15 Hours

**Spectroscopy – I:** Absorption and emission of electromagnetic radiation (emr) – LASER - Interaction of electromagnetic radiation with matter – Einstein coefficients; Microwave, IR and Raman spectroscopy of diatomic molecules – determination of molecular parameters – vibrational spectra of polyatomic molecules – IR and Raman active modes – overtone and combination bands – Fermi resonance – group frequencies and coupling interaction.

**Text Books**


Bokris J. O. M., Reddy A. K. N., ***Modern Electrochemistry, Vol I***, Plenum Press, New York, 1978.

Crow Dr., ***Principles and Applications of Electrochemistry***, Chapman Hall, UK, 1988,

Venkataraman R., Rengarajan K., Raghavan P. S., ***Electrochemistry***, 2007, 1st edition

Glasstone S., ***Thermodynamics for Chemists***, Eastern Wiley Publication, 2002.

Lee, Sears, Tercotte, ***Statistical Thermodynamics***, Addision Wesley Publishing Co., London, 1973, 1st Edition.

**Reference Books**

Antropov L., ***Theoretical electrochemistry***, MIR Publications, New Delhi, 1999.

Glasstone S., ***An Introduction to Electrochemistry***, Von Nostrand Co. Inc., Toronto, 2002.

Gupta M. C., ***Statistical Thermodynamics***, Wiley Eastern limited, New Delhi, 1993.

Kuriakose J. C., Rajaram, J., ***Thermodynamics***, Shoban lal Nagin Chand, New Delhi, India,1999.

Veera Reddy, K., ***Symmetry and spectroscopy of molecules***, Newage International (P) Ltd., 1998

**Pedagogy**

Chalk & Talk, E-Resources, Group Discussion

**Teaching aids**

Black Board, LCD Projector

**Course Contents and Lecture Schedule**

| Module No. | Topic | No. of Lectures | Content Delivery Methods |
|---|---|---|---|
| | **UNIT - I** | | |
| 1.1 | Theory of strong electrolytes – Interionic attraction theory – Debye-Huckel theory of strong electrolytes - Debye-Huckel model of ionic atmosphere | 3 | Chalk & Talk |
| 1.2 | Debye-Huckel Onsager equation-derivation, verification and modifications-Debye – Falkenhagen effect and Wien effect; Electrical double layers formation | 3 | E-Resources |
| 1.3 | Structure of electrified interfaces – Stern model. Debye-Huckel limiting law-extension- Huckel-Bronsted equation - Determination of activity coefficients using Bronsted equation | 3 | Discussion |
| 1.4 | Applications of conductivity measurements; Nernst equation and its significance – reversible and irreversible cells | 3 | Chalk & Talk |

| | | | |
|---|---|---|---|
| 1.5 | electrodes – SHE – Calomel – Glass electrode – Platinum electrode – Glassy carbon electrode – ion selective electrode and measurement of pH. | 3 | E-Resources |
| **UNIT - II** | | | |
| 2.1 | Over voltage – theories of over voltage-applications of over voltage-hydrogen and oxygen overvoltage; Butler-Volmer equation- Tafel equation | 3 | Discussion |
| 2.2 | Corrosion- principles of electrochemical corrosion – dry and wet corrosion and its mechanism – Pilling-Bedworth rule | 3 | Chalk & Talk |
| 2.3 | Types of corrosion- galvanic, aeration, stress, pitting corrosion and passivity – factor influencing corrosion – corrosion control- cathodic production - corrosion inhibitors. | 3 | E-Resources |
| 2.4 | Principles of Polorography - Cyclic Voltametry –quasi – reversible – irreversible voltamogram | 3 | E-Resources |
| 2.5 | electrochemical energy conversions-Nickel Cadmium, lead acid battery; Fuel cells – $H_2$ - $O_2$ Fuel cell – methyl alcohol fuel cell. | 3 | Chalk & Talk |
| **UNIT - III** | | | |
| 3.1 | Need for statistical mechanics or thermodynamics-Ensemble- types of ensemble – micro canonical - canonical and grand canonical ensemble | 3 | E-Resources |
| 3.2 | Phase space- microstates- probability and distribution- Maxwell Boltzmann classical distribution law- derivation in term of degeneracy | 3 | Chalk & Talk |
| 3.3 | Partition function (Q) – relation between partition function and the following thermodynamic functions – internal energy (E), Helmholtz free energy (A), Pressure (P), Enthalpy (H), Gibbs free energy (G), | 3 | Discussion |
| 3.4 | chemical potential (μi), heat capacity (Cv) and entropy(S); | 3 | Chalk & Talk |

| | | | |
|---|---|---|---|
| 3.5 | Derivation of Sackur-Tetrode – thermodynamic properties of monoatomic gases. | 3 | Chalk & Talk |
| **UNIT - IV** | | | |
| 4.1 | Quantum statistics- Bose-Einstein Statistics derivation- application of Bose-Einstein statistics for a photon gas | 3 | Discussion |
| 4.2 | Planck's radiation formula-Derivation of Rayleigh-Jeans law-Stefan Boltzman equation | 3 | E-Resources |
| 4.3 | Fermi-Dirac statistics derivation - Application of Fermi-Dirac statistics to electron gas in metals; Population inversion | 3 | Chalk & Talk |
| 4.4 | negative absolute temperature -heat capacity of diatomic gases-Einstein's theory and Debye_s theory of heat capacities of solids | 3 | Chalk & Talk |
| 4.5 | third law of thermodynamics and statistical entropy - hydrogen ortho and para nuclear states. | 3 | E-Resources |
| **UNIT - V** | | | |
| 5.1 | Absorption and emission of electromagnetic radiation (emr) – LASER – Interaction of electromagnetic radiation with matter | 3 | E-Resources |
| 5.2 | Einstein coefficients; Microwave, IR and Raman spectroscopy of diatomic molecules | 3 | Chalk & Talk |
| 5.3 | determination of molecular parameters – vibrational spectra of polyatomic molecules | 3 | Discussion |
| 5.4 | IR and Raman active modes – overtone and combination bands | 3 | E-Resources |
| 5.5 | Fermi resonance – group frequencies and coupling interaction | 3 | Chalk & Talk |
| | **Total** | **75** | |

**Course Designer**
**Mrs. A. Mumthaj**
Assistant Professor of Chemistry

| Course Code | Course Title | Category | Total Hours | Credits |
|---|---|---|---|---|
| 20PCHC2P | Physical Chemistry Practical | Core -VIII | 150 | 5 |

| Nature of Course | |
|---|---|
| Knowledge Oriented | ✓ |
| Skill Oriented | ✓ |
| Employability Oriented | |
| Entrepreneurship Oriented | |

| Course Relevance | |
|---|---|
| Local | |
| Regional | |
| National | |
| Global | ✓ |

**Preamble**

This lab course enables the students to acquire practical knowledge on physical chemistry experiments such as electrochemical, kinetics, surface chemistry and colorimetric estimations.

**Course Outcomes (CO)**

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

| No. | Course Outcome | Knowledge Level |
|---|---|---|
| **CO1** | Show the various types of conductometric titrations. | **K1,K2** |
| **CO2** | Operate the various types of potentiometric titrations. | **K1,K2,K3** |
| **CO3** | Connect the analytical skill on adsorption of oxalic acid. | **K1,K2,K3,K4** |
| **CO4** | Measure the analytical skill on adsorption of acetic acid | **K1,K2,K3,K4,K5** |
| **CO5** | Interpret the colorimetric estimation techniques. | **K1,K2,K3,K4,K5** |

**K1-Knowledge K2-Understand K3-Apply K4- Analyse K5- Evaluate**

**Mapping of CO with PO**

| | PO1 | PO2 | PO3 | PO4 | PO5 |
|---|---|---|---|---|---|
| **CO1** | **2** | **3** | **1** | **2** | **1** |
| **CO2** | **2** | **3** | **1** | **2** | **2** |
| **CO3** | **3** | **3** | **2** | **3** | **3** |
| **CO4** | **2** | **3** | **2** | **3** | **2** |
| **CO5** | **2** | **3** | **1** | **2** | **2** |

**1-Low 2-Medium 3-Strong**

**Mapping of CO with PSO**

| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|---|---|---|---|---|---|
| **CO1** | **3** | **3** | **1** | **1** | **2** |
| **CO2** | **3** | **3** | **1** | **1** | **2** |
| **CO3** | **3** | **3** | **3** | **3** | **3** |
| **CO4** | **3** | **3** | **3** | **3** | **3** |
| **CO5** | **3** | **2** | **1** | **2** | **1** |

**1-Low** **2-Medium** **3-Strong**

| S. No. | EXPERIMENTS |
|---|---|
| 1. | Estimation of HCl & CH3COOH by conductometrically |
| 2. | Estimation of HCl & NH4Cl by conductometrically |
| 3. | Estimation of Na2CO3 by conductometrically |
| 4. | Estimation of K2SO4 by conductometrically |
| 5. | Kinetics of base hydrolysis of an ester by conductometrically |
| 6. | Estimation of Fe(II) using KMnO4 by potentiometrically |
| 7. | Estimation of Fe(II) using CAS potentiometrically |
| 8. | Estimation of KI with KMnO4 by potentiometrically |
| 9. | Determination of pH of buffer solution by potentiometrically |
| 10. | Estimation of mixture of halides (KI and KCl) by potentiometrically |
| 11. | Adsorption of oxalic acid on to activated charcoal |
| 12. | Adsorption of acetic acid on to activated charcoal |
| 13. | Determination of concentration of KMnO4 soluion by spectrophotometrically. |

**Course Designer**
**Mrs. A. Mumthaj**
Assistant Professor of Chemistry

| Course code | Course Title | Category | Total Hours | Credits |
|---|---|---|---|---|
| 20PCHE21 | Analytical Chemistry | Elective - II | 75 | 5 |

| Nature of Course | |
|---|---|
| Knowledge Oriented | ✓ |
| Skill Oriented | ✓ |
| Employability Oriented | ✓ |
| Entrepreneurship Oriented | |

| Course Relevance | |
|---|---|
| Local | |
| Regional | |
| National | |
| Global | ✓ |

**Preamble**

Elicit electro analytical, thermo analytical and spectro analytical methods.

**Course Outcomes (CO)**

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

| No. | Course Outcome | Knowledge Level |
|---|---|---|
| **CO1** | Outline the principles of Precipitation Techniques and their applications | **K1, K2** |
| **CO2** | Make use of the minimization of errors, standard deviation, Student's test, Q test and T-test | **K1, K2,K3** |
| **CO3** | Examine the Electroravimetry, Coulometry, Voltammetry and Amperometry | **K1, K2,K3,K4** |
| **CO4** | Utilize the thermal analyses such as TGA, DTA and DSC. | **K1, K2,K3** |
| **CO5** | Evaluate fundamental concepts and applications of Spectroanalytical methods. | **K1, K2,K3,K4,K5** |

**K1-Knowledge K2-Understand K3-Apply K4- Analyse K5- Evaluate**

**Mapping of CO with PO**

| | PO1 | PO2 | PO3 | PO4 | PO5 |
|---|---|---|---|---|---|
| **CO1** | **2** | **3** | **2** | **2** | **2** |
| **CO2** | **1** | **3** | **3** | **2** | **3** |
| **CO3** | **2** | **3** | **2** | **2** | **2** |
| **CO4** | **1** | **3** | **3** | **3** | **2** |
| **CO5** | **3** | **1** | **3** | **3** | **3** |

**1-Low 2-Medium 3-Strong**

**Mapping of CO with PSO**

| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|---|---|---|---|---|---|
| CO1 | 3 | 2 | 2 | 1 | 2 |
| CO2 | 3 | 3 | 1 | 2 | 3 |
| CO3 | 3 | 3 | 2 | 1 | 2 |
| CO4 | 3 | 3 | 3 | 2 | 3 |
| CO5 | 3 | 3 | 3 | 1 | 3 |

**1-Low** **2-Medium** **3-Strong**

**Syllabus**

**UNIT I** 15 Hours

**Precipitation Techniques:** Introduction –properties and precipitating reagents-Colloidal precipitates-Co-precipitation –Post-precipitation – Precipitates from homogenous solutions – Surface adsorption –Drying and ignition of precipitates – Application of gravimetric methods.

**UNIT II** 15 Hours

**Error analysis:** Classification of errors –accuracy and precision – minimization of errors – significant figures – significant figures in computation – statistical treatment of data- mean, median, standard deviation, variance, relative standard deviation –spread, errors – standard deviation of computed results-reliability of results-Q test, T-test – confidence limit-comparison of results- Student's test –F-test T-test – comparison of the means of two samples- correlation and regression: linear regression (least square analysis).

**UNIT III** 15 Hours

**Electro analytical Methods:** Electro analytical Techniques: Electrogravimetry: Theory of electrogravimetric analysis - Electro analytical separation and determination of metal ions, Coulometry: Electrolytic cell - work electrodes - auxilliary electrode and reference electrode – Coulometric titrations. Voltammetry - Cyclic voltammetry – stripping voltammetry –chromopotentiometry - Amperometry; Amperometric titrations.

**UNIT IV** 15 Hours

**Thermo analytical Methods:** Thermal analysis; Theory and principles of DTA and TGA – factors affecting the position of DT and T G traces-application of DTA and TGA to the thermal behavior of the following compounds- crystalline copper sulphate, calcium oxalate monohydrate, calcium acetate monohydrate, - Comparison of DTA and TGA – principle and application of DSC –determination of degree of conversion of high alumina cement.

**UNIT V** 15 Hours

**Spectroanalytical methods:** ***Colorimetry***: Beer and Lambert's law – terminology – conditions for a satisfactory colorimetric analysis – methods of colour measurement or comparison - principles of colorimetric determinations of Cr, Fe, Mn - simultaneous spectrophotometric determination of Cr and Mn. ***Nephelometry and turbidometry*****:** Determination of sulphate and phosphate. ***Fluorimetry***: Principle – application of flourimetry in the determination of Ca, Cd and Zn and determination of codeine and morphine in a mixture. ***Flame spectrometry:*** Theory – interferences – AAS - applications in the determination of $Mg^{2+}$, $Ca^{2+}$ in tap water.

## Text Books

D. A. Skoog, D. M. West and F. J. Holler, ***Fundamentals of Analytical Chemistry***, Saunders College Publishing, Philadelphia, 1996, 7th Edition.

Willard HH, Merritt LL, Dean JA, Settle PA. ***Instrumental Methods of Analysis***, NewYork: Van Nostrand, 1988, 6th Edition.

## Reference Books

J. Basset et al., ***Vogel's Text book of Qualitative Inorganic Analysis***, Longman, ELBS, Essex, 1989, 5th Edition.

J. G. Dick, ***Analytical Chemistry***, Tata-McGraw Hill, 1973.

## Pedagogy

Chalk & Talk, E-Resources, Group Discussion

## Teaching aids

Black Board, LCD Projector

## Course Contents and Lecture Schedule

| Module No. | Topic | No. of Lectures | Content Delivery Methods |
|---|---|---|---|
| **UNIT - I** | | | |
| 1.1 | Introduction–properties and precipitating reagents- | 3 | Chalk & Talk |
| 1.2 | Colloidal precipitates-Co-precipitation – Post-precipitation | 3 | E-Resources |
| 1.3 | Precipitates from homogenous solutions | 3 | Discussion |
| 1.4 | Surface adsorption-Drying and ignition of precipitates | 3 | Chalk & Talk |

| | | | |
|---|---|---|---|
| 1.5 | Application of gravimetric methods. | 3 | E-Resources |
| **UNIT- II** | | | |
| 2.1 | Error analysis: Classification of errors – accuracy and precision –minimization of errors | 3 | Discussion |
| 2.2 | significant figures – significant figures in computation | 3 | Chalk & Talk |
| 2.3 | statistical treatment of data- mean, median, standard deviation, variance, relative standard deviation –spread, errors | 3 | E-Resources |
| 2.4 | standard deviation of computed results-reliability of results-Q test, T-test – confidence limit-comparison of results | 3 | Chalk & Talk |
| 2.5 | Student's test –F-test T-test – comparison of the means of two samples- correlation and regression: linear regression (least square analysis). | 3 | E-Resources |
| **UNIT- III** | | | |
| 3.1 | Electro analytical Techniques: Electrogravimetry: Theory of electrogravimetric analysis | 3 | E-Resources |
| 3.2 | Electro analytical separation and determination of metal ions. | 3 | Chalk & Talk |
| 3.3 | Coulometry: Electrolytic cell - work electrodes - auxilliary electrode and reference electrode | 3 | Discussion |
| 3.4 | Coulometric titrations-Voltammetry - Cyclic voltammetry. | 3 | Chalk & Talk |
| 3.5 | stripping voltammetry – chromopotentiometry - Amperometry; Amperometric titrations. | 3 | E-Resources |
| **UNIT- IV** | | | |
| 4.1 | Thermal analysis; Theory and principles of DTA and TGA | 3 | Discussion |
| 4.2 | Factors affecting the position of DT and T G traces. | 3 | E-Resources |

| | | | |
|---|---|---|---|
| 4.3 | application of DTA and TGA to the thermal behavior of the following compounds- crystalline copper sulphate, calcium oxalate monohydrate | 3 | Chalk & Talk |
| 4.4 | calcium acetate monohydrate. Comparison of DTA and TGA | 3 | Chalk & Talk |
| 4.5 | Principle and application of DSC – determination of degree of conversion of high alumina cement. | 3 | E-Resources |
| **UNIT- V** | | | |
| 5.1 | Colorimetry: Beer and Lambert's law – terminology – conditions for a satisfactory colorimetric analysis – methods of colour measurement or comparison. | 3 | E-Resources |
| 5.2 | principles of colorimetric determinations of Cr, Fe, Mn - simultaneous spectrophotometric determination of Cr and Mn. | 3 | Chalk & Talk |
| 5.3 | Nephelometry and turbidometry: Determination of sulphate and phosphate. | 3 | Discussion |
| 5.4 | Fluorimetry: Principle – application of flourimetry in the determination of Ca, Cd and Zn and determination of codeine and morphine in a mixture. | 3 | E-Resources |
| 5.5 | Flame spectrometry: Theory – interferences – AAS - applications in the determination of Mg2+, Ca2+ in tap water. | 3 | Chalk & Talk |
| | **Total** | **75** | |

**Course Designer**
**Dr. M.P. Kesavan**
Assistant Professor of Chemistry

| Course Code | Course Title | Category | Total Hours | Credits |
|---|---|---|---|---|
| 20PCHE22 | Computer Applications in Chemistry | Elective -II | 75 | 5 |

| Nature of Course | |
|---|---|
| Knowledge Oriented | ✓ |
| Skill Oriented | ✓ |
| Employability Oriented | ✓ |
| Entrepreneurship Oriented | |

| Course Relevance | |
|---|---|
| Local | |
| Regional | |
| National | |
| Global | ✓ |

**Preamble**

The course explains the concepts of internet programming, HTML, JAVA APPLET and their applications in chemistry. It gives hands-on experience on chemistry-related application soft wares.

**Course Outcomes (CO)**

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

| No. | Course Outcome | Knowledge Level |
|---|---|---|
| **CO1** | Outline Internet protocols, online usage of internet, search engine, e-publication and electronic mail. | **K1, K2** |
| **CO2** | Make use of HTML and Java programs to chemistry. | **K1, K2,K3** |
| **CO3** | Analyze the chemical structures in scientific manner and get the mass and NMR simulations; and also get an idea about computational chemistry. | **K1, K2,K3,K4** |
| **CO4** | Apply the knowledge of diffraction techniques to the study of structural chemistry; and understand the applications of shelx and PLATON software in crystallography. | **K1, K2,K3** |
| **CO5** | Evaluate the application of RASMOL and MATLAB in chemistry. | **K1, K2,K3,K4K5** |

**K1-Knowledge K2-Understand K3-Apply K4- Analyse K5- Evaluate**

**Mapping of CO with PO**

| | PO1 | PO2 | PO3 | PO4 | PO5 |
|---|---|---|---|---|---|
| **CO1** | **1** | **3** | **1** | **2** | **1** |
| **CO2** | **1** | **2** | **2** | **3** | **1** |
| **CO3** | **3** | **3** | **3** | **3** | **2** |
| **CO4** | **2** | **3** | **2** | **3** | **1** |
| **CO5** | **1** | **2** | **1** | **2** | **1** |

**1-Low 2-Medium 3-Strong**

**Mapping of CO with PSO**

| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|---|---|---|---|---|---|
| CO1 | 3 | 2 | 2 | 3 | 1 |
| CO2 | 3 | 1 | 2 | 3 | 1 |
| CO3 | 3 | 3 | 3 | 3 | 3 |
| CO4 | 3 | 2 | 1 | 2 | 2 |
| CO5 | 3 | 1 | 1 | 2 | 1 |

**1-Low** **2-Medium** **3-Strong**

**Syllabus**

**UNIT I** 15 Hours

**INTERNET**: Introduction- History- Importance of the Internet- Internet Access- Dial-Up connection, Direct connection and equipments - Internet protocol(TCP/IP,FTP HTTP, TELNET and WAP)-Internet addressing – Domain Name-Mail address-Uniform Resource Locator(URL)-Web Browsing- Searching the Web- Search Engines(Yahoo, Google)- Intranet – Searching and utilizing Popular websites in Chemistry. Online literature survey- accessing of e-journals. Preparing articles for e-publications. Online structure drawing- Collection of spectral data using databases.

**ELECTRONIC MAIL**: Introduction-Working of E-Mail - Word processor for E-Mail- Mailing Basics – Composing and sending of an E-Mail- Address Book – Signature- File Attachments- Customizing your Mail program – Advantages and Disadvantages of E-Mail - Tips for effective E-Mail use- Smile keys.

**UNIT II** 15 Hours

**HTML:** HTML - Need- Structure of HTML Document- HTML Tags- Horizontal line Tags- Background and Text color Tags- Font Tags- MARQUEES Tags- Adding pictures - Ordered and Unordered Lists- Creating Links- Construction of Periodic Table with required data for first ten elements- Frames – Developing and hosting of Web Pages for a given molecule / chemical.

**JAVA APPLETS:** - Simple and Java applets with graphics- Applications of applet to draw 2D and 3D view of molecules.

**UNIT III** 15 Hours

**Applications of chemdraw and chem 3D software in chemistry:** Introduction- Tool Pallets- Construction of the molecule using Chem Draw-Tools- Manipulating a molecule-Model display- Display type- Structure displays- Molecular Surface display- NMR simulation and interpretation-Naming IUPAC- Structure from Name and Name from Structure-Computational Concepts: - Computational methods: - Potential energy surface, geometry Optimizations property (calculations)-Molecular Mechanics Theory in brief - Animations- Difference between Chemdraw and Chem 3D.

**UNIT IV** 15 Hours

**Applications of SHELX program in chemistry:** Basics of Crystals-Symmetry and operations- Seven Crystal systems- Bravais lattices – X-Ray Diffractometers- Unit cell parameters- X-ray data- Deduction of Space group - Structure solution and refinement using SHELX- Structure building using PLATON- H-Bonding.

**UNIT V** 15 Hours

**Applications of RASMOL and MATLAB in chemistry**

**RASMOL:** Introduction- User commands– Identification of disulfide-bridges and visualization of :- d polar residues, the distribution of polar and non-polar amino acids, side chain of carboxylate and amine , the different structural motives like α-helix, β-sheet and β - turn, the amino acids bound to Zn, active site of carboxypeptidase A, the environment of the active center.

**MATLAB:** Introduction-advantages- getting started- windows for workspace, command interpretation, command history and current history- Addition- Use of sine and Cosine of angles(pi)- variable ‗ans'- order of operations- significant decimals- Representation of matrix- getting transpose of a matrix- display of images- saving images-solving linear equations(case m=n only).

**Text Books**

Alexis Leon and Mathews Leon, ***Fundamentals of Information Technology*** Leon TECH World, UBS Publishers & Distributors Ltd., 1999.

E. Balagurusmy, ***Programming with Java*** - ***A Primer***, Tata McGraw-Hill Publishing Company Ltd., New Delhi, 2003,2nd Edn., 15th Reprint

C. Xavier, ***World wide web design with HTML***, , Tata McGraw-Hill Publishing Company Ltd., New Delhi, 2000, 2nd Reprint.

**Reference Books**


Margaret Levine Young, ***Internet Complete Reference***, Tata McGraw-Hill Publishing Company Ltd., New Delhi, 2001.

Barbara Kassev, ***Using the Internet***, EE edition, New Delhi, 1998, IV Edition.

Alexis Leon and Mathews Leon, ***Internet for Everyone***, Leon TECH World, Publishers & Distributors Ltd., 2000.

John Zukowski, ***Mastering Java 2***, BPB Publications, New Delhi, 2002.

Patrick Naughten, The ***Java Hand Book***, Tata McGraw-Hill Publishing Company Ltd., New Delhi, 2002, 11th Reprint.

Herbert Schildt, ***Java 2- The Complete Reference***, Tata McGraw-Hill Publishing Company Ltd., New Delhi, 2001, 4th Edn.

Holzner, John Zukowski, ***Java 2 Complete***: Steven BPB Publications, New Delhi, 1999,1st Indian Edn..

Harley Hahn, The ***Internet Complete Reference***, Tata McGraw-Hill Publishing Company Ltd., New Delhi, 2001, 2nd Edn.

Chem Draw & Chem 3D – ***Manual***

Shelx, Rasmol and MATLAB- ***Manuals***.


**REFERENCES in the NET**

http://SCS99.unige.Che/eng/toc.html2.http://hackberry.chem.niu.edu:to/o/webpage.html

http://java.Sun.Com/applet/applets/chemical Models/index.html

http://ccl.osc.edu/chemistry.html5.http://www.umass.eud/microbio/rasmol/

http://www.Mdli.com/cgi/dynamic/welcome.html/

(for CHIME similar to Rasmol)

**Pedagogy**

Chalk & Talk, E-Resources, Group Discussion

**Teaching aids**

Black Board, LCD Projector

**Course Contents and Lecture Schedule**

| Module No. | Topic | No. of Lectures | Content Delivery Methods |
|---|---|---|---|
| | **UNIT – I** | | |
| 1.1 | INTERNET: Introduction- History- Importance of the Internet- Internet Access- Dial-Up connection, Direct connection and equipments –- Internet protocol(TCP/IP,FTP HTTP, TELNET and WAP) | 3 | Chalk & Talk |
| 1.2 | Internet addressing – Domain Name-Mail address-Uniform Resource Locator(URL)- Web Browsing- Searching the Web- Search Engines(Yahoo, Google)- Intranet | 3 | E-Resources |
| 1.3 | Searching and utilizing Popular websites in Chemistry. On line literature survey- accessing of e-journals. Preparing articles for e-publications. Online structure drawing- Collection of spectral data using databases. | 3 | Discussion |
| 1.4 | ELECTRONIC MAIL: Introduction- Working of E-Mail - Word processor for E-Mail- Mailing Basics – Composing and sending of an E-Mail- Address Book – Signature | 3 | Chalk & Talk |
| 1.5 | File Attachments- Customizing your Mail program –Advantages and Disadvantages of E-Mail - Tips for effective E-Mail use- Smile keys. | 3 | E-Resources |
| | **UNIT – II** | | |
| 2.1 | HTML - Need- Structure of HTML Document- HTML Tags- Horizontal line Tags- Background and Text color Tags- Font Tags | 3 | Discussion |
| 2.2 | MARQUEES Tags- Adding pictures - Ordered and Unordered Lists | 3 | Chalk & Talk |
| 2.3 | Creating Links- Construction of Periodic Table with required data for first ten elements- Frames | 3 | E-Resources |

| | | | |
|---|---|---|---|
| 2.4 | Developing and hosting of Web Pages for a given molecule / chemical. | 3 | Chalk & Talk |
| 2.5 | **JAVA APPLETS:** - Simple and Java applets with graphics- Applications of applet to draw 2D and 3D view of molecules. | 3 | E-Resources |
| **UNIT – III** | | | |
| 3.1 | **Chem- Draw and Chem 3D:** Introduction- Tool Pallets- Construction of the molecule using Chem Draw- Tools- Manipulating a molecule. | 3 | E-Resources |
| 3.2 | Model display- Display type- Structure displays- Molecular Surface display | 3 | Chalk & Talk |
| 3.3 | NMR simulation and interpretation- Naming IUPAC- Structure from Name and Name from Structure-Computational Concepts: - Computational methods | 3 | Discussion |
| 3.4 | Potential energy surface, geometry Optimizations property (calculations) | 3 | Chalk & Talk |
| 3.5 | Molecular Mechanics Theory in brief - Animations- Difference between Chemdraw and Chem 3D. | 3 | E-Resources |
| **UNIT – IV** | | | |
| 4.1 | Basics of Crystals- Symmetry and operations- Seven Crystal systems Bravais lattices | 3 | Discussion |
| 4.2 | X-Ray Diffractometers - Unit cell parameters. | 3 | E-Resources |
| 4.3 | X-ray data- Deduction of Space group | 3 | Chalk & Talk |
| 4.4 | Structure solution and refinement using SHELX | 3 | E-Resources |
| 4.5 | Structure building using PLATON- H-Bonding. | 3 | Chalk & Talk |

| UNIT –V | | | |
|---|---|---|---|
| 5.1 | RASMOL: - Introduction- User commands– Identification of disulfide-bridges and visualization of :-hydrophobic and polar residues, the distribution of polar and non-polar amino acids | 3 | E-Resources |
| 5.2 | side chain of carboxylate and amine , the different structural motives like α-helix, β-sheet and β - turn, the amino acids bound to Zn, active site of carboxypeptidase A, the environment of the active center | 3 | Chalk & Talk |
| 5.3 | MATLAB: - Introduction-advantages-getting started- windows for workspace, command interpretation, command history and current history | 3 | Discussion |
| 5.4 | Addition- Use of sine and Cosine of angles(pi)- variable _ ans'- order of operations- significant decimals- | 3 | Chalk & Talk |
| 5.5 | Representation of matrix- getting transpose of a matrix- display of images-saving images-solving linear equations(case m=n only). | 3 | E-Resources |
| | **Total** | **75** | |

**Course Designer**
**Ms. M. Rekha**
Assistant Professor of Chemistry

| Course Code | Course Title | Category | Total Hours | Credits |
|---|---|---|---|---|
| 20PCHC31 | Organic Chemistry - III | Core -IX | 90 | 5 |

| Nature of Course | |
|---|---|
| Knowledge Oriented | ✓ |
| Skill Oriented | ✓ |
| Employability Oriented | |
| Entrepreneurship Oriented | |

| Course Relevance | |
|---|---|
| Local | |
| Regional | |
| National | |
| Global | ✓ |

**Preamble**

The course explains the application of various reagents in organic synthesis and chemistry of steroids, vitamins, peptides and nucleic acid. It also explains the importance of green chemistry.

**Course Outcomes (CO)**

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

| No. | Course Outcome | Knowledge Level |
|---|---|---|
| **CO1** | Make use of chemical reagents in various organic transformation such as oxidation, reduction, catalysis etc., | **K1,K2,K3** |
| **CO2** | Apply the concepts and mechanism of photochemical and thermal reactions of carbonyl, alkenes and conjugated pi electrons compounds. | **K1,K2** |
| **CO3** | Analyze the structure and activity of compounds with steroid skeleton and vitamins | **K1,K2,K3,K4** |
| **CO4** | Explain the structure and synthesis of amino acids, peptides, proteins and nucleic acid | **K1,K2,K3,K4,K5** |
| **CO5** | Apply their knowledge to synthesis compounds in a greener way | **K1,K2,K3** |

**K1-Knowledge K2-Understand K3-Apply K4- Analyse K5- Evaluate**

**Mapping of CO with PO**

| | PO1 | PO2 | PO3 | PO4 | PO5 |
|---|---|---|---|---|---|
| **CO1** | **3** | **1** | **3** | **2** | **3** |
| **CO2** | **3** | **1** | **1** | **2** | **3** |
| **CO3** | **3** | **3** | **2** | **3** | **3** |
| **CO4** | **3** | **3** | **2** | **3** | **2** |
| **CO5** | **2** | **2** | **2** | **3** | **1** |

**1-Low 2-Medium 3-Strong**

**Mapping of CO with PSO**

| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|---|---|---|---|---|---|
| CO1 | 3 | 3 | 1 | 3 | 3 |
| CO2 | 3 | 3 | 2 | 2 | 3 |
| CO3 | 3 | 3 | 3 | 3 | 3 |
| CO4 | 3 | 2 | 2 | 1 | 2 |
| CO5 | 3 | 1 | 3 | 3 | 2 |

**1-Low** **2-Medium** **3-Strong**

**Syllabus**

**UNIT I** 18 Hours

**Reagents in Organic Synthesis:** Use of the following reagents in organic syntheses and functional group transformations – complex metal hydrides, Gilman's reagent, lithium dimethyl cuprate – lithium diisopropylamide (LDA) –– trimethyl silyliodide – tri-n-butyl tin hydride – Jones reagent – pyridinium chloro chromate – $SeO_2$ – peracids – DMSO – $Pb(OAc)_4$ – $HIO_4$ – Prevost and Woodward hydroxylation – Etard's reagent – Waker_s reagent – $RuO_4$ – $Hg(OAc)_2$ – Oppenauer oxidation – DDQ – $LiAlH_4$, $NaBH_4$, Lawessons reagent – Crown ethers – Thallium nitrate – Phase transfer catalysts – Birch reduction.

**UNIT II** 18 Hours

P**hotochemistry and Pericyclic reactions:** General principles – orbital symmetry considerations related to photochemical reactions, thermal versus photochemical reactions – principles of energy transfer – photochemical reactions of ketones – Norrish type I and type II reactions – Paterno Buchi reaction – Dienone photochemistry – photo reduction, photochemical oxidation, Barton reaction – photochemistry of alkenes and dienes. Pericyclic reactions Application of symmetry to orbital interactions – selection rules (Woodward and Hoffmann rules) – Electrocyclisation, cycloaddition and sigmatropic rearrangements – cheletropic reactions – Diels-Alder Reactions: Endoselectivity and regioselectivity – Explanation of these reaction in terms of correlation diagrams approach, FMO approach and Dewar – Zimmermann approach – (PMO) Huckel-Mobius concepts

**UNIT III** 18 Hours

**Chemistry of Steroids and Vitamins**: Introduction – Structural elucidation of Cholesterol – Androsterone and Testosterone (male sex hormones) – Oesterone, progesterone (Female sex hormone). Classification of Vitamins: Nomenclature of Vitamins – Strucure and Biological functions of vitamins: Vitamin A (Retinol), V itamin $B_2$ (Riboflavin), Vitamin $B_6$ (Pyridoxine), Vitamin $B_{12}$, Vitamin C, D and E (Structure elucidation and synthesis not required).

**UNIT IV** 18 Hours

**Chemistry of Peptides and Nucleic Acid** : (a) Polypeptides – Classification - the peptide linkage - Structure of amino acids – primary, secondary, tertiary and quaternary structure) – Solid phase peptide synthesis (Merifield) – use of protecting groups and reagents – Structural elucidation of glutathione, thyroxin and oxytocin.

(b) Nucleosides, Nucleotides and Nucleic acids – structure and synthesis of nucleosides and nucleotides – Elementary treatment on the structure of DNA and RNA.

**UNIT V** 18 Hours

**Green Chemistry**: Principles of green chemistry – planning a green synthesis in a laboratory – general interest for solvent free processes- Microwave synthesis: Introduction and characteristics of microwave heating – difference between conventional heating and microwave heating. Dielectric polarization – dipolar polarization – application and advantages of microwave heating over conventional heating.

## Text Books


I.L. Finar, ***Organic Chemistry Vol. II***, ELBS, UK , 2005, V Edition.

S.F. Dyke, ***Chemistry of Vitamins***, Interscience, Toronto, 1965.

O.P. Agarwal ***Chemistry of Natural products Vol. I and II***, Himalaya Publishing House, New Delhi, 2002.

V.K. Ahluwalia, M. Kidwai, ***New trends in Green Chemistry***, Anamaya Publishers, New Delhi, 2006, Second Edition.

Gurdeep Chatwal, ***Organic Chemistry of natural products Vol. I***, Himalaya Publishing House, 1997.

Morrison and Boyd, ***Organic Chemistry***, Prentice-Hall of India private limited, New Delhi, 6th Edition.


## Reference Books


Hermann Dugus, ***Bioorganic Chemistry,*** Springer International, New Delhi, 2004, 3rd Edition.

D.L. Nelson and M.M. Cox, ***Lehningers' Principal of Biochemistry***, W.H. Freeman and Company, New York, 2008, 5th Edition.

L.F Fieser and M. Fieser, ***Steroids,*** Reinhold Press, Atlanta, 1991.

**Pedagogy**

Chalk & Talk, E-Resources, Group Discussion

**Teaching aids**

Black Board, LCD Projector

**Course Contents and Lecture Schedule**

| Module No. | Topic | No. of Lectures | Content Delivery Methods |
|---|---|---|---|
| | **UNIT – I** | | |
| 1.1 | Use of the following reagents in organic syntheses and functional group transformations. | 3 | Chalk & Talk |
| 1.2 | complex metal hydrides, Gilman_s reagent, lithium dimethyl cuprate – lithium diisopropylamide (LDA). | 4 | E-Resources |
| 1.3 | Trimethyl silyliodide – tri-n-butyl tin hydride – Jones reagent – pyridinium chloro chromate. | 3 | Discussion |
| 1.4 | $SeO_2$ – peracids – DMSO – $Pb(OAc)_4$ – $HIO_4$ – Prevost and Woodward hydroxylation – Etard's reagent – Waker_s reagent – RuO4 – $Hg(OAc)_2$. | 4 | Chalk & Talk |
| 1.5 | Oppenauer oxidation – DDQ – $LiAlH_4$, $NaBH_4$, Lawessons reagent – Crown ethers – Thallium nitrate – Phase transfer catalysts – Birch reduction. | 4 | Chalk & Talk |
| | **UNIT – II** | | |
| 2.1 | General principles – orbital symmetry considerations related to photochemical reactions, thermal versus photochemical reactions. principles of energy transfer. | 4 | Discussion |
| 2.2 | photochemical reactions of ketones – Norrish type I and type II reactions – Paterno Buchi reaction – Dienone photochemistry – photo reduction, photochemical oxidation, Barton reaction. | 3 | Chalk & Talk |
| 2.3 | – photochemistry of alkenes and dienes. Pericyclic reactions Application of symmetry to orbital interactions – selection rules (Woodward and Hoffmann rules). | 4 | E-Resources |

| | | | |
|---|---|---|---|
| 2.4 | Electrocyclisation, cycloaddition and sigmatropic rearrangements – cheletropic reactions – Diels-Alder Reactions: Endoselectivity and regioselectivity. | 3 | Chalk & Talk |
| 2.5 | Explanation of these reaction in terms of correlation diagrams approach, FMO approach and Dewar – Zimmermann approach – (PMO) Huckel-Mobius concepts. | 4 | Chalk & Talk |
| **UNIT – III** | | | |
| 3.1 | Structural elucidation of Cholesterol – Androsterone and Testosterone (male sex hormones). | 4 | E-Resources |
| 3.2 | Oesterone, progesterone (Female sex hormone). Classification of Vitamins: Nomenclature of Vitamins | 4 | Chalk & Talk |
| 3.3 | Strucure and Biological functions of vitamins: Vitamin A (Retinol), Vitamin $B_2$ (Riboflavin) | 4 | Discussion |
| 3.4 | Vitamin $B_6$ (Pyridoxine), Vitamin $B_{12}$ | 3 | E-Resources |
| 3.5 | Vitamin C, D and E (Structure elucidation and synthesis not required). | 3 | Discussion |
| **UNIT – IV** | | | |
| 4.1 | Polypeptides – Classification - the peptide linkage. | 3 | Discussion |
| 4.2 | Structure of amino acids – primary, secondary, tertiary and quaternary structure. | 4 | E-Resources |
| 4.3 | Solid phase peptide synthesis (Merifield) – use of protecting groups and reagents – Structural elucidation of glutathione, thyroxin and oxytocin. | 4 | Chalk & Talk |
| 4.4 | Nucleosides, Nucleotides and Nucleic acids – structure and synthesis of nucleosides and nucleotides. | 4 | E-Resources |
| 4.5 | Elementary treatment on the structure of DNA and RNA. | 3 | Chalk & Talk |

| UNIT – V | | | |
|---|---|---|---|
| 5.1 | Principles of green chemistry – planning a green synthesis in a laboratory. | 3 | E-Resources |
| 5.2 | General interest for solvent free processes - Microwave synthesis: Introduction and characteristics of microwave heating. | 4 | Chalk & Talk |
| 5.3 | Difference between conventional heating and microwave heating. | 4 | Discussion |
| 5.4 | Dielectric polarization – dipolar polarization. | 4 | Discussion |
| 5.5 | Application and advantages of microwave heating over conventional heating. | 3 | Chalk & Talk |
| | **Total** | **90** | |

**Course Designer**
**Mr. G. Arivalagan**
Assistant Professor of Chemistry.

| Course Code | Course Title | Category | Total Hours | Credits |
|---|---|---|---|---|
| 20PCHC32 | Inorganic Chemistry -III | Core -X | 90 | 5 |

| Nature of Course | |
|---|---|
| Knowledge Oriented | ✓ |
| Skill Oriented | ✓ |
| Employability Oriented | |
| Entrepreneurship Oriented | |

| Course Relevance | |
|---|---|
| Local | |
| Regional | |
| National | |
| Global | ✓ |

**Preamble**

The course explains the various theories and reaction mechanism of coordination compounds and inorganic photochemical reactions. It also gives information on the applications of various spectral techniques in determining the structure and property of Inorganic compound/complexes.

**Course Outcomes (CO)**

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

| No. | Course Outcome | Knowledge Level |
|---|---|---|
| **CO1** | Explain various theories and properties of coordination compounds. | **K1,K2** |
| **CO2** | Examine the mechanism of co-ordination compounds. | **K1,K2,K3,K4** |
| **CO3** | Apply inorganic photochemical reactions to evaluate the reaction path and in photochemical energy conversion like solar cell, fuel cell etc. | **K1,K2,K3,K4,K5** |
| **CO4** | Outline the basic principles and instrumentation of spectral techniques like IR, Raman, NMR, NQR and electronic spectroscopy and analyze their application in determining the structure and property of Inorganic compound/complexes | **K1,K2,K3,K4** |
| **CO5** | Outline the principles of various spectral techniques like EPR, PES, IR, MBS etc and interpretation of the spectra. | **K1,K2,K3** |

**K1-Knowledge K2-Understand K3-Apply K4- Analyse K5- Evaluate**

**Mapping of CO with PO**

| | PO1 | PO2 | PO3 | PO4 | PO5 |
|---|---|---|---|---|---|
| **CO1** | **3** | **1** | **2** | **2** | **3** |
| **CO2** | **3** | **1** | **2** | **3** | **3** |
| **CO3** | **2** | **2** | **3** | **2** | **3** |
| **CO4** | **3** | **2** | **3** | **3** | **3** |
| **CO5** | **3** | **2** | **3** | **3** | **3** |

**1-Low 2-Medium 3-Strong**

**Mapping of CO with PSO**

| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|---|---|---|---|---|---|
| CO1 | 3 | 3 | 2 | 2 | 3 |
| CO2 | 3 | 2 | 2 | 3 | 2 |
| CO3 | 3 | 1 | 3 | 3 | 3 |
| CO4 | 3 | 3 | 3 | 3 | 3 |
| CO5 | 3 | 3 | 3 | 3 | 3 |

**1-Low** **2-Medium** **3-Strong**

**Syllabus**

**UNIT I** 18 Hours

**Coordination Chemistry-I**: Nomenclature of coordination complexes- Stereochemistry of coordination compounds: Geometrical isomerism- optical isomerism of complexes having C. N. 4, 6 – Stability constants – Factors affecting Stability constant in solution – Determination of Stability constant Spectrophotometric method - Chelate effect.

Theories of bonding – VBT – CFT – MO theories – Splitting of d-orbitals in Octahedral, Tetrahedral and Square planar geometries – CFSE calculation in terms of Dq - Factors affecting crystal field splitting – Spectrochemical series – Nephelauxetic effect - Magnetic properties of transition metal complexes – Para, Dia, ferro magnetism and antiferro magnetism- Calculation of spin-only magnetic moments.

**UNIT II** 18 Hours

**Coordination Chemistry-II**: Substitution reactions of octahedral complexes $S_N1$, $S_N2$, SNiCB - lability-inertness- square planar substitution reactions - Factors affecting reactivity of square planar complexes- Trans effect- Theories of Trans effect and its applications - Reactions of coordinated ligands - Acid hydrolysis - anation reactions and base hydrolysis. Mechanism of electron transfer reactions - Outer sphere, inner sphere electron transfer reactions - Marcus Theory and its applications. Synthesis of coordination compounds using electron transfer and substitution reaction.

**UNIT III** 18 Hours

**Inorganic Photochemistry:** Excited states of coordination complexes – properties of excited states charge transfer and energy transfer – photochemical pathways. Photoredox reactions of Co(III) and Cr(III) complexes – photosubstitution reactions – photoaquation, photoanation and photorearrangements - Role of TiO2 in solar energy conversion – Photoredox chemistry of Ruthenium bipyridyl and Ruthenium(II) poly pyridyl compounds-energy conversion and photochemical decomposition of water using Ru complexes- storage of solar energy

**UNIT IV** 18 Hours

**Physical Methods in Inorganic Chemistry-I:** Electronic spectra: selection rules – polarization – splitting of spectral terms – L.S Coupling scheme- Russel- Saunders method- Term Symbols -Orgel and Tanabe-Sugano diagram. – Evaluation of 10 Dq and beta $d^2$, $d^3$, $d^7$, $d^8$ systems IR and Raman spectra: Applications of IR and Raman. Selection rules to structure determination – IR spectral studies of carbonyl compounds. Nuclear magnetic resonance: Application of chemical shift and spin coupling to structure determination using multiple NMR (H,P,F) chemical exchange, dynamic processes in inorganic and organometallic compounds- Fluxional NMR of metal carbonyls and allyl complexes – paramagnetic NMR and contact and pseudo contact shifts.

**UNIT V** 18 Hours

**Physical Methods In Inorganic Chemistry-II:** Electron paramagnetic resonance spectroscopy: Applications of hyperfine splitting and g factor to structural elucidation- Zero field splitting-Krammer‘s Degeneracy- EPR spectra of Cu (II) and Mn (II) in various site symmetry- covalency of metal-ligand bonding by EPR study of dynamic processes in solids- Study of phase transition by Mn (II) – John Teller distortions in Cu (II) complexes. Mossbauer spectroscopy: Basic principles- Doppler effect- Isomer shift- Electron nuclear hyperfine interactions- Quadrupole and magnetic interactions in the study of structure and bonding in Iron and Tin complexes and in Biological systems.

**Text Books**


Shriver D. F. and Atkins, P.W, ***Inorganic Chemistry***, Oxford University Press, London, 1999.

Cotton F.A. and Wilkinson, G, ***Advanced Inorganic Chemistry***, Wiley-Interscience publications, John Wiley & Sons, New York, 1988, V Edn.

Gurdeep R. Chatwal & M. S. Yadav, ***Coordination Chemistry,*** Himalaya Publishing House, 1993, I Edn.

Figgis, B.N, ***Introduction to Ligand Fields***, Wiley Interscience, Eartern Ltd., New Delhi, 1964, I Edn.,

Banerjea, D, ***Coordination Chemistry***, Tata McGraw- Hill Publishing Co. Ltd., 1993.

Purcell, K. F. Kotz, J.C. Holt Saunders, ***Inorganic Chemistry***, Philedelphia, USA, 1977.

Pradeep. T, ***A Textbook of Nanoscience and Nanotechnology***, Tata, McGraw-Hill Education, India, 2003.

Drago, R. S. Van Nostrand and Reinhold, ***Physical methods in Chemistry,*** 1976.

Nakamoto, Kazuo, **Infrared and Raman Spectra of Inorganic and coordination compounds**, John Wiley and Sons, New York, 1986, IV edition.

Raymond Chang M, **Basic principles of Spectroscopy,** Mc Graw Hill, New Delhi, 1971.

Straughan B. P. and Walker S. ***Spectroscopy Vol.3,*** Chapman and Hall , NewDelhi, 1976,

T. Pradeep, ***Text book of nanoscience & Nanotechnology***, 2017.

**Reference Books**

Douglas and McDaniel ***A Concise of Inorganic Chemistry***, Oxford and IBH Publishing Company (P) Ltd., New Delhi, 2002.

E. Huheey, Ellen A. Keiter, Richard L. Keiter, ***Inorganic Chemistry,*** Pearson Education (Singapore) P.Ltd., Delhi, 2004, IV Edn.,

Wahid U. Malik, G. D. Tuli and R. D. Madan, ***Selected Topics in Inorganic Chemistry, S. Chand & Co. Ltd., New Delhi, 2006.***

William W*.* Porterfield, ***Inorganic Chemistry***, Elsevier, New Delhi, 2005, 2nd Edn.,

A.G. Sharpe***, Inorganic Chemistry, Addition***, Wesley Longman, UK, 2004, 3rd Edn.

Gary L. Miessler and Donald A. Tarr, ***Inorganic Chemistry***, Pearson Education, Inc., New Delhi, 2004, 3rd Edn.,

Raguse, ***Nano technology-Basic Science and Emerging Technologies,*** Overseas Press India (P). Ltd. New Delhi, 2005, Ist Edn, .

Mark Ratner and Daniel Ratnar***, A Gentle Introduction to the Next Nanotechnology,*** Big Idea, Pearson Education Inc., US and UK.

D.N. Sathyanarayana, ***Electronic Absorption Spectroscopy and Related Techniques,*** Universities Press (India) Limited, 2001.

**Pedagogy**

Chalk & Talk, E-Resources, Group Discussion

**Teaching aids**

Black Board, LCD Projector

**Course Contents and Lecture Schedule**

| Module No. | Topic | No. of Lectures | Content Delivery Methods |
|---|---|---|---|
| | **UNIT – I** | | |
| 1.1 | Nomenclature of coordination complexes- Stereochemistry of coordination compounds: Geometrical isomerism- optical isomerism of complexes having C. N. 4, 6. | 3 | Chalk & Talk |
| 1.2 | Stability constants – Factors affecting Stability constant in solution – Determination of Stability constant Spectrophotometric method - Chelate effect. | 4 | E-Resources |
| 1.3 | Theories of bonding – VBT – CFT – MO theories – Splitting of d-orbitals in Octahedral, Tetrahedral and Square planar geometries. | 4 | Discussion |
| 1.4 | CFSE calculation in terms of Dq - Factors affecting crystal field splitting – Spectrochemical series – Nephelauxetic effect. | 4 | E-Resources |
| 1.5 | Magnetic properties of transition metal complexes – Para, Dia, ferro magnetism and antiferro magnetism- Calculation of spin-only magnetic moments. | 3 | Discussion |
| | **UNIT – II** | | |
| 2.1 | Substitution reactions of octahedral complexes $S_N1$, $S_N2$, SNiCB. | 5 | Discussion |
| 2.2 | lability-inertness- square planar substitution reactions - Factors affecting reactivity of square planar complexes- | 4 | Chalk & Talk |
| 2.3 | Trans effect- Theories of Trans effect and its applications - Reactions of coordinated ligands - Acid hydrolysis - anation reactions and base hydrolysis. | 3 | E-Resources |
| 2.4 | Mechanism of electron transfer reactions - Outer sphere, inner sphere electron transfer reactions | 3 | Chalk & Talk |
| 2.5 | Marcus Theory and its applications. Synthesis of coordination compounds using electron transfer and substitution reaction. | 3 | E-Resources |

| UNIT – III | | | |
|---|---|---|---|
| 3.1 | Excited states of coordination complexes – properties of excited states charge transfer and energy transfer. | 4 | E-Resources |
| 3.2 | photochemical pathways. Photoredox reactions of Co(III) and Cr(III) complexes – photosubstitution reactions. | 4 | Chalk & Talk |
| 3.3 | Photoaquation, photoanation and photorearrangements - Role of TiO2 in solar energy conversion. | 4 | Discussion |
| 3.4 | Photoredox chemistry of Ruthenium bipyridyl and Ruthenium(II) poly pyridyl compounds. | 3 | Chalk & Talk |
| 3.5 | Energy conversion and photochemical decomposition of water using Ru complexes- storage of solar energy | 3 | Discussion |
| **UNIT – IV** | | | |
| 4.1 | Electronic spectra: selection rules – polarization – splitting of spectral terms – L.S Coupling scheme. | 3 | Discussion |
| 4.2 | Russel- Saunders method- Term Symbols -Orgel and Tanabe-Sugano diagram. – Evaluation of 10 Dq and beta d2, d3, d7, d8 systems. | 4 | E-Resources |
| 4.3 | IR and Raman spectra: Applications of IR and Raman. Selection rules to structure determination – IR spectral studies of carbonyl compounds. | 3 | Chalk & Talk |
| 4.4 | Nuclear magnetic resonance: Application of chemical shift and spin coupling to structure determination using multiple NMR (H,P,F) chemical exchange, dynamic processes in inorganic and organometallic compounds. | 5 | E-Resources |
| 4.5 | Fluxional NMR of metal carbonyls and allyl complexes – paramagnetic NMR and contact and pseudo contact shifts | 3 | Chalk & Talk |

| UNIT – V | | | |
|---|---|---|---|
| 5.1 | Electron paramagnetic resonance spectroscopy: Applications of hyperfine splitting and g factor to structural elucidation - Zero field splitting- Krammer‘s Degeneracy. | 5 | E-Resources |
| 5.2 | EPR spectra of Cu (II) and Mn (II) in various site symmetry- covalency of metal-ligand bonding by EPR study of dynamic processes in solids- Study of phase transition by Mn (II). | 3 | Chalk & Talk |
| 5.3 | John Teller distortions in Cu (II) complexes. | 2 | Discussion |
| 5.4 | Mossbauer spectroscopy: Basic principles- Doppler effect- Isomer shift. | 3 | Chalk & Talk |
| 5.5 | Electron nuclear hyperfine interactions- Quadrupole and magnetic interactions in the study of structure and bonding in Iron and Tin complexes and in Biological systems. | 5 | Chalk & Talk |
| | **Total** | **90** | |

**Course Designer**
**Dr. M. Nihath Nazleen**
Assistant Professor of Chemistry

| Course Code | Course Title | Category | Total Hours | Credits |
|---|---|---|---|---|
| 20PCHC33 | Physical Chemistry-III | Core -XI | 75 | 5 |

| Nature of Course | |
|---|---|
| Knowledge Oriented | ✓ |
| Skill Oriented | ✓ |
| Employability Oriented | |
| Entrepreneurship Oriented | |

| Course Relevance | |
|---|---|
| Local | |
| Regional | |
| National | |
| Global | ✓ |

**Preamble**

This course has been framed to enable the students to gain knowledge on basic and applications of group theory, spectroscopic techniques such as UV, PES, ESR, and NQR. It also gives information on nano science and technology.

**Course Outcomes (CO)**

On the completion of the course the student will be able to

| No. | Course Outcome | Knowledge Level |
|---|---|---|
| **CO1** | Summaries the fundamentals of group theory. | **K1, K2** |
| **CO2** | Analyze the applications of group theory. | **K1, K2,K3,K4** |
| **CO3** | Interpret the physical concepts of electronic and Photo electron Spectroscopy. | **K1, K2,K3,K4K5** |
| **CO4** | Apply the theory and applications of ESR, Mossbauer and NQR Spectroscopic techniques. | **K1, K2,K3** |
| **CO5** | Summarize the preparation, characterization and evaluate application of nanoparticles. | **K1, K2,K3,K4K5** |

**K1-Knowledge K2-Understand K3-Apply K4- Analyse K5- Evaluate**

**Mapping of CO with PO**

| | PO1 | PO2 | PO3 | PO4 | PO5 |
|---|---|---|---|---|---|
| **CO1** | **3** | **1** | **2** | **2** | **3** |
| **CO2** | **3** | **1** | **2** | **2** | **3** |
| **CO3** | **3** | **2** | **3** | **3** | **3** |
| **CO4** | **3** | **2** | **3** | **3** | **3** |
| **CO5** | **1** | **3** | **3** | **3** | **2** |

**1-Low 2-Medium 3-Strong**

**Mapping of CO with PSO**

| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|---|---|---|---|---|---|
| CO1 | 3 | 3 | 1 | 1 | 3 |
| CO2 | 3 | 3 | 2 | 2 | 3 |
| CO3 | 3 | 3 | 3 | 3 | 3 |
| CO4 | 3 | 3 | 3 | 3 | 3 |
| CO5 | 3 | 2 | 3 | 3 | 2 |

**1-Low** **2-Medium** **3-Strong**

**Syllabus**

**UNIT I** 15 Hours

**Group Theory I (Basics of Group Theory):** Introduction - Symmetry elements and symmetry operations - Definition of mathematical group - four cardinal properties of a group - closure, associative, idendity and inverse rule - cyclic group Abelian group ($H_2O$ only) and non-abelian group ($NH_3$ only) - Group multiplication table- $C_2v$ and $C_3v$; subgroup - similarity transformation - class of group - Point group - Assignment of point group of simple molecules. Matrix-introduction - matrix representation of the symmetry operations - identity (E), Proper axis of rotation (Cn), Vertical reflection (σv), Improper axis of rotation (Sn) and Inverse (i). Representation definition - reducible and irreducible representation of a group - block factorization. The great orthogonality theorem (GOT) - rules for writing (properties of) irreducible representations - Projection operator (definition only) - character table definition - construction of character table $C_2V$ and $C_3V$

**UNIT II** 15 Hours

**Group Theory II (Applications of Group Theory):** Prediction of symmetry of atomic orbitals - linear vector, rotation vector - symmetries of tensor like properties (α& g); Prediction of orbitals and hybridization in $BF_3$ and $CH_4$ molecules; Normal mode analysis - $H_2O$ and $NH_3$; Direct product representation and its applications - identification of IR and Raman active vibration of $H_2O$ and $N_2F_2$ - selection rules to predict allowed and forbidden electronic transition in UV-Visible spectra for example formaldehyde (HCHO); HMO energy calculation for ethylene and butadiene.

**UNIT III** 15 Hours

**Spectroscopy – II:** Electronic spectra of diatomic molecules - molecular quantum numbers - dissociation energy calculations - Birge-sponer extrapolation technique - pre-dissociation spectra - charge transfer spectra - Fortrat diagram - electronic spectra of molecules absorbance oscillator strength. Photoelectron spectroscopy (PES) - basic principles, spectrum, X-ray PES, (ESCA) - vibrational structure - PES of argon, oxygen and nitrogen.

**UNIT IV** 15 Hours

**Spectroscopy – III:** ESR spectroscopy - principle, g-factor, experimental method, spectrum, fine and hyperfine structures and applications (H-atom, CH3 radical, p-1,4 benzosemiquinone radical anion, naphthalene anion, Tempol). NQR spectroscopy - quadrupole movement, coupling constant, quadrupole transition-electric field gradient and molecular structure ($_7N^{14}$, $_5B^{11}$, $_{17}Cl^{36}$). Mossbauer spectroscopy - recoilless emission and resonance absorbtion, experimental method, isomeric shift and electric quadrupole splitting in $Fe^{57}$.

**UNIT V** 15 Hours

**Chemistry Of Nanoscience and Technology**: Introduction- Types of nano materials-Nanoparticles, nanotubes-Carbon nanotubes: SWCNT and MWCNT, nanowires, nanoribbons, nanorods, nano composites. Preparation methods-Chemical vapour deposition, Sol-Gel method, Electro deposition method, Ball milling method, Chemical reduction method, spin coating technique, Solvothernal synthesis, Colloidal method, Co-precipitation method, Flame spray synthesis (Arc Plasma)-Preparation of metal oxide nanoparticles. Characterization Techniques like SEM, TEM, AFM, XRD, UV-DRS, B.E.T analysis, DLS, PL -Applications of Nanoparticles.

**Text Books**


Cotton F. A., ***Chemical applications of group theory***, wiley Eastern Ltd., UK, 1971, 3rd Edition

Ramakrishnan. V. & Gopinathan M.S., ***Group theory in chemistry***, Vishal Publication, New Delhi, India, 1988.

Veera Reddy, K. ***Symmetry and spectroscopy of molecules***, Newage International (P) Ltd.,

Lehniger A. L. ***Principles of BioChemistry***, 1998 4th Edition.


**Reference Books**


G.M. Barrow, ***Introduction to molecular spectroscopy,*** McGraw-Hill, Newyork.

Banwell G.M., ***Fundamentals of molecular spectroscopy***, TMH company Ltd, 4th Edition.

Chang R., ***Basic principles of spectroscopy***, McGraw-Hill, 1971.

Straughan B.P., Walker S., ***Spectroscopy Vol. 1, 2, 3,*** Chapman and Hall, 1976.

Drago R.S., ***Physical methods in chemistry***, Saunder college publishing, 1999.

Raymond Chang, ***Physical Chemistry with application to biochemical system***, Mc Millan Publishing Company. Inc., New Delhi, 2002.

Graham L Patrick, ***An Introduction to Medicinal Chemistry***, Oxford University Press.

**Pedagogy**

Chalk & Talk, E-Resources, Group Discussion

**Teaching aids**

Black Board, LCD Projector

**Course Contents and Lecture Schedule**

| Module No. | Topic | No. of Lectures | Content Delivery Methods |
|---|---|---|---|
| | **UNIT – I** | | |
| 1.1 | Introduction - Symmetry elements and symmetry operations - Definition of mathematical group - four cardinal properties of a group - closure, associative, idendity and inverse rule. | 3 | Chalk & Talk |
| 1.2 | Cyclic group Abelian group ($H_2O$ only) and non-abelian group (NH3 only) - Group multiplication table- $C_2v$ and $C_3v$; subgroup - similarity transformation - class of group. | 3 | E-Resources |
| 1.3 | Point group - Assignment of point group of simple molecules. Matrix-introduction - matrix representation of the symmetry operations - idendity (E), Proper axis of rotation (Cn), Vertical reflection (σv), Improper axis of rotation (Sn) and Inverse (i). | 3 | Discussion |
| 1.4 | Representation definition - reducible and irreducible representation of a group - block factorization. The great orthogonality theorem (GOT) - rules for writing (properties of) irreducible representations. | 3 | E-Resources |
| 1.5 | Projection operator (definition only) - character table definition - construction of character table $C_2V$ and $C_3V$. | 3 | Discussion |
| | **UNIT – II** | | |
| 2.1 | Prediction of symmetry of atomic orbitals - linear vector, rotation vector - symmetries of tensor like properties (α & g). | 3 | Discussion |
| 2.2 | Prediction of orbitals and hybridization in $BF_3$ and $CH_4$ molecules; Normal mode analysis - $H_2O$ and $NH_3$ | 3 | Chalk & Talk |

| | | | |
|---|---|---|---|
| 2.3 | Direct product representation and its applications - identification of IR and Raman active vibration of $H_2O$ and $N_2F_2$. | 3 | E-Resources |
| 2.4 | Selection rules to predict allowed and forbidden electronic transition in UV-Visible spectra for example formaldehyde (HCHO). | 3 | E-Resources |
| 2.5 | HMO energy calculation for ethylene and butadiene | 3 | E-Resources |
| **UNIT – III** | | | |
| 3.1 | Electronic spectra of diatomic molecules - molecular quantum numbers. | 3 | E-Resources |
| 3.2 | Dissociation energy calculations - Birge-sponer extrapolation technique - | 3 | Chalk & Talk |
| 3.3 | Pre-dissociation spectra - charge transfer spectra - Fortrat diagram. | 3 | Discussion |
| 3.4 | electronic spectra of molecules absorbance oscillator strength Photoelectron spectroscopy (PES) - basic principles, spectrum, X-ray PES, (ESCA) - | 3 | E-Resources |
| 3.5 | vibrational structure - PES of argon, oxygen and nitrogen. | 3 | Discussion |
| **UNIT – IV** | | | |
| 4.1 | ESR spectroscopy - principle, g-factor, experimental method, spectrum, fine and hyperfine structures and applications (H-atom, $CH_3$ radical | 3 | Discussion |
| 4.2 | p-1,4 benzosemiquinone radical anion, naphthalene anion, Tempol). NQR spectroscopy | 3 | E-Resources |
| 4.3 | Quadrupole movement, coupling constant, quadrupole transition-electric field gradient and molecular structure ($_7N^{14}$, $_5B^{11}$, $_{17}Cl^{36}$). | 3 | Chalk & Talk |
| 4.4 | Mossbauer spectroscopy - recoilless emission and resonance absorption. | 3 | E-Resources |
| 4.5 | Experimental method, isomeric shift and electric quadrupole splitting in $Fe^{57}$. | 3 | Chalk & Talk |
| **UNIT – V** | | | |
| 5.1 | Introduction- Types of nano materials-Nanoparticles, nanotubes-Carbon nanotubes: SWCNT and MWCNT, nanowires. | 3 | E-Resources |

| | | | |
|---|---|---|---|
| 5.2 | Nanoribbons, nanorods, nano composites. Preparation methods-Chemical vapour deposition | 3 | Chalk & Talk |
| 5.3 | Sol-Gel method, Electrodeposition method, Ball milling method, Chemical reduction method, spin coating technique, Solvothernal synthesis, Colloidal method, Co-precipitation method, Flame spray synthesis (Arc Plasma). | 3 | Discussion |
| 5.4 | Preparation of metal oxide nanoparticles. Characterization Techniques like SEM, TEM, AFM. | 3 | E-Resources |
| 5.5 | XRD, UV-DRS, B.E.T analysis, DLS, PL - Applications of Nanoparticles. | 3 | Discussion |
| | **Total** | **75** | |

**Course Designer**

**Ms. A. Mumthaj**

Assistant Professor of Chemistry

| Course Code | Course Title | Category | Total Hours | Credits |
|---|---|---|---|---|
| 20PCHC3P | Inorganic Chemistry Practical | Core -XII | 150 | 5 |

| Nature of Course | |
|---|---|
| Knowledge Oriented | ✓ |
| Skill Oriented | ✓ |
| Employability Oriented | |
| Entrepreneurship Oriented | |

| Course Relevance | |
|---|---|
| Local | |
| Regional | |
| National | |
| Global | ✓ |

**Preamble**

This lab course enables the students to acquire laboratory skill on quantitative estimation of inorganic metal ions and qualitative analysis of inorganic cations present in the mixture of salts.

**Course Outcomes (CO)**

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

| No. | Course Outcome | Knowledge Level |
|---|---|---|
| CO1 | Estimate the amount of metal ions such as like Zinc, Magnesium and Copper present in the given solution by EDTA volumetric method. | K1,K2,K3,K4,K5 |
| CO2 | Calculate the amount of Nickel ions present in the given solution by direct and indirect EDTA volumetric methods. | K1,K2,K3,K4,K5 |
| CO3 | Analyse the familiar cations present in the given mixture of salts. | K1,K2,K3,K4 |
| CO4 | Analyse the less familiar cations present in the given salt mixture | K1,K2,K3,K4 |
| CO5 | Acquire the laboratory skill of quantitative as well as qualitative analysis of metal ions. | K1,K2,K3,K4,K5 |

**K1-Knowledge K2-Understand K3-Apply K4- Analyse K5- Evaluate**

**Mapping of CO with PO**

| | PO1 | PO2 | PO3 | PO4 | PO5 |
|---|---|---|---|---|---|
| CO1 | 3 | 3 | 3 | 3 | 3 |
| CO2 | 3 | 3 | 3 | 3 | 3 |
| CO3 | 2 | 3 | 3 | 3 | 3 |
| CO4 | 2 | 3 | 3 | 3 | 3 |
| CO5 | 3 | 3 | 3 | 3 | 2 |

**1-Low 2-Medium 3-Strong**

**Mapping of CO with PSO**

| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|---|---|---|---|---|---|
| **CO1** | **3** | **3** | **3** | **2** | **3** |
| **CO2** | **3** | **3** | **3** | **2** | **3** |
| **CO3** | **2** | **3** | **3** | **2** | **3** |
| **CO4** | **2** | **3** | **3** | **2** | **3** |
| **CO5** | **3** | **3** | **3** | **3** | **2** |

**1-Low** **2-Medium** **3-Strong**

**Syllabus**

I. COMPLEXOMETRIC TITRATIONS WITH EDTA

1. Estimation of ZINC
2. Estimation of MAGNESIUM
3. Estimation of COPPER
4. Estimation of NICKEL a) By Direct Method b) By Indirect Method

II. SEMI MICRO ANALYSIS

Semi micro analysis of samples containing two Familiar Cations and two Less Familiar Cations. – Maximum of Five samples.

**Reference Books**

J Mendham, RC Denney, JD Barnes, MJK Thomas, ***Vogel's A Text Book of Quantitative Chemical Analysis***, Pearson Education in South Asia, Panchsheel Park, New Delhi, 2008, Sixth Edition.

**Course Designer**

**Ms. A. Nihath Nazleen**
Assistant Professor of Chemistry

| Course Code | Course Title | Category | Total Hours | Credits |
|---|---|---|---|---|
| 20PCHC41 | Organic Chemistry- IV | Core -XIII | 75 | 4 |

| Nature of Course | |
|---|---|
| Knowledge Oriented | ✓ |
| Skill Oriented | ✓ |
| Employability Oriented | |
| Entrepreneurship Oriented | |

| Course Relevance | |
|---|---|
| Local | |
| Regional | |
| National | |
| Global | ✓ |

**Preamble**

The course explains the of heterocyclic compounds, terpenoids, alkaloids and antibiotics. It gives in-depth knowledge on the retro and asymmetric synthesis and molecular rearrangement reactions.

**Course Outcomes (CO)**

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

| No. | Course Outcome | Knowledge Level |
|---|---|---|
| **CO1** | Outline the chemistry of nitrogen and oxygen containing heterocyclic compounds and natural products. | **K1,K2** |
| **CO2** | Apply their knowledge on isolation, biological activity and structural studies of selective terpenoids and alkaloids. | **K1,K2,K3** |
| **CO3** | Outline synthetic route for complex organic molecules which find medicinal, industries of commercial importance. | **K1,K2** |
| **CO4** | Evaluate various methods to synthesize optically active compounds | **K1,K2,K3,K4,K5** |
| **CO5** | Apply their knowledge in writing the mechanism of molecular rearrangement reaction. | **K1,K2,K3** |

**K1-Knowledge K2-Understand K3-Apply K4- Analyse K5- Evaluate**

**Mapping of CO with PO**

| | PO1 | PO2 | PO3 | PO4 | PO5 |
|---|---|---|---|---|---|
| **CO1** | **3** | **3** | **1** | **2** | **2** |
| **CO2** | **3** | **3** | **3** | **3** | **3** |
| **CO3** | **3** | **3** | **3** | **3** | **3** |
| **CO4** | **3** | **2** | **3** | **3** | **3** |
| **CO5** | **3** | **1** | **2** | **1** | **3** |

**1-Low 2-Medium 3-Strong**

**Mapping of CO with PSO**

| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|---|---|---|---|---|---|
| CO1 | 3 | 3 | 1 | 2 | 3 |
| CO2 | 3 | 3 | 3 | 3 | 3 |
| CO3 | 3 | 2 | 2 | 3 | 3 |
| CO4 | 3 | 2 | 2 | 3 | 3 |
| CO5 | 3 | 3 | 3 | 1 | 3 |

**1-Low** **2-Medium** **3-Strong**

**Syllabus**

**UNIT I** 15 Hours

**Chemistry of Heterocyclic Compounds:** Heterocyclics – Nomenclature – Compounds containing two hetero atoms: Synthesis and reactivity of pyrazole, imidazole, oxazole, thiazole. diazines: the chemistry of pyridazine, pyrimidine and pyrazine – Comparison of basicity of diazines. Introduction to anthrocyanins and flavonoids.

**UNIT II** 15 Hours

**Chemistry of Terpenoids and Alkaloids:** Chemistry of terpenoids: General methods of determining structure of terpenoids – αpinene, Zingiberene, and Abietic acid. Chemistry of alkaloids: General methods of determining structure of alkaloids – Structure elucidation of (i) Morphine (ii) Reserpine. Antibiotics: Definition, Structural elucidation of penicillin, chloramphenicol.

**UNIT III** 15 Hours

**Advanced Organic Synthesis-I (Retro-synthesis)**: Disconnection Approach - Importance of organic synthesis-Planning synthesis – Synthons and types – synthetic equivalents – latent functionality Guideliness for best disconnection approach, Reactions involving functional group interconversions – Reterosynthetic analysis – concept of umpolung – two group C-X disconnections and synthetic strategies 1,2-, 1,3-, 1,4-, 1,5- and 1,6- difunctionalised disconnection. Steroselective and stereospecific reactions-Chemoselectivity–Stereoselectivity- Regioselectivity.

**UNIT IV** 15 Hours

**Advanced Organic Synthesis II (Asymmetric synthesis):** Definition of enantiomeric, disatereomeric excess – analytical methods to determine ee and de – strategy and classification of methods of asymmetric synthesis – Chiral substrates – Chiral auxiliaries – Chiral reagents – Chiral catalysts. Chiral catalysts and chiral reagents: BINAP-ruthenium (II) Mc Murray_s reagent – $Ti(i\text{-}PrO)_4$, and $K_2OS_2(OH)_4$ – Sharpless asymmetric epoxidation, – Heck reactions – Suzuki Coupling – Sonogashira coupling.

**UNIT V** 15 Hours

**Molecular Rearrangements:** Classification – Nucleophilic, electrophilic, and radical – Mechanism of Favorski, BenzilBenzilic acid, Bayer-Villiger, Wagner-Meerwin rearrangement, Carbanionic rearrangements, Stevan_s rearrangement, Sommelet-Hauser, Cope, and Wesly-Moser rearrangement, Fries Rearrangement. Acid catalyzed rearrangement – Arndt-Eistert synthesis – carbon to nitrogen migration – Hofmann rearrangement, Curtius rearrangement, Lossen rearrangement, Schmidt and Beckmann rearrangement.

**Text Books**


Jerry March, ***Advanced Organic Chemistry, Reaction mechanism and structure***, John Wiley and sons, New York, 1992, 4th Edition.

S. Warren, ***Organic synthesis - The disconnection approach***, John Wiley & Sons, UK, 2004.

Cary and Sundberg, ***Advanced Organic Chemistry, Part B, Reactions and Synthesis***, Plenum Press, 1990, 3rd Edition.

R. K. Mackei and D. M. Smith, ***Guide Book to Organic synthesis***, ELBS, 1982.

I.L. Finar, ***Organic Chemistry, Vol. II,*** ELBS, New York, 2005, 5th Edition.

W. Caruthers, Some ***Modern methods of organic synthesis***, Cambridge University.

C.H. Depuy and O.L. Chapman, ***Molecular reactions and Photo Chemistry***, Tata MacGraw Hill, 1975, Eastern and Economic Edition.


**Reference Books**


Graham Solomons, ***Organic Chemistry***, John Wiley and Sons INC, 1992, 5th Edition. Michael B. Smith, ***Organic Synthesis***, McGraw Hill, 1994, International Edition.

Clayden, Greeve, Warren and Wothers, ***Organic Chemistry***, OXFORD University Press, 2007.

A.J. Bellamy, ***An introduction to conservation of orbital symmetry***, Longman group Limited, 1974.

H. O. House, ***Modern synthetic reactions***, Cambridge University press, 1972, 3rd Edition.

W. Carruthers and I. Coldham, ***Modern methods of organic synthesis***, Cambridge University Press, 2004, 4th Edition.


**Pedagogy**

Chalk & Talk, E-Resources, Group Discussion

**Teaching aids**

Black Board, LCD Projector

**Course Contents and Lecture Schedule**

| Module No. | Topic | No. of Lectures | Content Delivery Methods |
|---|---|---|---|
| **UNIT – I** | | | |
| 1.1 | Heterocyclics – Nomenclature - Compounds containing two hetero atoms: Synthesis and reactivity of pyrazole, imidazole, oxazole, isoxazole, thiazole, isothiazole. | 7 | Chalk & Talk |
| 1.2 | Diazines: the chemistry of pyridazine, pyrimidine and pyrazine – Comparison of basicity of diazines - Chemistry of anthrocyanins and flavonoids. | 8 | E-Resources |
| **UNIT – II** | | | |
| 2.1 | Chemistry of terpenoids: General methods of determining structure of terpenoids – α-pinene, α-cadinene, Zingiberene, Abietic acid and Heliangine. | 8 | Discussion |
| 2.2 | Chemistry of alkaloids: Alkaloids and Drugs: General methods of determining structure of alkaloids – Structure elucidation of (i) Morphine (ii) Reserpine (iii) Lysergic acid. | 7 | Chalk & Talk |
| **UNIT – III** | | | |
| 3.1 | Disconnection Approach: Importance of organic synthesisPlanning synthesis, Synthons and types – synthetic equivalents – latent functionality - Guideliness for best disconnection approach. | 4 | E-Resources |
| 3.2 | Reactions involving functional group interconversions – Reterosynthetic analysis, concept of umpolung. | 4 | Chalk & Talk |
| 3.3 | Two group C-X disconnections and synthetic strategies 1,2-, 1,3-, 1,4-, 1,5- and 1,6- difunctionalised disconnection | 4 | Discussion |

| | | | |
|---|---|---|---|
| 3.4 | Steroselective and stereospecific reactions – Chemoselectivity – Stereoselectivity - Regioselectivity. | 3 | E-Resources |
| **UNIT – IV** | | | |
| 4.1 | Asymmetric synthesis: Definition of enantiomeric, disatereomeric excess – analytical methods to determine ee and de – strategy | 5 | Discussion |
| 4.2 | Classification of methods of asymmetric synthesis – chiral substrates – Chiral auxiliaries – chiral reagents – chiral catalysts | 5 | E-Resources |
| 4.3 | Chiral catalysts and chiral reagents: BINAP-ruthenium (II) Mc Murray`s reagent – $Ti(i\text{-}PrO)_4$, and $K_2Os_2(OH)_4$ – Sharpless asymmetric epoxidation, – Heck reactions – Suzuki Coupling – Sonogashira coupling. | 5 | Chalk & Talk |
| **UNIT – V** | | | |
| 5.1 | Classification – Nucleophilic, electrophilic, and radical – Mechanism of Favorski, Benzil-Benzilic acid, Bayer-Villiger, Wagner-Meerwin rearrangement | 5 | E-Resources |
| 5.2 | Carbanionic rearrangements, Stevan_s rearrangement, Sommelet-Hauser, Cope, and Wesly-Moser rearrangement, Fries Rearrangement. | 5 | Chalk & Talk |
| 5.3 | Acid catalyzed rearrangement – Arndt-Eistert synthesis – carbon to nitrogen migration – Hofmann rearrangement, Curtius rearrangement, Lossen rearrangement, Schmidt and Beckmann rearrangement. | 5 | Discussion |
| | **Total** | **75** | |

**Course Designer**
**Mr. G. Arivalagan**
Assistant Professor of Chemistry

| Course Code | Course Title | Category | Total Hours | Credits |
|---|---|---|---|---|
| 20PCHC42 | Inorganic Chemistry- IV | Core -XIV | 75 | 4 |

| Nature of Course | |
|---|---|
| Knowledge Oriented | ✓ |
| Skill Oriented | |
| Employability Oriented | |
| Entrepreneurship Oriented | |

| Course Relevance | |
|---|---|
| Local | |
| Regional | |
| National | |
| Global | ✓ |

**Preamble**

The course explains the synthesis, structure and reactivity of organometallic compounds and their catalytic applications, role of metal ion in biological systems and physical features of biochemistry.

**Course Outcomes (CO)**

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

| No. | Course Outcome | Knowledge Level |
|---|---|---|
| **CO1** | Define the terms EAN, 18, 16-electron rule classify the organometallic compounds, structure and properties of organometallic compounds such as metallocenes, alkenes, alkynes and arene complexes. | **K1, K2** |
| **CO2** | Discover and evaluate the synthesis, structure and reactivity of organometallic compounds. | **K1, K2,K3,K4, K5** |
| **CO3** | Explain the structures and work functions of iron sulphur proteins, blue copper proteins and cytochrome. | **K1,K2, K3** |
| **CO4** | Classify the Carboxypeptidase A, carbonic anhydrase, elements in biological systems and metals used for diagnosis. | **K1,K2, K4** |
| **CO5** | Develop their knowledge in physical features of biochemistry. | **K1, K2,K3** |

**K1-Knowledge K2-Understand K3-Apply K4- Analyse K5- Evaluate**

**Mapping of CO with PO**

| | PO1 | PO2 | PO3 | PO4 | PO5 |
|---|---|---|---|---|---|
| **CO1** | **3** | **2** | **3** | **3** | **3** |
| **CO2** | **3** | **2** | **3** | **3** | **3** |
| **CO3** | **2** | **3** | **2** | **3** | **2** |
| **CO4** | **2** | **3** | **2** | **3** | **2** |
| **CO5** | **2** | **3** | **1** | **2** | **1** |

**1-Low 2-Medium 3-Strong**

**Mapping of CO with PSO**

| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|---|---|---|---|---|---|
| CO1 | 3 | 3 | 2 | 2 | 3 |
| CO2 | 3 | 3 | 3 | 3 | 2 |
| CO3 | 2 | 3 | 2 | 3 | 3 |
| CO4 | 2 | 2 | 2 | 2 | 2 |
| CO5 | 2 | 1 | 2 | 2 | 2 |

**1-Low** **2-Medium** **3-Strong**

**Syllabus**

**UNIT I** 15 Hours

**Organometallic Chemistry – I:** Stability of organo metallic compounds- β hydrogen elimination- the sixteen and eighteen electron rule. Synthesis – structure and bonding in metal carbonyls – isoelectronic and isolobal analogy- use of IR in the structural elucidation of carbonyl compounds– metal nitrosyls – dinitrogen complexes. π donors-Carboxylic ligands and complexes. Synthesis structure bonding and reactivity of carbenes, carbines, metallocenes and other aromatic cyclopolyenes – Ferrocene – bonding and structure – sigma, pi and hapto nomenclature. Arene complexes – olefin – acetylene and pi allyl complexes.

**UNIT II** 15 Hours

**Organometallic Chemistry – II:** Catalysis involving organometallic compounds –properties of metals and ligands in homogeneous catalysis – oxidative addition and reductive elimination – hydrogen abstraction – activation of small molecules by complexation-agnostic interaction-insertionalkyl migration-insertion and elimination-catalytic reactions-hydrogenation of olefins – Wilkinson‘s catalyst – hydroformylation –syn-gas-water gas shift reactions- oxidation of olefins – Wacker process – propylene polymerization - Olefin metathesis -Ziegler natta catalyst -cyclo oligomerisation of acetylene , butadiene- Reppe‘s catalyst . Mansanto‘s acetic acid synthesis-Fischer-Tropsch‘s synthesis of Synthetic gasoline.

**UNIT III** 15 Hours

**Bioinorganic chemistry I:** Porphyrin ring system – metalloporphyrins – synthetic oxygen carriers –cytochromes – structures and work functions in respiration –iron-sulphur proteins (non-heme iron protein) – Copper containing proteins – classification – blue copper proteins – structure of blue copper electron transferases – copper proteins as oxidases – cytochrome C oxidase – mechanistic studies of C oxidase – Hemocyanin.

**UNIT IV** 15 Hours

**Bioinorganic chemistry II:** Carboxypeptidase A: structure, function – carbonic anhydrase: structure, function – inhibition and poisoning –in-vivo and in-vitro nitrogen fixation – essential and trace elements in biological systems –toxic effects of heavy metals (Pb, Cd, Hg and As) and detoxification – metals used for diagnosis- molecular mechanism of ion transport across the membrane – sodium and potassium ions pumps – chelate therapy – cis-platin.

**UNIT V** 15 Hours

**Physico-Chemical Principles and Biological Reactions:** Studies on biochemical equilibria: Buffer system of intracellular fluids – $H_2CO_3/HCO_3^-$, $HPO_4^{2-}/ H_2PO_4^-$- Application of Henderson-Hasselbach equation; Ion channels – membrane andstatic potentials - Role of $Na^+/K^+$ ions in neural communications $-Na^+/K^+$ ion pump; allosterismand oxygen saturation curves for hameoglobin and myoglobin – derivation of Hill equation.

## Text Books


Cotton F.A. and Wilkinson, G. ***Advanced Inorganic Chemistry***, Wiley-Interscience publications, John Wiley & Sons, New York, 1998, V Edition.

Wahid U. Malik, G.D. Tuli and R. D. Madan, ***Selected Topics in Inorganic Chemistry***, S. Chand & Co. Ltd., New Delhi, 2006.

Nakamoto, Kazuo, Paul J. McCarthy, ***Spectroscopy and Structure of Metal Chelate Compounds***, John Wiley and Sons. Inc., New York, 1986, IV edition.

Drago, R. S. Van Nostrand and Reinhold, ***Physical Methods in Chemistry***, 1976.

Purcell K.F. and Kotz J.C., ***Inorganic chemistry***, Holt Saunders, Philadelphia, 1977.


## Reference Books


Huheey, J. E., Ellen A. Keiter, Richard L. Keiter, **Inorganic chemistry**, pearson Education (Singapore) (P) Ltd., Delhi, 2004, IV Edition.

Wahid U. Malik, G.D. Tuli and R. D. Madan, **Selected Topics in Inorganic Chemistry**, S. Chand & Co.Ltd., New Delhi, 2006.

A.G. Sharpe, **Inorganic Chemistry**, Addition – Weskey Longman, UK, 2004, III Edition.

Gary L. Miessler and Donald A. Tarr, **Inorganic Chemistry**, Pearson Education, Inc., New Delhi, 2004, III Edition.

D. F. Shriver and P.W. Atkins, **Inorganic Chemistry**, Oxford University Press, London, 1999.

K. Hussain Reddy, **Bioinorganic Chemistry**, New Age International (P) Ltd., Delhi, 2005.

William W. Porterfield, **Inorganic Chemistry**, Elsevier, New Delhi, 2005, II Edition.

**Pedagogy**

Chalk & Talk, E-Resources, Group Discussion

**Teaching aids**

Black Board, LCD Projector

**Course Contents and Lecture Schedule**

| Module No. | Topic | No. of Lectures | Content Delivery Methods |
|---|---|---|---|
| | **UNIT – I** | | |
| 1.1 | Stability of organo metallic compounds- β hydrogen elimination. | 2 | Chalk & Talk |
| 1.2 | Synthesis – structure and bonding in metal carbonyls – isoelectronic and isolobal analogy. Sixteen and eighteen electron rule. | 3 | E-Resources |
| 1.3 | Use of IR in the structural elucidation of carbonyl compounds. Metal nitrosyls – dinitrogen complexes. π donors. | 4 | Discussion |
| 1.4 | Synthesis structure bonding and reactivity of carbenes, carbines, metallocenes and other aromatic cyclopolyenes | 3 | E-Resources |
| 1.5 | Ferrocene – bonding and structure – sigma, pi and hapto nomenclature. Arene complexes – olefin – acetylene and pi allyl complexes. | 3 | E-Resources |
| | **UNIT – II** | | |
| 2.1 | Catalysis involving organometallic compounds – properties of metals and ligands in homogeneous catalysis. | 3 | E-Resources |
| 2.2 | Oxidative addition and reductive elimination – hydrogen. Abstraction. Activation of small molecules by complexation-agnostic interaction, Insertion-alkyl migration-insertion and eliminationcatalytic reactions. | 3 | Discussion |
| 2.3 | Hydrogenation of olefins – Wilkinson‘s catalyst – hydroformylation –syn-gas water gas shift reactionsoxidation of olefins – Wacker process. | 3 | Chalk & Talk |
| 2.4 | Propylene polymerization – Olefin metathesis - Ziegler natta catalyst -cyclo oligomerisation of acetylene , butadiene. | 3 | Chalk & Talk |

| | | | |
|---|---|---|---|
| 2.5 | Reppe‘s catalyst. Mansanto‘s acetic acid synthesis, Fischer- Troppe‘s synthesis of Synthetic gasoline. | 3 | E-Resources |
| **UNIT – III** | | | |
| 3.1 | Porphyrin ring system metalloporphyrins –synthetic oxygen carriers –cytochromes. | 4 | E-Resources |
| 3.2 | Structures and work functions in respiration –iron-sulphur Proteins (non-heme iron protein)-Copper containing proteins – classification. | 5 | Chalk & Talk |
| 3.3 | Blue copper proteins-Structure of blue copper electron transferases – copper proteins as oxidases –cytochrome C oxidase – mechanistic studies of C oxidase – Hemocyanin. | 6 | Discussion |
| **UNIT – IV** | | | |
| 4.1 | Carboxypeptidase A: structure, function – carbonic anhydrase – inhibition and poisoning. | 3 | Discussion |
| 4.2 | In-vivo and in-vitro nitrogen fixation – essential and trace elements in biological systems - metals used for diagnosis. | 5 | E-Resources |
| 4.3 | Metal ion toxicity and detoxification – molecular mechanism of ion transport across the membrane. | 4 | Chalk & Talk |
| 4.4 | Sodium and potassium ions pumps chelate therapy – cisplatin. | 3 | E-Resources |
| **UNIT –V** | | | |
| 5.1 | Studies on biochemical equilibria: Buffer system of intracellular fluids $H_2CO_3/HCO_3^-$, $HPO_4^{2-}/ H_2PO_4^-$. | 6 | Chalk & Talk |
| 5.2 | Application of Henderson - Hasselbach equation; Ion channels – membrane and static potentials - Role of $Na^+/K^+$ ions in neural communications –$Na^+/K^+$ ion pump. | 5 | E-Resources |
| 5.3 | Allosterism and oxygen saturation curves for hameoglobin and myoglobin – derivation of Hill equation. | 4 | Discussion |
| | **Total** | **75** | |

**Course Designer**
**Ms. A. Nihath Nazleen**
Assistant Professor of Chemistry

| Course Code | Course Title | Category | Total Hours | Credits |
|---|---|---|---|---|
| 20PCHC43 | Physical Chemistry-IV | Core -XV | 75 | 5 |

| Nature of Course | |
|---|---|
| Knowledge Oriented | ✓ |
| Skill Oriented | |
| Employability Oriented | |
| Entrepreneurship Oriented | |

| Course Relevance | |
|---|---|
| Local | |
| Regional | |
| National | |
| Global | ✓ |

**Preamble**

The course enables the students to gain knowledge on theories and concepts of chemical kinetics, photochemistry, Radiation chemistry, surface chemistry and biophysical chemistry.

**Course Outcomes (CO)**

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

| No. | Course Outcome | Knowledge Level |
|---|---|---|
| **CO1** | Understand the fundamental concepts on kinetics and reaction rate. | **K1,K2** |
| **CO2** | Develop knowledge on various theories of chemical kinetics. | **K1,K2,K3** |
| **CO3** | Analyze the physical concepts of Photochemistry and Radiation chemistry. | **K1,K2,K3,K4** |
| **CO4** | Make use of the kinetics and theories of surface chemistry. | **K1,K2,K3** |
| **CO5** | Explain the concepts of biophysical chemistry. | **K1,K2,K3,K4,K5** |

**K1-Knowledge K2-Understand K3-Apply K4- Analyse K5- Evaluate**

**Mapping of CO with PO**

| | PO1 | PO2 | PO3 | PO4 | PO5 |
|---|---|---|---|---|---|
| **CO1** | **3** | **2** | **3** | **3** | **3** |
| **CO2** | **3** | **1** | **3** | **3** | **3** |
| **CO3** | **3** | **2** | **3** | **3** | **2** |
| **CO4** | **3** | **1** | **3** | **3** | **3** |
| **CO5** | **2** | **3** | **2** | **3** | **1** |

**1-Low 2-Medium 3-Strong**

**Mapping of CO with PSO**

| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|---|---|---|---|---|---|
| CO1 | 3 | 3 | 3 | 3 | 3 |
| CO2 | 3 | 3 | 3 | 3 | 3 |
| CO3 | 3 | 2 | 2 | 2 | 2 |
| CO4 | 3 | 3 | 3 | 2 | 3 |
| CO5 | 2 | 1 | 2 | 3 | 1 |

**1-Low** **2-Medium** **3-Strong**

**Syllabus**

**UNIT I** 15 Hours

**Chemical Kinetics – I**: Simple Collision theory- modification - Absolute reaction rate theory (ARRT) - Statistical and thermodynamics formulation - Comparison of ARRT with collision theory - Significance of entropy of activation- Relation between ΔH and Ea- Transmission coefficient; ARRT of termolecular reactions – Unimolecular reactions - Lindemann, Hinshelwood, RRKM and Slater treatments – solution kinetics – ARRT of reaction in solution – Influence of ionic strength on the rates of ionic reactions (salt effects).

**UNIT II** 15 Hours

**Chemical Kinetics – II:** Fast reactions-flow and relaxation techniques, Temperature Jump and pressure jump method - complex reactions – opposing, consecutive and parallel reactions; Chain reaction – kinetics and general characteristic – $H_2$-$Br_2$ reaction, Rice – Herzfeld mechanism for decomposition of acetaldehyde & ethane – Branched chain reaction – study of $H_2$-$O_2$ explosive reaction - homogeneous catalysis – acid, base catalysis.

**UNIT III** 15 Hours

**Photochemistry:** Photo physical processes in electronically excited molecules - Fluorescence, Phosphorescence and other deactivating processes. Stern-Volmer equation and its applications- electronically energy transfer mechanisms –photosensitization and chemiluminescence. Experimental techniques in photochemistry - light sourceschemical actinometry.

**Radiation chemistry:** Source of high energy - Interaction of high energy radiation with matterRadiolysis of water - definition of G value - mode of reactions of hydrated electrons$OH^-$ and $H^+$. Experimental techniques of radiation chemistry - Dosimetry.

**UNIT IV** 15 Hours

**Surface Chemistry:** Physisorption and Chemisorption – adsorption isotherm – derivation of Langmuir and Freundlich, derivation of B.E.T equation of multilayer adsorption – application of BET equation to surface area determination, derivation of Gibbs adsorption isotherm. Heterogeneous catalysis and their kinetics – chemical reactions on solid surfaces - Mechanism & Kinetics of unimolecular and bimolecular surface reactions – Langmuir – Hinshelwood, Langmuir –Ridel mechanism, ARRT of surface reactions; Basic concepts of Micelles and Reverse Micelles.

**UNIT V** 15 Hours

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

**Text Books**


Glasstone S., ***Textbook of Physical chemistry***, McMillan, Alasca, 1974, III Edition.

Daniels F., Alberty, R.A., ***Physical Chemistry***, John willey and sons , UK, 1974.

Moore, W.J., ***Physical Chemistry***, Orient Longman, UK, 1972, 5th Edition.

Lehniger A.L., ***Principles of BioChemistry***, 2006, 4th Edition.


**Reference Books**


Laidler K.J., ***Chemical Kinetics***, Tata McGraw Hill, UK, 2005, II Edition.

Frost A.A., Pearson R.G., ***Kinetics and Mechanism***, New York, 1990.

Wilkinson F., ***Chemical Kinetics and Reaction Mechanism***, Var Nostrard ReinholdCo., New York, 2000.

Rohatgi-Mukherjee K.K., ***Fundamentals of Photochemistry***, Wiley Eastern Ltd., New York, 1999, Revised edition.

Adamson A.M., ***Physical Chemistry of Surfaces***, John Willey, UK., 2002, V Edition.

Laider, K.S., ***Chemical kinetics***, TMH, New York, 2005, III Edition.

Raymond Chang, ***Physical Chemistry with application to biochemical system***, Mc Millan Publishing Company. Inc., New Delhi, 2002.

**Pedagogy**

Chalk & Talk, E-Resources, Group Discussion

**Teaching aids**

Black Board, LCD Projector

**Course Contents and Lecture Schedule**

| Module No. | Topic | No. of Lectures | Content Delivery Methods |
|---|---|---|---|
| | **UNIT – I** | | |
| 1.1 | Simple Collision theory- modification - Absolute reaction rate theory (ARRT) - Statistical and thermodynamics formulation. | 4 | Chalk & Talk |
| 1.2 | Comparison of ARRT with collision theory - Significance of entropy of activation- Relation between ΔH and Ea- Transmission coefficient. | 4 | E-Resources |
| 1.3 | ARRT of termolecular reactions – Unimolecular reactions - Lindemann, Hinshelwood, RRKM and Slater treatments – solution kinetics. | 4 | Discussion |
| 1.4 | ARRT of reaction in solution – Influence of ionic strength on the rates of ionic reactions (salt effects). | 3 | E-Resources |
| | **UNIT – II** | | |
| 2.1 | Fast reactions-flow and relaxation techniques. | 2 | E-Resources |
| 2.2 | Temperature Jump and pressure jump method - complex reactions – opposing, consecutive and parallel reactions. | 3 | Discussion |
| 2.3 | Chain reaction – kinetics and general characteristic – $H_2$-$Br_2$ reaction, Rice – Herzfeld mechanism for decomposition of acetaldehyde & ethane. | 5 | Chalk & Talk |
| 2.4 | Branched chain reaction – study of $H_2$-$O_2$ explosive reaction - homogeneous catalysis – acid, base catalysis. | 5 | Chalk & Talk |

| | | | |
|---|---|---|---|
| **UNIT – III** | | | |
| 3.1 | Photo physical processes in electronically excited molecules - Fluorescence, Phosphorescence and other deactivating processes. | 3 | E-Resources |
| 3.2 | Stern-Volmer equation and its applications - electronically energy transfer mechanisms –photosensitization and chemiluminescence. | 4 | Chalk & Talk |
| 3.3 | Experimental techniques in photochemistry - light sourceschemical actinometry. | 2 | Discussion |
| 3.4 | Source of high energy - Interaction of high energy radiation with matterRadiolysis of water - definition of G value. | 3 | Chalk & Talk |
| 3.5 | Mode of reactions of hydrated electrons$OH^-$ and $H^+$. Experimental techniques of radiation chemistry - Dosimetry. | 3 | E-Resources |
| **UNIT – IV** | | | |
| 4.1 | Physisorption and Chemisorption – adsorption isotherm – derivation of Langmuir and Freundlich. | 3 | Discussion |
| 4.2 | derivation of B.E.T equation of multilayer adsorption – application of BET equation to surface area determination, derivation of Gibbs adsorption isotherm. | 4 | Chalk & Talk |
| 4.3 | Heterogeneous catalysis and their kinetics – chemical reactions on solid surfaces - Mechanism & Kinetics of unimolecular and bimolecular surface reactions. | 4 | Chalk & Talk |
| 4.4 | Langmuir –Hinshelwood, Langmuir –Ridel mechanism, ARRT of surface reactions; Basic concepts of Micelles and Reverse Micelles. | 4 | E-Resources |

| UNIT –V | | | |
|---|---|---|---|
| 5.1 | Basic concepts of non-equilibrium thermodynamics- Onsager reciprocal relationship- Its application to biological systems. | 3 | Chalk & Talk |
| 5.2 | High energy metabolites- ATP and its role in bioenergetics- transfer of potential and coupled reaction. | 3 | Chalk & Talk |
| 5.3 | Biological energy conversion in catabolism and anabolism- role of singlet oxygen in biology. | 2 | Discussion |
| 5.4 | Biophysical applications of Mossbauer effect- NMR imaging- Applications of spin labeling in membrane research-, mechanism and application - Dendrimer. | 4 | E-Resources |
| 5.5 | Molecular recognition – An introduction to supramolecular chemistry and photochemistry. | 3 | E-Resources |
| | **Total** | **75** | |

**Course Designer**
**Ms. A. Mumthaj**
Assistant Professor of Chemistry

| Course Code | Course Title | Category | Total Hours | Credits |
|---|---|---|---|---|
| 20PCHC4P | Project Viva-Voce | Core -XVI | 150 | 4 |

| Nature of Course | |
|---|---|
| Knowledge Oriented | ✓ |
| Skill Oriented | ✓ |
| Employability Oriented | ✓ |
| Entrepreneurship Oriented | |

| Course Relevance | |
|---|---|
| Local | |
| Regional | |
| National | |
| Global | ✓ |

## Preamble

The research in chemistry requires the knowledge on laboratory synthesis, analysis, analytical data interpretation and able to communicate the scientific results both in oral, written and electronic format to both chemists and non-chemists. This course fulfills the said requirements.

## Course Outcomes (CO)

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

| No. | Course Outcome | Knowledge Level |
|---|---|---|
| **CO1** | Develop skills on preparation of novel materials through new synthetic routes. | **K1, K2** |
| **CO2** | Analyze the materials using various analytical techniques. | **K1, K2,K3** |
| **CO3** | Interpret the analytical data and able to correlate theoretical and experimental results. | **K1, K2,K3,K4** |
| **CO4** | Defend the laboratory scientific results both in oral, written and electronic format to both chemists and non-chemists. | **K1, K2,K3,K4** |
| **CO5** | Discuss research methodologies along with literature survey. | **K1, K2** |

**K1-Knowledge K2-Understand K3-Apply K4- Analyse K5- Evaluate**

## Mapping of CO with PO

| | PO1 | PO2 | PO3 | PO4 | PO5 |
|---|---|---|---|---|---|
| **CO1** | **3** | **2** | **3** | **2** | **3** |
| **CO2** | **3** | **3** | **3** | **2** | **3** |
| **CO3** | **3** | **3** | **3** | **2** | **3** |
| **CO4** | **3** | **2** | **3** | **3** | **3** |
| **CO5** | **3** | **1** | **2** | **3** | **3** |

**1-Low 2-Medium 3-Strong**

**Mapping of CO with PSO**

| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|---|---|---|---|---|---|
| **CO1** | **3** | **3** | **3** | **2** | **1** |
| **CO2** | **3** | **3** | **3** | **2** | **2** |
| **CO3** | **3** | **3** | **2** | **2** | **1** |
| **CO4** | **3** | **2** | **3** | **3** | **2** |
| **CO5** | **3** | **2** | **3** | **1** | **1** |

**1-Low** **2-Medium** **3-Strong**

**Marks**

| | |
|---|---|
| External Examiner: Viva: | 20 |
| External Examiner: Evaluation of Project: | 40 |
| Internal Examiner: Evaluation of Project: | 40 |
| Total: | 100 |

| Course Code | Course Title | Category | Total Hours | Credits |
|---|---|---|---|---|
| 20PCHE41 | Polymer Chemistry | Elective -III | 75 | 4 |

| Nature of Course | |
|---|---|
| Knowledge Oriented | ✓ |
| Skill Oriented | |
| Employability Oriented | ✓ |
| Entrepreneurship Oriented | |

| Course Relevance | |
|---|---|
| Local | |
| Regional | |
| National | |
| Global | ✓ |

**Preamble**

The course enables the students to gain knowledge on types of polymers, polymerization techniques and polymer processing.

**Course Outcomes (CO)**

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

| No. | Course Outcome | Knowledge Level |
|---|---|---|
| **CO1** | Outline the fundamentals of classification of polymers and chemistry of polymerization. | **K1,K2** |
| **CO2** | Develop knowledge on various types of individual polymers. | **K1,K2,K3** |
| **CO3** | Analyze the properties of polymers. | **K1,K2,K3,K4** |
| **CO4** | Make use of the polymerization techniques and degradation of polymers. | **K1,K2,K3** |
| **CO5** | Explain the basics and applications polymer processing. | **K1,K2,K3,K4,K5** |

**K1-Knowledge K2-Understand K3-Apply K4- Analyse K5- Evaluate**

**Mapping of CO with PO**

| | PO1 | PO2 | PO3 | PO4 | PO5 |
|---|---|---|---|---|---|
| **CO1** | **3** | **3** | **2** | **2** | **2** |
| **CO2** | **3** | **3** | **2** | **2** | **2** |
| **CO3** | **3** | **3** | **2** | **1** | **2** |
| **CO4** | **3** | **3** | **3** | **3** | **2** |
| **CO5** | **3** | **3** | **3** | **3** | **2** |

**1-Low 2-Medium 3-Strong**

**Mapping of CO with PSO**

| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|---|---|---|---|---|---|
| CO1 | 3 | 3 | 3 | 3 | 2 |
| CO2 | 2 | 2 | 3 | 3 | 2 |
| CO3 | 2 | 2 | 3 | 3 | 2 |
| CO4 | 2 | 3 | 3 | 3 | 2 |
| CO5 | 3 | 3 | 3 | 3 | 2 |

**1-Low** **2-Medium** **3-Strong**

**Syllabus**

**UNIT I** 15 Hours

**Classification of polymers and chemistry of polymerization:** Classification of polymers - linear polymers, non-linear polymers, branched polymers, cross linked polymers, homo chains, hetero chains, homo polymers, co polymers, block polymers and graft polymers. Chemistry of polymerization - Types of polymerization-mechanism-chain, growth, free radical, ionic, co-ordination, ring opening, metathetical, group transfer, polyaddition and polycondensation polymerizations.

**UNIT II** 15 Hours

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

**UNIT III** 15 Hours

**Properties of polymers:** Configuration of polymer chain-geometrical structure-syndiotatic, isotatic and atatic polymers. Glass transition temperature - Definition-factors affecting glass transition temperature-relationships between glass transition temperature and (a) molecular weight, (b) melting point and (c) plasticizer-importance of glass transition temperature - heat distortion temperature. Molecular weight and size of polymers - Number average, weight average, sedimentation and viscosity average molecular weights-molecular weights and degree of polymerization-poly dispersity-molecular weight distribution in polymers-size of polymer molecules.

**UNIT IV** 15 Hours

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

**UNIT V** 15 Hours

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

## Text Books


B.K. Sharma, ***Polymer Chemistry***, Goel Publishing House, Meerut, 1989.

P.J. Flory, ***Principles of Polymer Chemistry***, Cornell Univ. press, Ithaca, 1953.

F.W. Billmeyer, ***Text Book of Poymer Science***, John Wiley and sons, New York, 1984, 3rd Edition.


## Reference Books


V.R. Gowariker, N.V. Viswanathan, Jayadev Sreedher, ***Polymer Science***, Wiley Eastern Ltd., New Delhi 1986.

G. Odian, ***Principles of Polymerisation***, John Wiley and sons, New York, 1981, 2nd Edition.

D.W. van Krevelen, P.J. Hoftyrager, ***Properties of Polymers***, Elsevier, New York, 1976.

Harry R. Allcock, F. W. Lampe, J.E. Mark, ***Contemporary Polymer Chemistry***, Pearson, Prentice Hall, New Delhi, 2005, 3rd Edition.


## Pedagogy

Chalk & Talk, E-Resources, Group Discussion

## Teaching aids

Black Board, LCD Projector

**Course Contents and Lecture Schedule**

| Module No. | Topic | No. of Lectures | Content Delivery Methods |
|---|---|---|---|
| **UNIT – I** | | | |
| 1.1 | Classification of polymers: linear polymers, non-linear polymers, branched polymers, cross linked polymers. | 4 | Chalk & Talk |
| 1.2 | Homo chains, hetero chains, homo polymers, co polymers, block polymers and graft polymers. | 4 | E-Resources |
| 1.3 | Chemistry of polymerization: Types of polymerization-mechanism-chain,growth, free radical, ionic, co-ordination, ring opening polymerization. | 4 | Discussion |
| 1.4 | Metathetical, group transfer, polyaddition and polycondensation polymerizations. | 3 | E-Resources |
| **UNIT – II** | | | |
| 2.1 | Monomers required general methods of preparation, repeat units and uses of the following polymers and resins-polyethylene, polystyrene, polyacrylonitrile, polymethymethacrylate, PVC. | 5 | E-Resources |
| 2.2 | Polytetrafluoroethylene, polyisoprenes, polybutadienes and polychloroprene, polyesters. | 3 | Discussion |
| 2.3 | Polycarbonates, polyimides, polyamides (Kevlar), polyurethanes, Polyethyleneglycols. | 3 | Chalk & Talk |
| 2.4 | Phenolformaldehyde, urea-formaldehyde, melamineformaldehyde and epoxy resins-silicone polymers. | 4 | E-Resources |
| **UNIT – III** | | | |
| 3.1 | Configuration of polymer chain geometrical structure syndiotatic, isotatic and atatic polymers. | 3 | E-Resources |
| 3.2 | Glass transition temperature: Definition-factors affecting glass transition temperature | 2 | E-Resources |

| | | | |
|---|---|---|---|
| 3.3 | Relationships between glass transition temperature and (a) molecular weight, (b) melting point and (c) plasticizer. | 2 | E-Resources |
| 3.4 | Importance of glass transition temperature- heat distortion temperature. | 2 | Discussion |
| 3.5 | Molecular weight and size of polymers: Number average, weight average, sedimentation and viscosity. | 3 | Chalk & Talk |
| 3.6 | Average molecular weights-molecular weights and degree of polymerization-poly dispersity-molecular weight distribution in polymers-size of polymer molecules. | 3 | E-Resources |
| **UNIT – IV** | | | |
| 4.1 | Polymerization techniques: Bulk, solution, suspension, emulsion, melt condensation and interfacial polycondensation polymerizations. | 5 | Discussion |
| 4.2 | Degradation: Types of degradation - thermal, mechanical, ultrasonic and photodegradation. | 4 | E-Resources |
| 4.3 | Photostabilizers - oxidative degradation – antioxidants - hydrolytic degradation | 4 | Chalk & Talk |
| 4.4 | Uses of polymers: Electronics and biomedicine. | 2 | E-Resources |
| **UNIT –V** | | | |
| 5.1 | Plastics (thermo and thermosetting), elastomers, fibres, compounding. | 4 | Chalk & Talk |
| 5.2 | Plasticisers, colorants, flame retardants. | 3 | Chalk & Talk |
| 5.3 | Compression and injection mouldings - film extrusion and calendaring. | 4 | Discussion |
| 5.4 | Die casting and rotational casting - thermofoaming-reinforcing. | 4 | E-Resources |
| | **Total** | **75** | |

**Course Designer**
**Dr. M.P. Kesavan**
Assistant Professor of Chemistry

| Course Code | Course Title | Category | Total Hours | Credits |
|---|---|---|---|---|
| 20PCHE42 | Conducting Polymers | Elective -III | 75 | 4 |

| Nature of Course | |
|---|---|
| Knowledge Oriented | ✓ |
| Skill Oriented | |
| Employability Oriented | ✓ |
| Entrepreneurship Oriented | |

| Course Relevance | |
|---|---|
| Local | |
| Regional | |
| National | |
| Global | ✓ |

**Preamble**

The course enables the students to understand basic concepts and synthetic methods, electrochemical synthesis, semiconducting and metallic polymers, doping and catalytic conducting polymers.

**Course Outcomes (CO)**

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

| No. | Course Outcome | Knowledge Level |
|---|---|---|
| **CO1** | Summarise the basic concepts and synthetic methods of polymers. | **K1,K2** |
| **CO2** | Analyze the electrochemical synthesis of polymers. | **K1,K2,K3,K4** |
| **CO3** | Apply the concepts of semiconducting and metallic polymers. | **K1,K2,K3** |
| **CO4** | Interpret the change in electronic properties of polymer by doping. | **K1,K2,K3,K4K5** |
| **CO5** | Apply the concepts of conducting polymers in catalysis. | **K1,K2,K3** |

**K1-Knowledge K2-Understand K3-Apply K4- Analyse K5- Evaluate**

**Mapping of CO with PO**

| | PO1 | PO2 | PO3 | PO4 | PO5 |
|---|---|---|---|---|---|
| **CO1** | **3** | **3** | **2** | **1** | **2** |
| **CO2** | **3** | **3** | **3** | **3** | **2** |
| **CO3** | **3** | **3** | **3** | **1** | **2** |
| **CO4** | **3** | **3** | **3** | **1** | **2** |
| **CO5** | **3** | **3** | **3** | **3** | **2** |

**1-Low 2-Medium 3-Strong**

**Mapping of CO with PSO**

| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 |
|---|---|---|---|---|---|
| CO1 | 3 | 3 | 3 | 2 | 1 |
| CO2 | 3 | 3 | 3 | 2 | 1 |
| CO3 | 2 | 3 | 3 | 2 | 1 |
| CO4 | 2 | 3 | 3 | 2 | 1 |
| CO5 | 2 | 2 | 3 | 2 | 1 |

**1-Low** **2-Medium** **3-Strong**

**Syllabus**

**UNIT I** 15 Hours

Basic Concepts and Synthetic methods: Basics of conducting polymers – Organic conjugated unsaturated hydrocarbons - Chemical Synthesis of conducting polymers – Other synthetic methods.

**UNIT II** 15 Hours

Electrochemical Synthesis: Electrochemical synthesis of conducting polymers – monomers, electrolytic condition, electrodes and mechanism; Electrochemical synthesis of derivatives of poly pyrrole, polythiophene, polyazulene, polycarbazole, polyindole, polyaniline and polyphenylene.

**UNIT III** 15 Hours

Semiconducting and Metallic Polymers: Structural basis for semiconducting and metallic polymers – introduction; Organic meta polymers - Synthetic route, isomers and electronic structure (polymers like polyacetylene, poly(p-phenylene), polypyrrole, polythiophene, etc.,).

**UNIT IV** 15 Hours

Doping: Electrochemical doping; deadline to the development of conducting polymers; role of reduction and oxidation potential in doping; polyacetylene as electrode materials.

**UNIT V** 15 Hours

Catalytic Conducting Polymers: Catalytic properties of conducting polymers; catalysis of electron donor-acceptor complexes; electrocatalysis by semiconducting polymers.

**Text Books**

Terje A. Skotheim, Ronald L. Elsenbaumer, John R. Reynolds, ***Handbook of conducting Polymers***, Marcel Dekkar, 1995, Second Edition.

Raymond B Seymour, ***New Concepts in Polymer Science***, Polymeric Composites, VSP, 1990.

**Reference Books**

Hari Singh Nalwa (Edn), ***Handbook of Organic Conductive Molecules and Polymers***, Wiley, 1997.

Jean-Pierre Farges, ***Organic Conductors***, Marcel Dekkar, 1994.

David B Cotts, Z Reyes, ***Electrically Conductive Organic Polymers for Advanced Applications***, William Andrew Inc, 1987.

Larry Rupprecht, ***Conductive Polymers and Plastics***, William Andrew Inc, 1999.

Wallace Gordon, Gordon G Wallace, Geoffrey M Spinks, ***Conductive Electroactive Polymers***, CRC Press, 2002.

**Pedagogy**

Chalk & Talk, E-Resources, Group Discussion

**Teaching aids**

Black Board, LCD Projector

**Course Contents and Lecture Schedule**

| Module No. | Topic | No. of Lectures | Content Delivery Methods |
|---|---|---|---|
| **UNIT – I** | | | |
| 1.1 | Basics of conducting polymers - Organic – conjugated unsaturated hydrocarbons. | 6 | Chalk & Talk |
| 1.2 | Chemical Synthesis of conducting polymers – Other synthetic methods. | 9 | E-Resources |
| **UNIT – II** | | | |
| 2.1 | Electrochemical synthesis of conducting polymers – monomers, electrolytic condition, electrodes and mechanism. | 6 | Chalk & Talk |
| 2.2 | Electrochemical synthesis of derivatives of polypyrrole, polythiophene, polyazulene. | 5 | Discussion |
| 2.3 | Polycarbazole, polyindole, polyaniline and polyphenylene. | 4 | E-Resources |
| **UNIT – III** | | | |
| 3.1 | Structural basis for semiconducting and metallic polymers – introduction. | 6 | Discussion |
| 3.2 | Organic meta polymers - Synthetic route, isomers and electronic structure (polymers like polyacetylene, poly(p-phenylene), polypyrrole, polythiophene, etc.,). | 9 | E-Resources |

| | | | |
|---|---|---|---|
| **UNIT – IV** | | | |
| 4.1 | Electrochemical doping; deadline to the development of conducting polymers. | 5 | E-Resources |
| 4.2 | Role of reduction and oxidation potential in doping. | 5 | Discussion |
| 4.3 | Polyacetylene as electrode materials. | 5 | Chalk & Talk |
| **UNIT –V** | | | |
| 5.1 | Catalytic properties of conducting polymers. | 5 | Discussion |
| 5.2 | Catalysis of electron donor-acceptor complexes | 5 | Chalk & Talk |
| 5.3 | Electrocatalysis by semiconducting polymers. | 5 | E-Resources |
| | **Total** | **75** | |

**Course Designer**
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