Appendix

# Centre for Integrated Studies

## Cochin University of Science and Technology

**Scheme of Examination and Syllabus for the**

**Five Year Integrated M.Sc. Chemistry Approved by the Combined Board of Studies in Physical and Mathematical Sciences and**

**Chemical and Biological Sciences on 27-11-2025**

**(2022 admission)**

## Programme Objective

The five-year Integrated M. Sc in Chemistry aims to impart a sound foundation in basic sciences with a focus on transdisciplinary subjects in order to build human resources for innovative research in Chemical Science and train competent manpower who can take challenges in teaching and research.

## Program Outcomes

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

**PO 1:** acquire systematic and coherent understanding of the fundamental concepts.

**PO 2:** demonstrate comprehensive knowledge and understanding of both theoretical and experimental/applied chemistry in various fields.

**PO 3:** design and perform the chemical synthesis and characterize the products.

**PO 4:** design and execute experimental routines for detection and quantification of chemical entities.

**PO 5:** analyze the kinetics and energetics of chemical processes and infer the mechanism.

**PO 6:** demonstrate the basic principles of instrumental methods of analysis.

**PO 7:** operate advanced instruments and related softwares to execute in-depth analysis of chemical problems.

**PO 8:** design and develop new molecules/processes with industrial and societal applications.

**PO 9:** acquire skills for future employment in academia and industry.

**PO 10:** demonstrate knowledge relevant to the regional, national and international development needs.

# SEMESTER: 1

***Semester Credit: 23 (Core: 13; Elective: 0) Cumulative Credit: 23***

| Course Code | Course Name | Course Type | Credits | L-T-P | CE | ESE | Total Marks |
|---|---|---|---|---|---|---|---|
| ENG10101 | English - I | Core | 2 | 2-1-0 | 50 | 50 | 100 |
| | **Language** | | | | | | |
| MAL10101 | Malayalam - I | Core | 2 | 2-1-0 | 50 | 50 | 100 |
| HIN10101 | Hindi - I | | | | | | |
| FLG10101 | German-I | | | | | | |
| CHE10101 | Atomic Structure and Chemical Bonding | Core | 3 | 3-1-0 | 50 | 50 | 100 |
| PHY10101 | Mechanics | Core | 3 | 3-1-0 | 50 | 50 | 100 |
| BIO10101 | General Biology | Core | 3 | 3-1-0 | 50 | 50 | 100 |
| MAM10101 | Calculus-I | Core | 4 | 4-1-0 | 50 | 50 | 100 |
| CHE10102 | Inorganic Quantitative Analysis Lab | Core | 2 | 0-0-6 | 100 | - | 100 |
| PHY10102 | Physics Lab (Mechanics) | Core | 2 | 0-0-6 | 100 | - | 100 |
| BIO10102 | General Biology Lab | Core | 2 | 0-0-6 | 100 | - | 100 |

## SEMESTER: 2

***Semester Credit: 23 (Core: 23; Elective: 0) Cumulative Credit: 46***

| Course Code | Course Name | Course Type | Credits | L-T-P | CE | ESE | Total Marks |
|---|---|---|---|---|---|---|---|
| ENG10201 | English - II | Core | 2 | 2-1-0 | 50 | 50 | 100 |
| | **Language** | | | | | | |
| MAL10201<br>HIN10201<br>FLG10201 | Malayalam - II<br>Hindi – II<br>German-II | Core | 2 | 2-1-0 | 50 | 50 | 100 |
| CHE10201 | Periodicity, Nuclear Chemistry, Metallurgy and Acid Base Chemistry | Core | 3 | 3-1-0 | 50 | 50 | 100 |
| PHY10201 | Waves and Optics | Core | 3 | 3-1-0 | 50 | 50 | 100 |
| BIO10201 | Biochemistry | Core | 3 | 3-1-0 | 50 | 50 | 100 |
| MAM10201 | Linear Algebra, Group Theory | Core | 4 | 4-1-0 | 50 | 50 | 100 |
| CHE10202 | Inorganic Qualitative Analysis Lab | Core | 2 | 0-0-6 | 100 | - | 100 |
| PHY10202 | Physics Lab (Waves and Optics) | Core | 2 | 0-0-6 | 100 | - | 100 |
| BIO10202 | Biochemistry Lab | Core | 2 | 0-0-6 | 100 | - | 100 |

## SEMESTER: 3

***Semester Credit: 25 (Core: 25; Elective: 0) Cumulative Credit: 71***

| Course Code | Course Name | Course Type | Credits | L-T-P | CE | ESE | Total Marks |
|---|---|---|---|---|---|---|---|
| CHE10301 | Introductory Organic Chemistry | Core | 3 | 3-1-0 | 50 | 50 | 100 |
| PHY10301 | Electricity and Magnetism-I | Core | 3 | 3-1-0 | 50 | 50 | 100 |
| BIO10301 | Cell Biology | Core | 3 | 3-1-0 | 50 | 50 | 100 |
| MAM10301 | Calculus-II | Core | 4 | 4-1-0 | 50 | 50 | 100 |
| MAM10302 | Mathematical Methods-I | Core | 4 | 4-1-0 | 50 | 50 | 100 |
| EVS10301 | Environmental Science | Core | 2 | 2-1-0 | 50 | 50 | 100 |
| CHE10302 | Organic Qualitative Analysis Lab | Core | 2 | 0-0-6 | 100 | - | 100 |
| PHY10302 | Physics Lab (Electricity and Magnetism) | Core | 2 | 0-0-6 | 100 | - | 100 |
| BIO10302 | Cell Biology Lab | Core | 2 | 0-0-6 | 100 | - | 100 |

## SEMESTER: 4

***Semester Credit: 25 (Core: 25; Elective: 0) Cumulative Credit: 96***

| Course Code | Course Name | Course Type | Credits | L-T-P | CE | ESE | Total Marks |
|---|---|---|---|---|---|---|---|
| CHE10401 | Introductory Physical Chemistry | Core | 3 | 3-1-0 | 50 | 50 | 100 |
| PHY10401 | Quantum Physics and Relativity | Core | 3 | 3-1-0 | 50 | 50 | 100 |
| BIO10401 | Molecular Biology and Genetics | Core | 3 | 3-1-0 | 50 | 50 | 100 |
| MAM10401 | Mathematical Methods-II | Core | 4 | 4-1-0 | 50 | 50 | 100 |
| STA10401 | Probability and Statistics | Core | 4 | 4-1-0 | 50 | 50 | 100 |
| COM10401 | Basic Computer Science | Core | 2 | 2-1-0 | 50 | 50 | 100 |
| CHE10402 | Physical Chemistry Lab | Core | 2 | 0-0-6 | 100 | - | 100 |
| PHY10402 | Physics Lab (Modern Physics) | Core | 2 | 0-0-6 | 100 | - | 100 |
| BY10402 | Molecular Biology and Genetics Lab | Core | 2 | 0-0-6 | 100 | - | 100 |

## SEMESTER: 5

***Semester Credit: 20 (Core: 20; Elective: 0) Cumulative Credit: 116***

| Course Code | Course Name | Course Type | Credits | L-T-P | CE | ESE | Total Marks |
|---|---|---|---|---|---|---|---|
| 20-802-0501 | Analytical Chemistry-I (Analytical Techniques, Instrumental Methods, Molecular Spectroscopy) | Core | 3 | 3-1-0 | 50 | 50 | 100 |
| 20-802-0502 | Inorganic Chemistry-I (Chemistry of Main Group Elements) | Core | 3 | 3-1-0 | 50 | 50 | 100 |
| 20-802-0503 | Organic Chemistry-I (Functional Group Chemistry) | Core | 3 | 3-1-0 | 50 | 50 | 100 |
| 20-802-0504 | Physical Chemistry-I (Equilibrium Thermodynamics) | Core | 3 | 3-1-0 | 50 | 50 | 100 |
| 20-802-0505 | Mathematics for Chemists | Core | 2 | 2-1-0 | 50 | 50 | 100 |
| 20-802-0506 | Inorganic Chemistry Lab | Core | 2 | 0-0-6 | 100 | - | 100 |
| 20-802-0507 | Organic Chemistry Lab | Core | 2 | 0-0-6 | 100 | - | 100 |
| 20-802-0508 | Open Ended Lab-I | Core | 2 | 0-0-6 | 100 | - | 100 |

# SEMESTER: 6

***Semester Credit: 20 (Core: 20; Elective: 0) Cumulative Credit: 136***

| Course Code | Course Name | Course Type | Credits | L-T-P | CE | ESE | Total Marks |
|---|---|---|---|---|---|---|---|
| 20-802-0601 | Inorganic Chemistry-II (Coordination Chemistry) | Core | 3 | 3-1-0 | 50 | 50 | 100 |
| 20-802-0602 | Organic Chemistry-II (Structure, Stereochemistry and Conformational Analysis) | Core | 3 | 3-1-0 | 50 | 50 | 100 |
| 20-802-0603 | Physical Chemistry-II (Electrochemistry, Solid State and Liquid State) | Core | 3 | 3-1-0 | 50 | 50 | 100 |
| 20-802-0604 | Industrial Chemistry | Core | 3 | 3-1-0 | 50 | 50 | 100 |
| 20-802-0605 | Computer Programming and Numerical Methods | Core | 2 | 2-1-0 | 50 | 50 | 100 |
| 20-802-0606 | Advanced Physical Chemistry Lab-I | Core | 2 | 0-0-6 | 100 | - | 100 |
| 20-802-0607 | Industrial Chemistry Lab | Core | 2 | 0-0-6 | 100 | - | 100 |
| 20-802-0608 | Open Ended Lab-II | Core | 2 | 0-0-6 | 100 | - | 100 |

## SEMESTER: 7

***Semester Credit: 21 (Core: 16; Elective: 5) Cumulative Credit: 157***

| Course Code | Course Name | Course Type | Credits | L-T-P | CE | ESE | Total Marks |
|---|---|---|---|---|---|---|---|
| 25-802-0701 | Inorganic Chemistry -III (Concepts and Developments) | Core | 3 | 3-1-0 | 50 | 50 | 100 |
| 25-802-0702 | Organic Chemistry-III (Reactivity and Mechanisms) | Core | 4 | 4-1-0 | 50 | 50 | 100 |
| 25-802-0703 | Theoretical Chemistry-I (Quantum Chemistry) | Core | 3 | 3-1-0 | 50 | 50 | 100 |
| 25-802-0704 | Theoretical Chemistry-II (Group Theory and Spectroscopy) | Core | 4 | 4-1-0 | 50 | 50 | 100 |
| 25-802-0705 | Advanced Chemical Synthesis and Separation Lab | Core | 2 | 0-0-6 | 100 | - | 100 |
| 25-802-0706 | Open Ended Lab-III | Core[c] | - | 0-0-6 | 50 | - | - |
| 25-802-0707 | Supramolecular Chemistry | Elective | 3 | 2-1-0 | 50 | 50 | 100 |
| 25-802-0708 | Green Chemistry | Elective | 3 | 2-1-0 | 50 | 50 | 100 |
| 25-802-0709 | Polymer Chemistry | Elective | 3 | 2-1-0 | 50 | 50 | 100 |
| 25-802-0710 | Bonds and Bands in Solids | Elective[a] | 2 | 2-1-0 | 50 | 50 | 100 |
| 25-802-0711 | Professional and Career Development in Chemistry | Audit[b] | - | 2-0-0 | - | - | - |

## SEMESTER: 8

***Semester Credit: 24 (Core: 20; Elective: 4) Cumulative Credit: 181***

| Course Code | Course Name | Course Type | Credits | L-T-P | CE | ESE | Total Marks |
|---|---|---|---|---|---|---|---|
| 25-802-0801 | Inorganic Chemistry-IV (Chemistry of d- and f- Block Elements) | Core | 3 | 3-1-0 | 50 | 50 | 100 |
| 25-802-0802 | Organic Chemistry -IV (Reactions, Reagents and Synthesis) | Core | 4 | 4-1-0 | 50 | 50 | 100 |
| 25-802-0803 | Organic Chemistry -V (Spectroscopy of Organic Compounds) | Core | 3 | 2-1-0 | 50 | 50 | 100 |
| 25-802-0804 | Physical Chemistry-III (Statistical and Nonequilibrium Thermodynamics) | Core | 3 | 3-1-0 | 50 | 50 | 100 |
| 25-802-0805 | Theoretical Chemistry-III (Chemical Bonding and Computational Chemistry) | Core | 3 | 2-0-2 | 50 | 50 | 100 |
| 25-802-0806 | Advanced Physical Chemistry Lab-II | Core | 2 | 0-0-6 | 100 | - | 100 |
| 25-802-807 | Open Ended Lab-IV | Core[c] | 2 | 0-0-4 | 50 | - | 100[c] |
| 25-802-808 | Bioanalytical Chemistry | Elective | 2 | 2-1-0 | 50 | 50 | 100 |
| 25-802-809 | Advanced Photochemistry | Elective | 2 | 2-1-0 | 50 | 50 | 100 |
| 25-802-810 | Theory of Orbital Interactions in Chemistry | Elective | 2 | 1-1-3 | 50 | 50 | 100 |
| 25-802-0811 | Material Chemistry | Elective | 4 | 3-0-2 | 50 | 50 | 100 |

## SEMESTER: 9

***Semester Credit: 19 (Core: 16; Elective: 3) Cumulative Credit: 200***

| Course Code | Course Name | Course Type | Credits | L-T-P | CE | ESE | Total Marks |
|---|---|---|---|---|---|---|---|
| 25-802-0910 | Analytical Chemistry-II (Advanced Analytical Techniques and Instrumental Methods) | Core | 4 | 4-1-0 | 50 | 50 | 100 |
| 25-802-0902 | Inorganic Chemistry -V (Organometallic and Bioinorganic Chemistry) | Core | 3 | 3-1-0 | 50 | 50 | 100 |
| 25-802-0903 | Organic Chemistry-VI (Chemistry of Natural Products) | Core | 3 | 3-1-0 | 50 | 50 | 100 |
| 25-802-0904 | Physical Chemistry-IV (Chemical Kinetics, Reaction Dynamics, Catalysis and Surface Chemistry) | Core | 3 | 3-1-0 | 50 | 50 | 100 |
| 25-802-0905 | Physical Chemistry-V (Advanced Electrochemistry) | Core | 3 | 2-1-0 | 50 | 50 | 100 |
| 25-802-0906 | Transition Metals: Chemistry and Applications in Organic Synthesis | Elective | 3 | 3-1-0 | 50 | 50 | 100 |
| 25-802-0907 | Spectroscopic Techniques | Elective | 3 | 3-1-0 | 50 | 50 | 100 |
| 25-802-0908 | New Methods and Strategies in Organic Synthesis and Dynamic Stereochemistry | Elective | 3 | 3-1-0 | 50 | 50 | 100 |
| 25-802-0909 | Advanced Techniques in Organic Synthesis: Theory and Practice | Elective | 3 | 3-1-0 | 50 | 50 | 100 |

# SEMESTER: 10

***Semester Credit: 18 (Core: 18; Elective: 0) Cumulative Credit: 215***

| Course Code | Course Name | Course Type | Credits | L-T-P | CE | ESE | Total Marks |
|---|---|---|---|---|---|---|---|
| 25-802-1001 | Project Dissertation and Viva Voce | Core | 16 | - | - | 300 | 300 |

[a]-MOOC Course
[b]-Value Added Course
[c]-Sum of marks obtained in CE of Sem 7 and Sem 8
L-T-P ≡ Lecture-Tutorial-Practical Hours
CE ≡ Continuous Evaluation; ESE ≡ End Semester Evaluation

**CORE**

**CHE10101**

**ATOMIC STRUCTURE AND CHEMICAL BONDING**

**Credit 3** **48 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Describe the major discoveries that led to the foundation of quantum mechanics | Understand |
| C.O. 2:<br>Correlate the concepts of quantum mechanics to atomic structure | Apply |
| C.O. 3:<br>Correlate the concepts of atomic structure to properties of atoms | Analyse |
| C.O. 4:<br>Apply the concept of atomic orbitals to build molecular orbitals | Apply |
| C.O. 5:<br>Evaluate the structure and bonding of any molecule | Analyse |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | x | | | | | | | | | |
| C.O. 2 | x | x | | | | | | | | |
| C.O. 3 | x | x | | | | | | | | |
| C.O. 4 | x | x | | | | | | | | |
| C.O. 5 | x | x | | | | | | | | |

| **UNIT I** | **10 hrs** |
|---|---|
| Black body radiation, Planck's law, Hydrogen spectrum, Bohr's theory, its limitations, Photoelectric effect, Double slit experiment, Heisenberg's uncertainty principle and its significance, Wave-Particle duality, de Broglie equation.<br>Limitations of classical mechanics in describing the properties of microscopic particles. | |
| **UNIT II** | **10 hrs** |
| Schrödinger's wave equation, significance of $\psi$ and $\psi^2$, Quantum numbers and their significance. Sign of wave functions. Radial and angular wave functions. Radial and angular distribution curves. Shapes of s, p, d and f orbitals. Contour boundary and probability diagrams. | |
| **UNIT III** | **8 hrs** |
| Quantization, Electronic Transitions, Quantum Theory, Atomic Energy States, Pauli's Exclusion Principle, Hund's rule of maximum multiplicity, Aufbau's principle and its limitations, Variation of orbital energy with atomic number. Electronic energy level diagram and electronic configurations of hydrogen-like and polyelectronic atoms and ions. Excited states. | |

| UNIT IV | 10 hrs |
|---|---|
| Ionic bond: General characteristics, types of ions, size effects, radius ratio rule and its limitations. Packing of ions in crystals. Born-Lande equation with derivation and importance of Kapustinskii expression for lattice energy. Madelung constant, Solvation energy, Covalent bond, Lewis structure, Valence shell electron pair repulsion theory (VSEPR), shapes of simple molecules and ions containing lone pairs and bond pairs of electrons, multiple bonding ($\sigma$ and $\pi$ bond approach) and bond lengths, Ionic character in covalent compounds: Bond moment and dipole moment. | |
| **UNIT V** | **10 hrs** |
| Valence Bond theory, Hybridization, equivalent and non-equivalent hybrid orbitals. Bent's rule, Resonance and resonance energy, Molecular orbital theory. bonding, non- bonding, antibonding molecular orbitals (concept only) elementary pictorial approach of homo- and hetero-diatomic molecules $H_2$, $B_2$, $C_2$, $O_2$, $N_2$, CO, NO and $CO_2$, $H_2O$ etc. molecular orbitals, sigma and pi bonds. multiple bonding, Concept of Bond order, bond length, bond strength, bond energy, Formal charge, Molecular Electron Configurations, Metallic Bond: Qualitative idea of valence bond and band theories. Semiconductors and insulators, Van der Waal's forces, ion-dipole, dipole–dipole interactions, London forces, Hydrogen bonding; Effect of chemical forces on physical properties | |

Recommended Text Books:


1. Lee, J.D. Concise Inorganic Chemistry, 5th Ed., John Wiley & Sons, 1999.
2. Douglas, B.E. and Mc Daniel, D.H., Concepts & Models of Inorganic Chemistry, 3rd Ed., Oxford, 1994.
3. Atkins, P.W. and Paula, J. Physical Chemistry, 8th Ed., Oxford Press, 2006.
4. Day, M.C. and Selbin, J. Theoretical Inorganic Chemistry, 2nd Ed., ACS Publications, 2002.
5. Huheey, J. E., Keiter, E. A. and Keiter, R. L. Inorganic Chemistry, Principle and structure and reactivity, 4th Ed., Harper Collins College Publishers, New York,1993.
6. Shriver, D. F., Atkins, P. W. and Langford, C. H. Inorganic Chemistry, 4th Ed., W.H. Freeman & Company, 2006.
7. Housecroft, C. and Sharpe, G., Inorganic Chemistry, 4th Ed., Pearson, 2012.
8. Levine, I. N. Physical Chemistry, 6th Ed., McGraw-Hill Education, 2008.

**CORE/LAB**

**CHE10102**

**QUANTITATIVE ANALYSIS LAB**

**Credit 2** **96 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Develop basic concepts of quantitative volumetric analysis | Understand |
| C.O. 2:<br>Estimate the amount of a given substance by acidimetry, alkalimetry and permanganometry | Apply |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | x | x | | | | | | | x | |
| C.O. 2 | x | x | | x | x | | | | x | |

| **UNIT-I** | **96 hrs** |
|---|---|
| I. Acidimetry and Alkalimetry<br>1. Strong acid- Strong base<br>2. Strong base –Weak acid<br>3. Strong acid-Weak base<br>4. Estimation of hardness of water<br>II. Redox Titration (Permanganometry)<br>1. Estimation of Oxalic acid<br>2. Estimation of Mohr’s salt<br>3. Estimation of Ferrous iron<br>4. Estimation of Manganese dioxide in pyrolusite | |

**Recommended Text Books:**

1. Vogel’s Textbook of Quantitative Chemical Analysis, 6$^{th}$ Ed., Pearsons Education Ltd.
2. Laboratory Manual, CHE 10102, Department of Applied Chemistry, CUSAT

**CORE**

**CHE10201**

**PERIODICITY, NUCLEAR CHEMISTRY, ACID BASE CHEMISTRY AND METALLURGY**

**Credit 3** **48 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Correlate the physical and chemical properties of elements based on their periodic classification | Analyse |
| C.O. 2:<br>Analyse the properties, stability, mode of decay and kinetics of a given nucleus/nuclear process | Apply |
| C.O. 3:<br>Describe the radioactivity phenomena and its applications | Understand |
| C.O. 4:<br>Compare the strength of various acids and bases | Apply |
| C.O. 5:<br>Explain the occurrence of minerals and metallurgical principles for isolation and purification | Apply |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | x | x | | | | | | | | |
| C.O. 2 | x | x | | | x | | | | | |
| C.O. 3 | x | x | | | x | | | | | |
| C.O. 4 | x | x | | | x | | | | | |
| C.O. 5 | x | x | | | x | | | | | |

| **UNIT I** | **10 hrs** |
|---|---|
| Atomic weights, Development of periodic law, The modern periodic table, Basis of periodic classification, orbital types and periodic table, Commonality in electronic configurations, Atomic sizes, ionization energy, Electron negativity, Electron Affinity, Polarizability and polarizing power, Relative orbital energies and overlap, Trends associated with properties – Physical and chemical, Anomalies in periodic properties. Predicting Chemistry of super heavy elements. | |
| **UNIT II** | **14 hrs** |
| Nuclear radius, Nuclear Forces, Nuclear Spin, Magnetic dipole moment, Elementary Particles, Binding Energy, Nuclear models – Shell model- magic number, periodicity in nuclear properties, Liquid drop model – fission and fusion, Nuclear Stability, Exchange theory, n/p ratio, Nuclear Radiations, Nuclear reactions, Types of nuclear reactions, Decay Kinetics, Half-life, Radioactive | |

| | |
|---|---|
| disintegration series. Fission: Fission products and Fission yield curve, Fission energy, theory of nuclear fission, nuclear reactor, breeder reactor<br>- nuclear reactors in India. Fusion reactions, hydrogen bomb and energy of sun. | |
| **UNIT III** | **8 hrs** |
| Transuranium elements: Synthesis, separation and properties of transuranium elements. Radioisotopes: Co-precipitation, ion-exchange, solvent extraction as a tracer, Synthesis of labeled compounds (any two), isotopic dilution and radiopharmaceuticals. Neutron activation analysis, Principles of determination of age of rocks and minerals, radio carbon dating principles, Isotope dilution and neutron activation analysis. | |
| **UNIT IV** | **8 hrs** |
| Acid Base concepts, Bronsted-Lowry definition, Lux Flood Definition, Solvent system definition, Lewis Definition, Usanovich Definition, Generalized concept, Measures of acid base concept, Acid Base anomalies, Pearson's HSAB concept, acid-base strength and hardness and softness, Symbiosis, theoretical basis of hardness and softness, electronegativity and hardness. | |
| **UNIT V** | **8 hrs** |
| Occurrence of metals based on standard electrode potential, methods of concentration of ores, reduction to free metal, electrometallurgy, hydrometallurgy, and synthesis of ultrapure elements. Refining of metals, electrolytic, ion exchange, zone refining, vapour phase refining and oxidative refining. Thermodynamics of the oxidation of metals to metaloxides- Ellingham diagrams. Extractive metallurgy of U, Th, Ti. | |

**Recommended Text Books:**


1. Mingos, D. M. P., Essential trends in inorganic chemistry, Oxford University press 1998.
2. Wulfsberg, G., Inorganic Chemistry, VIVA,2002.
3. Greenwood, N. N., Earnshaw, A., Chemistry of Elements, Maxwell Macmillan International Edition, Pergamon Press, 1989.
4. Cotton, F.A., Wilkinson, G, Advanced Inorganic Chemistry. Wiley-VCH,1999.
5. Huheey, J. E., Keiter, E. A., Kieter, R. L., Medhi, O. K., Inorganic Chemistry Principles Structure and Reactivity, Pearson Education, 4th edition,2009.
6. Shriver, D. F., Atkins, P. W. and Langford, C. H. Inorganic Chemistry, $4^{th}$ Ed., W.H. Freeman & Company,2006.
7. Douglas, B.E. and Mc Daniel, D.H., Concepts & Models of Inorganic Chemistry, $3^{rd}$ Ed., Oxford, 1994.
8. G.L. Miessler, P.J. Fischer, D.A. Tarr, Inorganic Chemistry, $5^{th}$ ed., Pearson, 2014.
9. Sharma, B. K., Industrial Chemistry (including Chemical Engineering), GOEL Publishing House,1997.
10. Arnikar, H. J., Essentials of Nuclear Chemistry, Wiley Eastern Ltd., New Delhi, 1982.

**CORE/LAB**

**CHE10202**

**INORGANIC QUALITATIVE ANALYSIS LAB**

**Credit 2** **96 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Develop basic concepts of inorganic qualitative analysis | Understand |
| C.O. 2:<br>Identify acid radicals and basic radicals from a given sample mixture | Apply |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | x | x | | | | | | | x | |
| C.O. 2 | x | x | | x | x | | | | x | |

| **UNIT I** | **96 hrs** |
|---|---|
| Systematic qualitative analysis of mixtures containing two acid and two basic radicals from the list given below by semi micro method<br>$Pb^{2+}$, $Cu^{2+}$, $Bi^{2+}$, $Cd^{2+}$, $Fe^{2+}$, $Fe^{3+}$, $Al^{3+}$, $Zn^{2+}$, $Mn^{2+}$, $Co^{2+}$, $Ni^{2+}$, $Ca^{2+}$, $Sr^{2+}$, $Ba^{2+}$, $Mg^{2+}$, $NH_4^+$; $CO_3^{2-}$ $SO^{2-}$, $NO^-$, $F^-$, $Cl^-$, $CO^{2-}$, CH $COO^-$, $PO^{3-}$, $CrO^{2-}$ | |

**Recommended Text Books:**

1. A.I. Vogel, A Text Book of Qualitative Inorganic Analysis, Longman,1966.
2. Laboratory Manual, CHE 10202, Department of Applied Chemistry, CUSAT.

**CORE**

**CHE10301**

**INTRODUCTORY ORGANIC CHEMISTRY**

**Credit 3** **48 hours**

| **Course Outcome**<br>After the completion of the course the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Assign the nomenclature of simple organic molecules following IUPAC rules | Apply |
| C.O. 2:<br>Illustrate different bonding models to predict the three dimensional structure of molecules. | Analyse |
| C.O. 3:<br>Apply the concepts of isomerism and analyse the conformation and configuration of organic molecules | Analyse |
| C.O. 4:<br>Describe the different types of organic reactions | Understand |
| C.O. 5:<br>Develop an insight into the importance of organic chemistry in life | Understand |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | x | x | | | | | | | | |
| C.O. 2 | x | x | | | | | | | | |
| C.O. 3 | x | x | | | | | | | | |
| C.O. 4 | x | x | | | | | | | | |
| C.O. 5 | x | x | | | | | | | | |

| **UNIT I** | **6 hrs** |
|---|---|
| Nomenclature of organic compounds. Rules of IUPAC system of nomenclature of common organic compounds – alkanes, alkenes, alkynes, cycloalkanes, bicycloalkanes, alkyl halides, alcohols and phenols. Aldehydes, ketones, carboxylic acids and its derivatives, amines, nitro compounds, heterocyclic compounds. | |
| **UNIT II** | **10 hrs** |
| Structure and Models of bonding: Study of Lewis Structures, Formal Charge, VSEPR, Hybridization, localised σ and π bonds, polar covalent bonding, Bond dipoles, molecular dipoles and quadrupoles, polarizability, Resonance, Bond Lengths and Bond energy. | |
| **UNIT III** | **10 hrs** |
| Stereochemistry: Concept of Configuration, Classification of Stereoisomers, Optical isomerism, Chirality, Wedge formula, Fischer projection, Newman projection, perspective formula. Relative and absolute configurations, sequence rules, D & L, R & S systems of nomenclature. Enantiomers, meso | |

| | |
|---|---|
| form, diastereoisomers, epimers, anomers. Geometrical Isomerism: E-Z notation - determination of configuration.<br>Conformational analysis: Strain in molecules, acyclic molecules, cyclohexane, substituted cyclohexanes- A values. | |
| **UNIT IV** | **12 hrs** |
| Basic introduction to Organic reactions: Classification and an overview of organic reactions. Electron pushing diagrams. Basics of reaction coordinate diagrams, intermediates, transitions states, exothermic and endothermic reactions, activation energy, rates of reactions and rate determining step. Hammond's postulate. Nucleophilic substitutions - $S_N1$, $S_N2$, substitutions on aromatic carbon, Addition reactions - polar and non-polar addition - addition of Bromine and hydrogen halides to double bonds - Markownikoff's rule and peroxide effect., Elimination - E1, E2, E1cb, pyrolytic elimination. Basic introduction to rearrangements and Pericyclic Reactions. | |
| **UNIT V** | **10 hrs** |
| Organic Chemistry in life: Natural products (structure and classification) – Terpenes, Steroids and alkaloids. Biomolecules (structure and function): carbohydrates, amino acids, proteins and nucleic acids. Pharmaceuticals and Drugs, Dyes and Chemistry of Vision. Introduction to polymer science – Monomers and Polymerisaton. Mechanisms of Radical and condensation polymersiations. | |

**Recommended Text Books:**


1. Clayden J., Greeves, N. Warren, S., Organic Chemistry (2 Ed), Oxford University Press, 2001.
2. Bruice, P.Y. Organic Chemistry, 7th Ed., Prentice Hall Inc., 2013.
3. Morrison, R.T. Boyd, R.N. and Bhattacharjee, S.K. Organic Chemistry, 6th Ed., Pearson Education Inc., 2014.
4. McMurry, J. Organic Chemistry, 5th Edition, Brooks/Cole, 2000.
5. March, J., Smith, D., March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 7th Ed., Wiley, 2013
6. Carroll, F.A. Perspectives on Structure and Mechanism in Organic Chemistry, 2nd Ed., Wiley, 2010.

**CORE/LAB**

**CHE10302**

**ORGANIC QUALITATIVE ANALYSIS LAB**

**Credit 2** **96 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Identify the functional group(s) present in a given organic compound. | Understand |
| C.O. 2:<br>Categorize the unknown organic compound based on functional group analysis and prepare the corresponding derivative. | Analyse |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | x | x | | | | | | | x | |
| C.O. 2 | x | x | | x | x | | | | x | |

| **UNIT I** | **96 hrs** |
|---|---|
| Identification of simple organic compounds<br>Preparation of derivatives | |

**Recommended Text Books:**


1. Pavia, D.L. Lampman, G.M. Kriz, G.S. and Engel, R.G. Introduction to Organic Laboratory Techniques: A small scale Approach, 2nd Ed., 2007.
2. Dey, B.B. Sitaraman, M.V. and Govindachari, T.V. Laboratory Manual of Organic Chemistry, 3rd Ed., Viswanathan, 1957.
3. Furniss, B.S. Hannaford, A.J. Smith, P.WG. Tatchell, A.R. Vogel's Textbook of Practical Organic Chemistry, 5th Ed., Longman, 1989.
4. Mann, F.G. Saunders, B.C. Practical Organic Chemistry, 4th Ed., Pearson Education India, 2009.
5. Clark, H.T. A handbook of organic analysis, Longman, 1966.
6. Laboratory Manual, CHE 10302, Department of Applied Chemistry, CUSAT

**CORE**

**CHE10401**

**INTRODUCTORY PHYSICAL CHEMISTRY**

**Credit 3** **48 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Differentiate the properties of real gases from those of a perfect gas, and construct an equation of state that describes their properties. | Apply |
| C.O. 2:<br>Predict changes in thermodynamic parameters during a process and predict the spontaneity. | Apply |
| C.O. 3:<br>Apply the laws of chemical kinetics and photochemistry to calculate rate/ rate constants/quantum yield of different types of reactions. | Apply |
| C.O. 4:<br>Understand the details of the structure of solid surfaces and the extent to which a surface is covered and the variation of the extent of coverage with the pressure and temperature | Apply |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | x | x | | | x | | | | | |
| C.O. 2 | x | x | | | x | | | | | |
| C.O. 3 | x | x | | | x | | | | | |
| C.O. 4 | x | x | | | x | | | | | |

**UNIT I** **8 hrs**

Real gases- Deviation from ideal behavior- Compressibility factor, Van der Waals equation, Virial equation, PV isotherms, Continuity of states, Law of corresponding states, Critical phenomena and critical constants.

**UNIT II** **10 hrs**

State functions, Reversible and irreversible processes, Isothermal and adiabatic processes, First, second and third laws of thermodynamics, Concepts of work, heat, Internal energy, enthalpy, Heat capacity, entropy, Gibbs energy, Helmholtz energy- Changes during isothermal and adiabatic reversible and irreversible processes. Joule Thomson effect- Inversion temperature, Application of J.T effect - Liquefaction of gases.

Entropy and free energy as criteria for spontaneity and equilibrium. Nernst Heat theorem and Unattainability of absolute zero.

| UNIT III | 6 hrs |
|---|---|
| Theories of acids and bases- Arrhenius Theory, Lewis theory and Bronsted Theory, Hard and soft acids, pH, PKa, PKb, Ionic product of water, Common ion effect, Solubility product, Acid strength, Degree of hydrolysis of salts, Buffer solutions, Mechanism of buffer action, Henderson equation. | |
| **UNIT IV** | **12 hrs** |
| Rate laws, Order and molecularity, Zero, first, second and third order reactions-Integration of rate laws, Half-life period, Temperature dependence of rate constant-Arrhenius equation Photochemistry-Photochemical laws, Beer Lambert Law, Quantum yield, Jablonski Diagram -Photophysical and photochemical processes, Fluorescence, Phosphorescence-, Chemiluminescence, Bioluminescence, Photosensitisation, Photosynthesis. | |
| **UNIT V** | **12 hrs** |
| Adsorption- Physisorption and chemisorption, Adsorption 16 Isotherms- Langmuir, Freundlich and BET isotherms (Qualitative approach), Application of isotherms for surface area determination, Catalysis- homogeneous and heterogeneous (introduction) Enzyme catalysis- Michael Menton equation.<br>Colloids- Lyophilic and Lyophobic colloids, Preparation of colloids, Kinetic, optical and electrical properties, Electrical double layer Models for double layer: Heimboltz, Gouy Champman and Stern, Zeta potential. Stability of colloids, Protective colloids- Gold number, Flocculation, Hardy Schulze rule, Surfactants, micelles, Critical miscelle concentration, Factors affecting CMC Reverse miscelle, Donnan membrane equilibrium, Dorn effect, Sedimentation potential and streaming potential, Emulsions, Gels, Sols | |

**Recommended Text Books:**


1. Peter Atkins and Julio de Paula, Physical Chemistry, Oxford University Press, $8^{th}$ and 10th Edn, 2017.
2. D.A McQuarrie, J.D Simon, Molecular Thermodynamics, Viva Student Edn. 2010.
3. I.N Levine, Physical Chemistry, McGraw Hill, Indian Edn, 2011.
4. W. J. Moore and R. G. Pearson, Kinetics and Mechanism, Wiley, New York.
5. K. J. Laidler, Chemical-Kinetics, McGraw Hill, New York.

**CORE/LAB**

# CHE10402

# PHYSICAL CHEMISTRY LAB

**Credit 2** **96 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Verify the concepts and laws in physical chemistry | Evaluate |
| C.O. 2:<br>Execute and perform experiments based on pH metry, potentiometry, conductometry and colorimetry to quantify and obtain other physical properties of the chemical species | Evaluate |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | x | x | | | | | | | x | |
| C.O. 2 | x | x | | x | x | | | | x | |

| **UNIT I** | **96 hrs** |
|---|---|
| 1. pH METRY<br>Strong acid X strong base, Strong acid X weak base, Weak acid X Strong base<br>2. POTENTIOMETRY<br>Strong acid X strong base, Strong acid X weak base, Weak acid X Strong base, $KMnO_4$ X$Fe^{2+}$<br>3. CONDUCTOMETRY<br>Strong acid X strong base, Strong acid X weak base, Weak acid X Strong base<br>4. COLORIMTERY<br>Estimation of iron, chromium, nickel, Manganese, Copper, phosphate in soft drinks | |

**Recommended Text Books:**


1. Gurtu, J. N., Gurtu, A., Advanced Physical Chemistry Experiments, 6th Ed.,Pragati Prakashan,2014.
2. Yadav, J. B., Advanced Practical Physical Chemistry, 36th Ed., KrishnaPrakashan, 2016.
3. Laboratory Manual, CHE 10402, Department of Applied Chemistry, CUSAT.

**CORE**

**20-802-0501**

**ANLYTICAL CHEMISTRY-I**

**(ANALYTICAL TECHNIQUES, INSTRUMENTAL METHODS, MOLECULAR SPECTROSCOPY)**

**Credit 3** **48 hours**

| **Course Outcome**<br>After the completion of the course the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Perform various statistical evaluation of experimental data | Analyse |
| C.O. 2:<br>Explain the theory, instrumentation and applications of various chromatographic, spectroscopic, thermal and surface analytical methods | Apply |
| C.O. 3:<br>Predict the type of spectroscopic/chromatographic method for the analysis of the given compound/mixture | Apply |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | x | | | | | | | | | |
| C.O. 2 | x | x | | | | | | | | |
| C.O. 3 | x | x | x | | | | | | | |

| **UNIT I** | **6 hrs** |
|---|---|
| Significant figures, Accuracy, Precision, Error, Types of errors- Determinate and Indeterminate errors, Distribution of random errors, Mathematical Expression for error- Absolute and Relative error, Methods to reduce error, Statistical tools for expressing precision- Standard deviation, Relative standard deviation, Variance, Comparison of results- Students t test, f test, Criteria for rejecting a value-Q test, Confidence interval, Correlation and Regression, Linear regression analysis | |
| **UNIT II** | **10 hrs** |
| Chromatography-classification-column, paper, thin layer chromatography, selection of mobile and stationary phase, Theory and instrumentation of HPLC, LC-MS, GC, GC-MS, ion exchange chromatography, gel permeation chromatography, supercritical fluid chromatography and size exclusion chromatography, Important applications of chromatographic techniques<br>Solvent extraction and Solid phase extraction<br>Distribution law-Liquid-liquid extractions, synergistic extraction. Counter current extraction, super critical fluids, Electrophoresis- theory and applications. | |

| UNIT III | 12 hrs |
|---|---|
| Introduction to spectroscopy, spectroscopy and its importance in chemistry, interaction of electromagnetic radiation with matter, Difference between atomic and molecular spectra. Energy levels in molecules, different types of spectroscopic techniques, Basic instrumentation of spectrometers, optical systems used in spectroscopy – Sources, Filters, Monochromators, Detectors, Single and Double beam optics, Signal to noise ratio, bandwidth and band pass.<br>Instrumentation of NMR, FT IR, UV-Visible, Laser Raman spectroscopy and fluorescence spectroscopy. | |
| **UNIT IV** | **10 hrs** |
| Atomic absorption spectroscopy – Absorption of radiant energy by atoms, Instrumentation, Interferences in AAS, Analytical applications of AAS.<br>Atomic Emission spectroscopy – Principle – Types – Flame atomic emission spectroscopy, Flame photometry, ICP-AES, Instrumentation and applications of ICP-AES. | |
| **UNIT V** | **10 hrs** |
| Introduction to surface characterisation techniques-SEM, AFM, TEM, XRD,<br>Principle and applications of SEM, TEM, AFM and XRD<br>Introduction to thermal methods of analysis-TG, DTA and DSC. | |

**Recommended Text Books:**


1. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Saunders College Pub., 2007.
2. J.H. Kennedy, Analytical Chemistry: Principles, Saunders College Pub., 1990.
3. G.H. Jeffery, J. Bassett, J. Mendham, R.C. Denney, Vogel's Text Book of Quantitative Chemical Analysis, 5th Edn., John Wiley& sons,1989.
4. G.D. Christian, J.E. O'Reilly, Instrumental Analysis, Allyn & Bacon, 1986.
5. F.W. Fifield, D. Kealey, Principles and Practice of Analytical Chemistry, Blackwell Science, 2000.
6. Contemporary Instrumental Analysis, Kenneth A. Rubinson, Judith F. Rubinson, Prentice Hall, New Jersey, 2000.
7. Wilson & Wilson's, Comprehensive Analytical Chemistry, Volume 47, Modern Instrumental Analysis, Edited by S. Ahuja, N. Jespersen, Reed Elsevier India Private Ltd., Noida, 2006.
8. Journal of Chromatography Library, Volume 3, Liquid Column Chromatography-A Survey of Modern Techniques and Applications, Edited by Z. Deyl, K. Macek, J. Janak, Elsevier Scientific Publishing Company, Amsterdam, 1975.
9. Gas Chromatography, John Willett, John Wiley & Sons, Singapore, 1991.

10. Fundamentals of Analytical Chemistry, Doughlas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, 9th Ed., Cengage Learning, 2014.

**CORE**

**20-802-0502**

**INORGANIC CHEMISTRY – I**

**(CHEMISTRY OF MAIN GROUP ELEMENTS)**

**Credit 3** **48 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Describe the general periodic behaviour and occurrence of the main group elements | Understand |
| C.O. 2:<br>Interpret the types of bonding based on the electronic configuration | Apply |
| C.O. 3:<br>Explain the reactivity and physicochemical properties based on the type of bonding | Analyse |
| C.O. 4:<br>Compare the structure, bonding and reactivity of the main group elements with the related organic compounds and transition metal complexes | Apply |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | x | x | | | x | | | | | |
| C.O. 2 | x | x | | | x | | | | | |
| C.O. 3 | x | x | | | x | | | | | |
| C.O. 4 | x | x | | | x | | | | | |
| C.O. 5 | x | x | | | x | | | | | |

| **UNIT I** | **12 hrs** |
|---|---|
| s- Block elements- Hydrogen, Hydrogen Bonding, Hydrates, Hydrogen ions, acids and bases,<br>Group 1 elements - General Behavior, Occurrence and abundance, Electronic Configuration and types of bonding, Flame colors and spectra, Color of compounds, Alkali metals in liquid ammonia and other solvents, Oxides, Hydroxides, hydrides, alkoxides, amido complexes, Ionic salts and M+ ions in solution, Alkali metal complexes, Organolithium compounds.<br>Group 2 elements – General Behavior, Occurrence and abundance, Electronic Configuration and types of bonding, Elemental Beryllium, Binary Compounds, Coordination compounds with oxygen and nitrogen ligand, organoberyllium compounds, Compounds of Magnesium, calcium, strontium-, oxides, halides, hydrides, carbides, ionic salts and complexes, alkoxides.<br>Grignard reagents – preparation and properties. | |

| UNIT II | 12 hrs |
|---|---|
| p- Block elements – Group 13 elements- General Behavior, Occurrence and abundance, Electronic Configuration and types of bonding, oxides, halides, Complex Compounds, Chemistry of oxidation states I and II, Boranes- Preparation, Classifications, Structure and Bonding, Tetrahydroborate ion, Boron Halides, Boron – Nitrogen Compounds, Boron – Oxygen Compounds.<br>Organometallic compounds of Al Group 14 elements – General Behavior, Occurrence and abundance, Electronic Configuration and types of bonding, Carbon- Properties, Allotropes, Carbon Halides, Carbon Oxides, Compounds with C-N bond, C-S bond, Carbon compounds as ligands. Oxygen compounds of Silicon, Organo compounds, Silanes and Silenes, Organometallic compounds of Si and Sn. Inorganic Polymers. | |
| **UNIT III** | **8 hrs** |
| Group 15 elements - General Behavior, Occurrence and abundance, Group trends and stereochemistry, Electronic Configuration and types of bonding, Active Nitrogen, Nitrogen fixation natural and artificial, Nitrogen compounds-Nitrides, Ammonia, Hydrazine, Oxides of Nitrogen, Oxo acids and anions, Halogen Compounds, nitrogen compounds as ligands, Halides of Phosphorous, Oxides of Phosphorous, Sulfides and other chalcogenides of phosphorous, Phosphonium, Phosphorous – Nitrogen Compounds, Phosphorus-nitrogen compounds: Phosphazenes and poly phosphazenes.<br>Organic compounds of Phosphorous, Compounds with element-element bonds, Oxo anions of Phosphorous, Phosphate in bio systems, Phosphorous compounds as ligands, Compounds of Ar, Sb and Bi. | |
| **UNIT IV** | **8 hrs** |
| Group 16 elements - General Behavior, Occurrence and abundance, Electronic Configuration and types of bonding, Group trends and stereochemistry, Types of oxides, Chemical properties of Dioxygen, Singlet oxygen, ozone, Peroxo compounds, Superoxide, Halo compounds, Oxygen compounds as ligands, Sulfanes, polysulfides, Sulphur-Nitrogen Compounds, Tetrasulphur tetranitride, disulphur dinitride and polythiazyl. SxNy compounds. S-N cations and anions. Sulphur-phosphorus compounds: Molecular sulphides such as $P_4S_3$, $P_4S_7$, $P_4S_9$ and $P_4S_{10}$. Halogen compounds of sulphur, Oxides, oxohalides and oxo acids of Sulphur, Sulphur compounds as ligands. | |
| **UNIT V** | **8 hrs** |
| Group 17 elements- General Behavior, Occurrence and abundance, Electronic Configuration and types of bonding, Halogen bonding, Preparation, C-T complexes of Halogen, Halides, Molecular halides, Halides and halogen compounds as ligands, Oxides and oxo acids, Interhalogen and poly halogen compounds, Oxohalogen fluorides. Group 18 elements - General Behavior, Occurrence and abundance, Electronic Configuration and types of bonding, Halogen compounds. | |

**Recommended Text Books:**

1. Mingos, D. M. P., Essential Trends in Inorganic Chemistry, Oxford University Press 1998.
2. Wulfsberg G., Inorganic Chemistry, VIVA, 2002.
3. Greenwood, N. N., Earnshaw, A., Chemistry of the Elements, Maxwell Macmillan International Edition, Pergamon Press, 1989.
4. Cotton, F.A., Wilkinson, G, Advanced Inorganic Chemistry. Wiley-VCH, 1999
5. Huheey, J. E., Keiter, E. A., Kieter, R. L., Medhi, O. K., Inorganic Chemistry Principles Structure and Reactivity, Pearson Education, 4th edition, 2009.
6. Lee, J. D., A New Concise Inorganic Chemistry, ELBS, 1998

**CORE**

**20-802-0503**

**ORGANIC CHEMISTRY-I**

**(FUNCTIONAL GROUP CHEMISTRY)**

**Credit 3** **48 hours**

| **Course Outcome**<br>After the completion of the course the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Correlate structure of organic compounds with their properties | Apply |
| C.O. 2:<br>Describe the synthesis and reactions of different classes of organic compounds | Apply |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | x | | | | | | | | | |
| C.O. 2 | | | x | | | | x | x | | |

| **UNIT I** | **8 hrs** |
|---|---|
| Alkyl and aryl halides - Classification, physical properties, preparation methods, reactions. | |
| **UNIT II** | **10 hrs** |
| Alcohols, phenol and ethers - Classification, physical properties, preparation methods, reactions – with hydrogen halide, order of reactivity of 1°, 2° and 3° alcohols, with $PCl_3$, dehydration, with active metals, ester formation, formation of alkyl sulfonates, oxidation – primary, secondary and tertiary alcohols, chemoselective oxidants for alcohols – Oppenauer's oxidation, Moffatt-Pfitzner oxidation, Des-Martin oxidation, Alcohols as acids and bases. Ascent and decent in alcohol series Dihydric alcohols: Oxidative cleavage– Lead tetra acetate, Periodic acid- Pinacol - Pinacolone rearrangement –mechanism.<br>Phenols - Preparation, physical properties, - Acidity of phenols, reactions, rearrangement of phenol derivatives-Fries rearrangement, Claisen rearrangement Ethers – preparation, physical properties, reactions – cleavage by acids. Synthesis and Reactions of Epoxides, Cleavage of ether linkages by HI- Ziesels method of estimation of methoxy groups. | |
| **UNIT III** | **10 hrs** |
| Carbonyl compounds A: Aldehydes and Ketones<br>Physical properties, preparation, reactions – Cannizaro reaction, Aldol condensation, Wittig reaction, nucleophilic addition - addition of cyanide, derivatives of ammonia, Grignard reagent, alcohols, oxidation and reduction – Baeyer-Villiger oxidation-Cannizzaro's reaction, Meerwein-Ponndorf Verley reduction, Clemmensen reduction, Wolff-Kishner reduction, $LiAlH_4$ and $NaBH_4$ reductions, | |

| | |
|---|---|
| α, β – unsaturated carbonyl compounds – Claisen, Claisen-Schmidt, Dieckmann, Benzoin, Aldol, Perkin and Knoevenagel condensations, nucleophilic and electrophilic addition – Michael addition and Robinson annulation, Mannich reaction. Alkylation of carbonyl compounds via enamines.<br>Compounds containing active methylene groups. | |
| **UNIT IV** | **10 hrs** |
| Carbonyl compounds B: Carboxylic Acids and acid chlorides & esters<br>Physical properties – Acidity of carboxylic acids – effect of substituents, preparation, reactions – salt formation and decarboxylation, preparation and reactions of functional derivatives, halogenation of aliphatic acids - Hell- Volhard- Zelinsky reaction.<br>Methods of formation and chemical reactions of anthranilic acid, cinnamic acid, acrylic acid, oxalic acid, malonic acid, citric acid, adipic acid, maleic acid, fumaric acid. Preparation and reactions of benzene sulphonic acid, benzene sulphonyl chloride and ortho and para toluene sulphonyl chlorides-uses. Esters, hydroxyl acids, lactones.<br>Synthetic uses of malonic ester, acetoacetic ester and cyanoacetic ester. Keto-enol<br>tautomerism of ethyl acetoacetate. | |
| **UNIT V** | **10 hrs** |
| Nitrogen containing compounds<br>Amines- isomerism- stereochemistry of amines, distinguish between primary, secondary and tertiary amines- Structural features affecting basicity of aliphatic and aromatic amines. Quaternary amine salts as phase-transfer catalysts. Comparative study of aliphatic and aromatic amines. Preparation of alkyl and arylamines (reduction of nitro compounds, nitriles), reductive amination of aldehydic and ketonic compounds, Gabriel-Phthalimide reaction, Diazonium salts preparation, synthetic transformations of aryl diazonium salts, azo coupling.<br>Mechanisms of Sandmeyer's and Gatterman reactions- Schiemann and Gomberg reactions Preparation and uses of Phenyl hydrazine. Diazomethane and diazoacetic ester - preparation, structure and synthetic uses -Arndt Eistert<br>synthesis- mechanism –Wolff rearrangement. Amides - preparation and reactions. | |

**Recommended Text Books:**


1. Bruice, P.Y. Organic Chemistry, 7th ed., Prentice Hall Inc., 2013.
2. Morrison, R.T. Boyd, R.N. and Bhattacharjee, S.K. Organic Chemistry, 6th Ed., Pearson Education Inc., 2014.
3. Clayden, J. Green, N. Warren, S. and Wothers, P. Organic Chemistry, 2nd Ed., Oxford University Press, 2012
4. McMurry, J. Organic Chemistry, 5th Ed., Brooks/Cole, 2000.

5. Bruckner, R. Advanced Organic Chemistry: Reaction Mechanisms, 1st Ed., Academic Press, 2001.
6. Carey, F.A. and Sundberg, R.J. Advanced Organic Chemistry (parts A and B), 5th Ed., Springer, 2008.
7. Norman, R.O.C. Principles of Organic Synthesis, 2nd Ed., Chapman and Hall, 1978.
8. Solomons, T.W.G. Fryhle, C.B., Snyder, S. A. Organic Chemistry, 12th Ed., Global, 2017.
9. Smith Janice G., Organic Chemistry 3rd Edn., McGraw-Hill, 2011.

**20-802-0504**

**PHYSICAL CHEMISTRY I**

**(Equilibrium Thermodynamics)**

**Credit 3** **48 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Predict changes in thermodynamic parameters during a process and predict the spontaneity. | Apply |
| C.O. 2:<br>Describe the significance of chemical potential in physical and chemical processes | Apply |
| C.O. 3:<br>Understand the thermodynamics of phase transitions and interpret the phase diagram of a given system | Analyze |
| C.O. 4:<br>Interpret dependence of chemical equilibrium on pressure, temperature and concentration | Analyze |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | x | x | | | x | | | | | |
| C.O. 2 | x | x | | | x | | | | | |
| C.O. 3 | x | x | | | x | | | | | |
| C.O. 4 | x | x | | | x | | | | | |

| **UNIT I** | **8 hrs** |
|---|---|
| Language and Mathematics of Thermodynamics.<br>Recap of first and second law. The Clausius inequality, Free energy functions - Variation with temperature and pressure. Gibbs Helmholtz equation. Relation between thermodynamic functions. Maxwell relations-significance.<br>Third law of thermodynamics: Nernst Heat Theorem, Calculation of absolute entropy, Unattainability of absolute zero. | |
| **UNIT II** | **10 hrs** |
| Thermodynamic systems of variable composition – Partial molar properties. Chemical Potential, Significance of Chemical potential, Gibbs Duhem Equation and Duhem Margules Equation. Thermodynamics of mixing. Excess functions, Concepts of activity and fugacity, Standard states. | |
| **UNIT III** | **10 hrs** |
| Physical transformation of Pure substances- Stability of a phase, Phase transitions and phase boundaries- Thermodynamic aspects, Ehrenfest Classification of Phase transitions. Phase rule – Application to one component systems- Water, S, $CO_2$ and He. | |

| UNIT IV | 10 hrs |
|---|---|
| Thermodynamics of Binary systems: Binary liquids- Ideal solutions, Raoults law, Henry's Law, Deviations from ideality, Real and Regular solutions, Excess functions, Ideal Dilute Solutions-Colligative Properties- van't Hoff factor. Liquid-vapour equilibria of binary systems – Vapour pressure-composition diagrams and Temperature composition diagrams. Distillation of binary mixtures –Azeotrope formation.<br>Liquid-liquid equilibria- Partially miscible and immiscible liquids- CST, Nernst Distribution Law, Partition co-efficient, Principle of Steam distillation.<br>Solid-liquid Equilibria-Cooling curve, Eutectic system, Deep Eutectic solvents, Application, Compound formation with Congruent and Incongruent melting points. Salt hydrate water systems, Solid-Vapour Equilibria- $CuSO_4$-water system. Three component systems | |
| **UNIT V** | **10 hrs** |
| Chemical Equilibria: Chemical Equilibria and free energy, Equilibrium Constant, Applications of free energy function to physical and chemical changes- Le Chateliers Principle. Effect of temperature and pressure on the chemical equilibrium- van't Hoff reaction isotherm and isochore. | |

**Recommended Text Books:**


1. Peter Atkins and Julio de Paula, Physical Chemistry, Oxford University Press, 8th and10th Edn, 2017.
2. D.A McQuarrie, J.D Simon, Molecular Thermodynamics, Viva Student Edn. 2010.
3. I.N Levine, Physical Chemistry, McGraw Hill Indian Edn, 2011.
4. I. M. Klotz & R. M. Rosenberg, Chemical Thermodynamics, Wiley, 7th Edn, 2008.
5. L. K. Nash, Elements of Chemical Thermodynamics, Addison Wesley, 2nd Edn, 2013.
6. F. Daniels and R. A. Alberty, Physical Chemistry, Wiley Publishers, 4th Edn 2004.

**CORE**

**20-802-0505**

**MATHEMATICS FOR CHEMISTS**

**Credit 2** **32 hours**

| **Course Outcome**<br>After the completion of the course the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Solve mathematical problems | Apply |
| C.O. 2:<br>Apply the principles of mathematics to chemical systems/processes | Analyse |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | x | x | | | | | | | | |
| C.O. 2 | x | x | | | | | | | | |

| **UNIT I** | **4 hrs** |
|---|---|
| Numbers: Real and Complex number algebra. Vector algebra. | |
| **UNIT II** | **6 hrs** |
| Functions & Variables: Differential calculus-first- and higher-order derivatives, evaluation of minimum and maximum, limits & continuity. Partial differentiations. Exact and inexact differentials. Numerical differentiation. The gamma and delta functions.<br>Integral Calculus: Indefinite and definite integrals, improper integrals. Methods of integration. Surface and volume integrals. Numerical integrations. | |
| **UNIT III** | **8 hrs** |
| Differential Equations: Ordinary first- and second-order differential equations.<br>Partial differential equations. Solution of inexact differential equations by the method of integrating factors. Power series and extended power series solutions.<br>Numerical solutions | |
| **UNIT IV** | **8 hrs** |
| Special functions: Hermite, Legendre and Laguerre polynomials, recursion relations. Matrices and Determinants. Eigenvalues and eigenvectors.<br>Orthogonal transformation. Rank & inverse ofmatrix. | |
| **UNIT V** | **6 hrs** |
| Solution of Linear Systems: Gaussian elimination, Cramer's rule. Gauss-Jordan elimination. Gauss-Seidel and Jacobi methods. Solution of non-Linear Systems: Newton-Raphsonmethod.<br>Curve fittings. Permutation & Combination. Probability. Stirling's approximation. Lagrange multipliers. | |

**Recommended Text Books:**


1. Mortimer, R. G, Mathematics for Physical Chemistry. 3rdEdn., Academic Press.2014
2. Kreyszig, E., Advanced Engineering Mathematics. 9thEdn. Wiley,2015
3. Turrell, G., Mathematics for Chemistry and Physics, 2ndEdn., Academic Press,2004
4. McQuarrie, D. A., Mathematics for Chemists and Physicists, 4thEdn.,Wiley,2007.

**CORE/LAB**

**20-802-0506**

**INORGANIC CHEMISTRY LAB**

**Credit 2** **96 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Estimate the amount of a given metal ion by complexometric reactions | Apply |
| C.O. 2:<br>Identify the cation from the given mixture | Apply |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | x | x | | x | x | | | | | |
| C.O. 2 | x | x | x | x | x | | | | | |

| **UNIT I** | **96 hrs** |
|---|---|

1. Complexometry
2. Estimation of Zinc Estimation of Magnesium
3. Estimation of different metal ions from a mixture – use of masking agents
4. Analysis of less common ions
5. Separation and identification of two less familiar metal ions such as Tl, W, Se, Mo, Ce, Th, Ti, Zr, V, U and Li from a mixture of salts.

**Recommended Text Books:**


1. Vogel's Textbook of Quantitative Chemical Analysis 6th Ed., Pearsons EducationLtd.
2. A.I. Vogel, G. Svehla, Vogel's Qualitative Inorganic Analysis, 7th Edn., Longman,1996.
3. V.V. Ramanujam, Inorganic Semimicro Qualitative Analysis, The National Pub.Co., 1974.
4. Laboratory Manual, CHE 10506, Department of Applied Chemistry, CUSAT.

**CORE/LAB**

**20-802-0507**

**ORGANIC CHEMISTRY LAB**

**Credit 2** **96 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Prepare organic compounds through one step synthesis and purify and recrystallize the product | Analyse |
| C.O. 2<br>Apply analytical techniques for the quantitative and qualitative analysis of organic molecules | Apply |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | x | x | | x | | | | | | |
| C.O. 2 | x | x | | x | | | | | | |

| **UNIT I** | **96 hrs** |
|---|---|
| One step synthesis of Organic Compounds Estimation of organic compounds<br>Separation of organic binary mixtures –liquid-liquid extraction, column chromatography.<br>Purity assessment of the isolated components by TLC & GC. | |

**Recommended Text Books:**


1. Pavia, D.L. Lampman, G.M. Kriz, G.S. and Engel, R.G. Introduction to Organic Laboratory Techniques: A small scale Approach, 2nd Ed., 2007.
2. Dey, B.B. Sitaraman, M.V. and Govindachari, T.V. Laboratory Manual of Organic Chemistry, 3rd Ed., Viswanathan, 1957.
3. Furniss, B.S. Hannaford, A.J. Smith, P.WG. Tatchell, A.R. Vogel's Textbook of Practical Organic Chemistry, 5th Ed., Longman, 1989.
4. Mann, F.G. Saunders, B.C. Practical Organic Chemistry, 4th Ed., Pearson Education India, 2009.
5. Clark, H.T. A handbook of organic analysis, Longman, 1966.
6. Laboratory Manual, CHE 10707, Department of Applied Chemistry, CUSAT.

**CORE/LAB**

**20-802-0508**

**OPEN ENDED LAB-I**

**Credit 2** **96 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Design experiments and validate the hypothesis of an independent research problem. | Evaluate |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | x | x | | | | x | x | x | x | |

| **UNIT I** | **96 hrs** |
|---|---|
| The students shall perform literature review/ experiments/analysis for validating the hypothesis.<br>The students shall submit a project report and appear for viva-voce. | |

**CORE**

**20-802-0601**

**INORGANIC CHEMISTRY – II**

**(COORDINATION CHEMISTRY)**

**Credit 3** **48 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Explain the properties of transition metals and lanthanides | Apply |
| C.O. 2:<br>Describe and explain the structure, bonding and magnetism in transition metal complexes using crystal field theory and ligand field theory | Analyse |
| C.O. 3:<br>Describe various metal-ligand interactions in terms of sigma- and pi-bonding | Evaluate |
| C.O. 4:<br>Explain the stability of transition metal complexes, their reactivity, and the mechanisms of ligand substitution and redox reactions | Analyse |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | x | x | | | x | | | | | |
| C.O. 2 | x | x | | | x | | | | | |
| C.O. 3 | x | x | | | x | | | | | |
| C.O. 4 | x | x | | | x | | | | | |

| **UNIT I** | **8 hrs** |
|---|---|
| General periodic trends of d and f block elements, Metallic property, Chemistry of variable oxidation states, properties of d configuration - $d^0$ to $d^{10}$, Type of compounds. Lanthanides and Actinides- Stable oxidation states, lanthanide and actinide contraction, Occurrence and recovery; Separation of Lanthanides; difference between 4f and 5f orbitals. | |
| **UNIT II** | **10 hrs** |
| Werner's theory, Bonding in coordination compounds: Valence bond description and its limitations. valence bond theory (inner and outer orbital complexes), Crystal Field Theory (CFT). measurement of 10 Dq (Δo), CFSE in weak and strong fields, pairing energies, factors affecting the magnitude of 10 Dq (Δo, Δt). Octahedral vs. tetrahedral coordination, tetragonal distortions from octahedral geometry Jahn-Teller theorem, Jahn – Teller effect in octahedral complexes, square planar geometry. | |
| **UNIT III** | **10 hrs** |
| Factors affecting the crystal-field parameters. Spectrochemical series, colour and spectral behaviours. magnetism of first-row transition metal complexes, stabilization of unusually low and high oxidation | |

| | |
|---|---|
| states of metals, Ligand field theory and Qualitative aspect of MO Theory, Effect of π-donor and π-acceptor ligands in LFSE, back bonding. Application of crystal filed theory, lattice energies, ionic radii, site preferences in spinels. Structural and stereoisomerism in complexes with coordination numbers 4 and 6. | |
| **UNIT IV** | **12 hrs** |
| Definition and Classification with appropriate examples based on nature of metal-carbon bond (ionic, s, p, and multicentre bonds), metal-metal multiple bonding, Concept of hapticity of organic ligands. Metal carbonyls: 18 electron rule, EAN rule as applied to carbonyls, electron count of mononuclear, polynuclear and substituted metal carbonyls of 3d series. Preparation and Structures of mononuclear and binuclear carbonyls of Cr, Mn, Fe, Co and Ni. π-acceptor behaviour of CO, synergic effect and use of IR data to explain extent of back bonding. Zeise's salt: Preparation and structure, evidences of synergic effect and comparison of synergic effect with that in carbonyls.<br>Organo-lithium aluminium, magnesium, zinc and titanium compounds – their preparations, properties, reactions, bonding and applications. "Sandwitch" compound: Ferrocene – its preparation, reactions and structure. | |
| **UNIT V** | **8 hrs** |
| Introduction to inorganic reaction mechanisms. Substitution reactions in square planar complexes, Trans-effect, theories of trans effect, Mechanism of nucleophilic substitution in square planar complexes, Thermodynamic and Kinetic stability, Labile and inert complexes, Kinetics of octahedral substitution, Ligand field effects and reaction rates. | |

**Recommended Text Books:**


1. Purcell, K.F & Kotz, J.C. Inorganic Chemistry, 2nd Ed., W.B. Saunders Co, 1991.
2. Huheey, J. E., Keiter, E. A. and Keiter, R. L. Inorganic Chemistry, Principle and structure and reactivity, 4th Ed., Harper Collins College Publishers, New York, 1993.
3. Lippard, S.J. & Berg, J.M. Principles of Bioinorganic Chemistry 2nd Ed., University Science Books, 1994.
4. Cotton, F.A. & Wilkinson, G, Advanced Inorganic Chemistry. 6th Ed., Wiley- Interscience, 1999.
5. Basolo, F, and Pearson, R.C., Mechanisms of Inorganic Chemistry, 2nd Ed., John Wiley & Sons, NY, 1967.
6. Greenwood, N.N. & Earnshaw A., Chemistry of the Elements, 2nd., Ed. Butterworth-Heinemann,1997.
7. Miessler, G.L. & Tarr, D. A. Inorganic Chemistry, 5th Ed., Pearson Publication, 2013.
8. Sharpe, A.G. Inorganic Chemistry, 4th Indian Reprint, Pearson Education, 2005.

9. Douglas, B. E.; McDaniel, D.H. and Alexander, J.J. Concepts and Models in Inorganic Chemistry 3rd Ed., John Wiley and Sons, NY, 1994.
10. Powell, P. Principles of Organometallic Chemistry, 2nd Ed., Springer, 1991.
11. Shriver, D. F., Atkins, P. W. and Langford, C. H. Inorganic Chemistry, 4$^{th}$ Ed., W.H. Freeman & Company, 2006.
12. Crabtree, Robert H. The Organometallic Chemistry of the Transition Metals. 6th Ed., New York, NY: John Wiley, 2014.
13. W. L. Jolly, Modern Inorganic Chemistry, McGraw-Hill International, 2$^{nd}$ Edition, New York, 1991.

**CORE**

**20-802-0602**

**ORGANIC CHEMISTRY-II**

**(STRUCTURE, STEREOCHEMISTRY AND CONFORMATIONAL ANALYSIS)**

**Credit 3** **48 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Appraise Molecular Orbital Theory and group orbital concepts to sketch MO's of common organic molecules and reactive intermediates | Analyze |
| C.O. 2:<br>Apply the concepts of isomerism and analyse the conformation and configuration of organic molecules. | Apply |
| C.O. 3:<br>Analyze the conformational effects on the reactivity of various reactions | Analyze |
| C.O. 4:<br>Understand the conformation and stereo-electronic effects of carbohydrates | Understand |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | x | x | | | x | | | x | | |
| C.O. 2 | x | x | | | x | | | x | | |
| C.O. 3 | x | x | | | x | | | x | | |
| C.O. 4 | x | x | | | x | | | x | | |

| **UNIT I** | **10 hrs** |
|---|---|
| MO theory and Frontier orbitals: Qualitative Molecular Orbital Theory, Group orbitals, Hyper conjugation, Negative – Hyperconjugation, Anomeric effect.<br>Conjugated Systems, Huckels rule and Modern theory of Aromaticity. Substituent effects on frontier orbitals. Study of Structure and Stability of Reactive intermediates: Carbocations, Carbanions, Carbenes, Nitrenes, and Radicals.<br>Study of Bonding Weaker than Covalent Bonds: Ion pairing interactions, ion –dipole interactions, dipole – dipole interactions, Hydrogen bonding, Factors affecting strength and stability of hydrogen bonds, cations – π, polar – π, π- stacking, π-donor – acceptor interactions, induced dipole interactions, the hydrophobic effect. | |
| **UNIT II** | **10 hrs** |
| Geometrical & Optical isomerism: origin of chirality, chiral centres and configuration, axes and planes, helicity. Topicity relationships, enantiotopic and diastereotopic, groups and faces, prochiral | |

| | |
|---|---|
| centres and faces. Symmetry, stereochemistry and time scale. Allenes, cumulenes, biphenyls, and spirans.<br>Compounds containing chiral atoms other than carbon. Topological and Supramolecular stereochemistry.<br>Brief introduction to CD and ORD techniques, octant rule, axial haloketone rule, and sign of Cotton effect. | |
| **UNIT III** | **8 hrs** |
| Conformational analysis: Strain, types of strain including *B, F, I,* Pitzer strain, Beyer strain. Acyclic $sp^3$–$sp^3$, $sp^3$-$sp^2$ systems, structure and stability of small, medium, and large rings, cyclohexane, substituted cyclohexanes, A values, cyclohexenes, decalins, bicyclic systems. | |
| **UNIT IV** | **10 hrs** |
| Reaction Mechanisms and Conformational Effects on Reactivity – Ester Hydrolysis, Alcohol Oxidations, SN2 Reactions, Elimination Reactions, Epoxidation by Intramolecular closure of Halohydrins, Epoxide Openings ($S_N2$), Electrophilic Additions to Olefins, Rearrangement Reactions, Conformational and Stereoelectronic Effects on Reactivity. Baldwins rules for ring closure. | |
| **UNIT V** | **10 hrs** |
| General introduction to carbohydrates: Structure and stereochemistry of monosaccharides, disaccharides, mutarotation, glyoxal, stepping up and stepping down, reducing and non-reducing sugars, glycosidic linkage, O & N glycosides. Conformation and Stereo-electronic Effects of carbohydrates: *D* and *L* sugars, Chair conformation, Endo/Exo-anomeric effect, Reverse anomeric effect, Glycosidic torsion angles, Hydroxymethyl group conformation. Conformation and stability of aldohexoes, structure and conformation of ribose and deoxyribose. | |

**Recommended Text Books:**

1. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th ed. 2013, Wiley
2. T H. Lowry and K.S. Richardson: Mechanism and Theory in Organic Chemistry, 3rd ed. 1997, Benjamin-Cummings Publishing Company.
3. F. A. Carey and R. J. Sundberg: Advanced Organic Chemistry (parts A and B), 5th Edition 2008, Springer.
4. E. V. Anslyn and D. A. Dougherty: Modern Physical Organic Chemistry. Ist ed. 2006, University Science Books,
5. F. A. Carroll: Perspectives on structure and mechanism in organic chemistry, 2$^{nd}$ edition, 2011 Wiley.
6. N. S. Issacs: Physical Organic Chemistry, Second Edition, 2nd Edition, 1995, Prentice Hall.
7. A. Pross: Theoretical and Physical Principles of Organic Chemistry, I Edition,1995, Wiley.

8. J. Clayden, N. Green, S. Warren and P. Wothers: Organic Chemistry, 2nd Edition. 2012, Oxford University Press.
9. P.S.Kalsi: Stereochemistry, Conformation and Mechanism, 3rd Edn., New Age Publications
10. E. L. Eliel and S. H. Wilen: Stereochemistry in Organic Compounds, 1994, John Wiley.
11. S. H. Pine: Organic Chemistry, 5th edition, 2008, McGraw Hill
12. I. Flemming: Molecular orbitals and organic chemical reactions, student edition, 2009, Wiley.
13. J. McMurry, Organic Chemistry, Fifth Edition, 2000, Brooks/Cole .
14. D. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications, Second Edition, 1994, Wiley Eastern Limited, New Delhi.

**CORE**

**20-802-0603**

**PHYSICAL CHEMISTRY- II**

**(ELECTROCHEMISTRY, SOLID STATE AND LIQUID STATE)**

**Credit 3** **48 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Describe the theories effecting ionic conductance and apply the concepts to calculate conductance of a given system. | Apply |
| C.O. 2:<br>Describe the mechanism of electronic conductance process in charged interfaces. | Apply |
| C.O. 3:<br>Describe the regular arrangement of atoms in crystals and the symmetry of their arrangement. | Analyze |
| C.O. 4:<br>Understand properties of solids and liquids, and see how their mechanical, electrical, optical, and magnetic properties stem from the properties of their constituent atoms and molecules. | Analyze |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | x | x | | | x | | | | | |
| C.O. 2 | x | x | | | x | | | | | |
| C.O. 3 | x | x | | | x | | | | | |
| C.O. 4 | x | x | | | x | | | | | |

| **UNIT I** | **8 hrs** |
|---|---|
| Introduction- Ionics, Electrodics, Electrochemical Cells, Electrodes, Electrolytes, Half Reactions, Electrochemical Work, Equilibrium electrochemistry-Halfreactions and electrodes, Types of cells, Types of electrodes- Standard hydrogen electrode, Calomel electrode, Quinhydrone electrode. Ion – Solvent, Ion – Ion Interactions, Ionic and Electronic Conductance, Conductance Measurement, Equivalent Conductance, Kohlrausch's Law, Ostwalds dilution law, Ionic Mobility, Walden's rule, abnormal conductance, Conductometeric titrations. | |
| **UNIT II** | **12 hrs** |
| Transport Number- Factors Influencing, measurement- Hittorf's and moving boundary methods. Debye-Huckel Theory, Ionic Atmosphere, time of Relaxation, Mechanism of Electrolytic Conductance, Debye Huckel Onsager equation for strong electrolytes. Electrode – Ion interface, liquid junction potential, Double Layer, Overvoltage (Elementary idea). | |

| | |
|---|---|
| The electromotive force, Standard potentials, Applications of standard potentials, Determination of solubility product and activity co-efficient, pH determination, Potentiometric titrations, Redox indicators principle. Activity and Activity Coefficient of Electrolytes. Corrosion of metals- different forms of corrosion and prevention. Electrochemical Theory of corrosion – methods of prevention. Fuel Cell, Batteries (Elementary idea). | |
| **UNIT III** | **12 hrs** |
| Symmetry as a universal theme, Molecular symmetry, Symmetry elements and operations, Point groups, Matrix representation of symmetry operations, character, Definition of a mathematical group, Abelian group, Cyclic group, symmetry operations as group elements, symmetry and isomerism, Symmetry classification of molecules into point groups (Schoenflies symbol). Group multiplication table. Crystal structures and symmetry, Crystallographic point groups, space group, unit cells, Miller indices, Seven crystal systems and Bravais lattices, Simple, body centered and face centered systems, Packing in solids- packing diagrams, close packing,- hcp and ccp structures, XRD, Braggs equation – derivation, Powder and rotating crystal technique. Identification of cubic crystals based on interplanar ratio. | |
| **UNIT IV** | **8 hrs** |
| Ionic solids with formula MX (CsCl, NaCl, Zinc Blende and Wurtzite Structures), MX2 (Fluorite and Antfluorite Structures, Cadmium Halides, CaF2, Rutile, Anti-rutile, betacristobalite), other crystal systems (Bismuth tri-iodide, Corundum, Rhenium Trioxide etc.), Mixed oxides (Spinel, Perovskite, Ilmenite). The properties of solids , Mechanical properties Electrical properties, Impact on nanoscience: Nanowires, Optical properties , Magnetic properties.<br>Point Defects in crystals- stoichiometric and non-stoichiometric defects, Line defect, surface defects, Liquid Crystals- Classification and application. | |
| **UNIT V** | **8 hrs** |
| Vapour pressure , Surface tension - determination of vapour pressure. Parachor – determination, application to structure elucidation of compounds, Viscosity - determination of molecular mass from viscosity measurements. Refraction – refractive index, molar refraction and optical exaltation – application to structure elucidation, Concept of superhydrophobicity/super-leophilcity.. | |

**Recommended Text Books**


1. J. Bockris and A.K.N. Reddy, Modern Electrochemistry, 2nd Edn., Wiley, New York, 1998
2. R. Crow, Principles and Applications of Electrochemistry, Paper back edn, $4^{th}$ edn, 1994.
3. S. Glasstone, An Introduction to Electrochemistry, Paperback edn., 2007
4. L.V. Azaroff, Introduction to Solids, Mc Graw Hill, 1960.
5. A. R. West, Solid State Chemistry, Wiley Student (Indian) Ed., (2014)

6. A.K. Galwey, Chemistry of Solids, Chapman and Hall, London, 1967. 35
7. Lesley Smart and Elaine Moore, Solid State Chemistry, Chapman and Hall, 1995.
8. H. V. Keer, Principles of the Solid State Wiley Eastern Ltd, New Delhi, 1993.
9. C. N. R. Rao and J. Gopalakrishnan, New Directions in Solid State Chemistry. 2nd edn, Cambridge Uty Press, 1997.

**CORE**

**20-802-0604**

**INDUSTRIAL CHEMISTRY**

**Credit 3** **48 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Describe the sustainable management of chemicals | Apply |
| C.O. 2:<br>Preform quality analysis of chemical products | Analyze |
| C.O. 3:<br>Evaluate the factors influencing the industrial scale up of chemical synthesis | Evaluate |
| C.O. 4:<br>Explain and prepare flow chart for preparation of chemicals | Analyze |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | x | x | | x | x | x | x | x | | |
| C.O. 2 | x | x | | x | x | x | x | x | | |
| C.O. 3 | | x | | x | x | x | x | x | | |
| C.O. 4 | | x | x | x | x | x | x | x | | |

| **UNIT I** | **10 hrs** |
|---|---|
| Source of Chemicals, Organic Chemicals, Inorganic Chemicals, Recycling of materials, waste minimization, E factor and atom economy, Reduction of material use. Water management – water for industry, sources of water, water conditioning methods, municipal waste water, Industrial waste water – treatment. Energy Management- energy required by chemical industries, sources of energy, cost of energy, types of energy requirement, use of energy, efficient utilization of energy., energy, risk and hazards. Sustainable use of- chemical feedstocks, water, energy. Environmental pollution control – methods of pollution control, economics of pollution control, industrial health and hygiene. | |
| **UNIT II** | **10 hrs** |
| Industrial Processes in practice – Basic chemical data, Flow charts; chemical process selection, design and operation, Plant location, safety, construction of plant, process system engineering. Case study of chemical industry of regional importance. Pharmaceutical Industries – Classification, methods of preparation, radioisotopes in medicine, biological hormones, steroids, vitamins, plant and animal isolates, drug design (basic understanding). | |
| **UNIT III** | **10 hrs** |
| Fuel Industries – Calorific value, modern concept of fuels, classification, criteria for selection, comparison of gas, liquid and solid fuels, properties, methods of processing various fuels, solid fuels | |

| | |
|---|---|
| , Gaseous fuels, Petroleum – occurrence, mining, product of refining, Processing, color and constituency, classification and composition, grading of petroleum, determination of flash point, knocking, antiknock compounds, octane number, cetane number, chemical treatment to upgrade liquid fuel, Petrochemicals. | |
| **UNIT IV** | **10 hrs** |
| Agrichemical Industries- Fertilizers – Fertilizer type, need for fertilizer, essential requirements, plant nutrients and regulators, soil fertility, pH of soil, classification of fertilizer, natural fertilizers, nitrogenous fertilizer, Phosphate fertilizers, NPK fertilizers, effect of fertilizer- pollution. Insecticides classification, DDT, BHC, Gammexane, Endosulfan. Attractant and repellants.<br>Introduction to nutraceuticals: definitions, synonymous terms, claims for a compound as nutraceutical, regulatory issues. Study of Properties, structure and functions of various Nutraceuticals (3 examples) formulation of functional food, stability, analysis. Food as remedies, Anti-nutritional Factors present in Foods, Nutraceutical Industry and Market Information.<br>Synthetic uses of malonic ester, acetoacetic ester and cyanoacetic ester. Keto-enol tautomerism of ethyl acetoacetate. | |
| **UNIT V** | **8 hrs** |
| Rubber Industries – Chlorinated and oxygenated rubber, latex, coagulation, crude natural rubber, vulcanization, physical and chemical properties. Synthetic rubbers-SBR, silicone rubber, reclaimed rubber, foam rubber, rubber cement, applications, Rubber derivatives. Leather – manufacture, tanning of leather – vegetable tanning, chrome tanning, oil tanning. Synthetic Fibers – properties, preparation, requirements, difference between synthetic and natural fiber. Rayon, Nylon, Orlon, Teflon. | |

**Recommended Text Books:**


1. C. A. Heaton, An Introduction to industrial chemistry, 2nd edition, 1991,Blackie.
2. George T. Austin, Shreve's Chemical Process Industries, 5th edition, 1984, McGraw Hill International.
3. B. K. Sharma, Industrial Chemistry (including Chemical Engineering), 1997, GOEL Publishing House.
4. M. Farhat Ali, Bassam El Ali, Handbook of Industrial Chemistry: Organic Chemicals, 2005, McGraw Hill Professional.
5. Fritz Ullmann, Ullmann's Encyclopedia of Industrial Chemistry, 1999-2014, John Wiley and Sons, Inc.
6. A. K. De, Environmental Chemistry, 7th edition, 2013, New Age International Publishers.
7. G. E. J. Poinern, A Laboratory Course in Nanoscience and Nanotechnology, 2015, CRC Press Taylor & Francis Group

**CORE**

**20-802-0605**

**MATHEMATICS FOR CHEMISTS**

**Credit 2** **32 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Describe different numerical methods and apply them to solve simple chemical problems | Apply |
| C.O. 2:<br>Write FORTRAN programmes for solving simple chemical problems using the numerical methods | Analyze |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | x | x | | | | | | | | |
| C.O. 2 | x | x | | | | | x | | | |

| **UNIT I** | **6 hrs** |
|---|---|
| Programming in FORTRAN: Program design (algorithm), organization of program, data types and integer constants, complex constanta, logical constants, variables, implicit and explicit data typing, expressions and hierarchy of operations, mix-mode arithmatic, library functions, input/output specification, formatting, unconditional transfers, conditional statements and constructs, GO TO/ IF statements, relational operators, block if structure, else if construct, do loops, nesting, variables and arrays, parameter/data statements, common blocks, read/write by opening files, subroutines and construction of large program. | |
| **UNIT II** | **6 hrs** |
| Numerical Methods: Taylor's theorem, Expansion of functions, Remainder, Mean value and Extreme value theorems, Discrete average value theorem. Numerical Differentiation (first, second and higher derivatives) - Truncation and Round-off errors, Step size dilemma, Difference table (Pascal's triangle). | |
| **UNIT III** | **4 hrs** |
| Numerical Integration - Riemann sum, Quadrature rule, Interpolating polynomials (Lagrange's), Weights, Mid-point, Trapezoidal, Simpson's rule of integration, Adams' Predictor-Corrector method. Roots of equations- Newton- Raphson and Secant methods, Bisection and False-point methods, Bracketing. | |
| **UNIT IV** | **8 hrs** |
| Numerical solution of ordinary differential equations- Initial value problems, Euler's method, Taylor and Runge-Kutta methods, Modified Euler and Hugen's method, Error estimates. Curve fitting- Least | |

| | |
|---|---|
| square fit algorithm, Monotone and convex data. Linear systems- Forward, Backward substitution, LU- factorization, pivoting (only basics), Gaussian Elimination, Gauss-Jordan Elimination, Jacobi and Gauss-Seidel methods. Eigenvalue problems. Statistical analysis of data. | |
| **UNIT V** | **8 hrs** |
| Programming Laboratory (Linux OS, vi editon): Students are instructed to write programs on some of the numerical methods taught. Programming in FORTRAN (FORTRAN 77 Standard)<br>Examples of numerical algorithms – algebraic equations, numerical integration, curve fitting, matrix computations | |

**Recommended Text Books:**


1. Schatzman, M., Numerical Analysis: A Mathematical Introduction, 2ndEdn. Oxford University Press,2012
2. McCormick, J. M., Salvadori, M. G., Numerical Methods in Fortran, Prentice Hall of India,2009
3. Burden, R. L., Faires, J. D., Numerical Analysis, 2ndEdn. Brooks/Cole,2012.
4. Epperson, J. F., An Introduction to Numerical Methods and Analysis, John Wiley and Sons, Inc.,2014
5. Maron, M. J., Numerical Analysis: A Practical Approach, , Macmillan,2008.
6. Hildebrand, F. B., Introduction to Numerical Analysis, McGraw Hill, New York,2007.
7. Xavier, C., Fortran 77 and Numerical Methods, 2ndEdn., New Age International Publishers,2011
8. Rajaraman, V., Computer Programming in Frotran, PHI Learning,1995.
9. Mollah,S.A., Numerical Analysisand Computational Programming, Allied Publishers Ltd,2011.

**CORE/LAB**

**20-802-0606**

**ADVANCED PHYSICAL CHEMISTRY LAB – I**

**Credit 2** **96 hours**

| **Course Outcome**<br>After the completion of the course the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Verify the concepts and laws in physical chemistry. | Evaluate |
| C.O. 2:<br>Execute and perform experiments based on CST, Rast method, Transition temperature and Hall effect for the determination of various physical properties. | Evaluate |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | x | | | | | | | | x | |
| C.O. 2 | xx | | | x | x | | | | x | |

**UNIT I** **96 hrs**

1. Enzyme Kinetics
2. C.M.C. determination
3. CST

   Determination of mutual solubility of phenol-water system Influence of KCl, Succinic acid on CST of phenol-water system- Estimation of concentration of unknown solution
4. RAST METHOD

   Determination of molal depression constant of naphthalene -determination of molecular weight of solute
5. TRANSITION TEMPERATURE

   Determination of transition temperature of salt hydrate-water system

   Determination of molecular weight of solute ;Viscosity, molecular weight of polymers
6. Intermolecular hydrogen bonding in benzyl alcohol using infrared spectroscopy
7. HALL EFFECT EXPERIMENT.

**Recommended Text Books:**


1. J. N. Gurtu, and A. Gurtu Advanced Physical Chemistry Experiments, 6th Ed., Pragati Prakashan,2014.
2. J. B. Yadav, Advanced Practical Physical Chemistry, 36th Ed., Krishna Prakashan, 2016.
3. Laboratory Manual, CHE 10606, Department of Applied Chemistry, CUSAT.

**CORE/LAB**

**20-802-0607**

**INDUSTRIAL CHEMISTRY LAB**

**Credit 2** **96 hours**

| **Course Outcome**<br>After the completion of the course the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Prepare and analyze industrially important chemical products | Create |
| C.O. 2:<br>Prepare the treatment methods for conversion of natural resources to value added chemicals | Create |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | | | x | x | | | | x | x | |
| C.O. 2 | | | x | x | | | | x | x | |

| **UNIT I** | **96 hrs** |
|---|---|
| 1. Preparation of soap and detergents<br>2. Preparation of margarine<br>3. Preparation and physical property measurement of natural, synthetic rubber, fiber.<br>4. Extraction of essential oils<br>5. Extraction of natural flavors<br>6. Preparation of Biogas<br>7. Waste water treatment<br>8. Preparation and characterization of nanomaterials<br>9. Preparation of silicon from Rice Husk<br>10. Galvanization/powder coating. | |

**Recommended Text Books:**


1. J. N. Gurtu, and A. Gurtu Advanced Physical Chemistry Experiments, 6th Ed., Pragati Prakashan,2014..
2. J. B. Yadav, Advanced Practical Physical Chemistry, 36th Ed., Krishna Prakashan, 2016.
3. Laboratory Manual, CHE 10606, Department of Applied Chemistry, CUSAT.

**CORE/LAB**

**20-802-0608**

**OPEN ENDED LAB-II**

**Credit 2** **96 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Design experiments and validate the hypothesis of an independent research problem. | Evaluate |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | x | x | | | | x | x | x | x | |

| **UNIT I** | **96 hrs** |
|---|---|
| 1. The students shall perform literature review/ experiments/analysis for validating the hypothesis.<br>2. The students shall submit a project report and appear for viva-voce. | |

**CORE**

**25-802-0701**

**INORGANIC CHEMSITRY-III**

**(CONCEPTS AND DEVELOPMENTS)**

**Credit 3** **48 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Identify the structure-activity relationship of simple molecules based on their qualitative molecular orbitals. | Analyze |
| C.O. 2:<br>Predict the stability and topology of different polyhedral boranes and related compounds. | Analyze |
| C.O. 3:<br>Assess the strength of various acids and bases and their reactivity. | Analyze |
| C.O. 4:<br>Explain behavior of different non-aqueous solvent systems towards different reactions. | Apply |
| C.O. 5:<br>Interpret the structure and properties of compounds of sulfur, nitrogen, phosphorous and group 14 elements. | Apply |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | x | x | | | x | | | | | |
| C.O. 2 | x | x | | | x | | | | | |
| C.O. 3 | x | x | | | x | | | | | |
| C.O. 4 | x | x | | | x | | | | | |
| C.O. 5 | x | x | | | x | | | | | |

| **UNIT I** | **10 hrs** |
|---|---|
| Qualitative molecular orbital theory, symmetry of molecular orbitals, MOs for homo and heteronuclear diatomic molecules, $H_2$ to $F_2$, HF, CO, NO, $BeH_2$, $CO_2$, $H_2O$, $BH_3$, $NH_3$, $B_2H_6$, $B_3N_3H_6$, $S_3N_3$, $N_3P_3Cl_6$, $Si_2H_2$. Importance of frontier molecular orbitals, Shape, energy and reactivity of molecules. | |
| **UNIT II** | **10 hrs** |
| Electronic structure and allotropes of boron, boron halides, boron heterocycles, borazine Structure and bonding in polyhedral boranes and carboranes, styx notation; electron count in polyhedral boranes; Wade's rule; topological approach to boron hydride structure. Importance of icosahedral framework of boron atoms in boron chemistry. Closo, nido and arachno structures. Synthesis of | |

| | |
|---|---|
| polyhedral boranes; electron counting in polycondensed polyhedral boranes, mno rule. Carboranes, metallocarboranes; Boron halides, boron heterocycles, borazine. | |
| **UNIT III** | **10 hrs** |
| Relative strength of acids, Pauling rules, Lux-Flood concept, Lewis concept, Generalized acid-base concept, Measurement of acid base strength, Lewis acid – base interactions, steric and solvation effects, acid–base anomalies, Pearson's HSAB concept, acid-base strength and hardness and softness, Symbiosis, theoretical basis of hardness and softness, electronegativity and hardness. | |
| **UNIT IV** | **8 hrs** |
| Chemistry in non-aqueous solvents reactions in $NH_3$, liquid $SO_2$, solvent character, reactions in $SO_2$, acetic acid, solvent character, reactions in $H_2SO_4$ and some other solvents. Molten salts, Green solvent: supercritical $CO_2$, Ionic liquids and deep eutectic solvents. | |
| **UNIT V** | **10 hrs** |
| Sulphur-Nitrogen compounds: Tetrasulphur tetranitride, disulphur dinitride and polythiazyl. SxNy compounds. S-N cations and anions. Sulphur-phosphorus compounds: Molecular sulphides such as $P_4S_3$, $P_4S_7$, $P_4S_9$ and $P_4S_{10}$. Phosphorusnitrogen compounds: Phosphazenes and poly phosphazenes. Transition metal dichalcogenides, MoS2. Structure, bonding and reactivity of 2D and 3D Carbon, Silicon and Germanium materials. Carbon nitrides, fullerenes, carbon nanotubes (CNT's) and graphenes. | |

**Recommended Text Books:**


1. G.L. Miessler, P.J. Fischer, D.A. Tarr, Inorganic Chemistry, 5th ed., Pearson, 2014.
2. E. Huheey, E. A. Keiter, R. L. Keiter, Inorganic Chemistry: Principles of Structure and Reactivity, 4th ed., Harper Collin College Publishers, 1993.
3. F. A. Cotton, G. Wilkinson, C. A, Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th ed., Wiley-Interscience: New York, 1999.
4. D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, 3rd ed., ELBS, 1999.
5. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd ed., Wiley, 1994.
6. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2nd ed., Butterworth- Heinemann, 1997.
7. C.E. Housecroft, A.G. Sharpe, Inorganic Chemistry, 5th ed., Pearson, 2018.
8. E. Wiberg, A.F. Holleman, N. Wiberg, Inorganic Chemistry, Academic Press, 2001.
9. A. V. Kolobov, J. Tominaga, Two-Dimensional Transition Metal Dichalcogenides, Springer, 2016.

10. Yu-Chuan Lin, Properties of Synthetic Two-dimensional Materials and Heterostructures, Springer, 2018.
11. Changzheng Wu, Xiaojun Wu, et al, Inorganic Two-dimensional Nanomaterials: Fundamental Understanding, Characterization and Energy Applications, RSC, 2017
12. D.R. MacFarlane, Mega Kar, J.M. Pringle, Fundamentals of ionic liquids, Wiley-VCH, 2017.
13. Yizhak Marcus, Deep Eutectic Solvents, Springer, 2019.
14. J.M. DeSimone and W. Tumas, Green Chemistry Using Liquid and Supercritical Carbon dioxide, D.U.P, 2003.
15. F. M. Kerton , R. Marriott , et al., Alternative Solvents For Green Chemistry, 2nd ed., RSC, 2013.

**CORE**

**25-802-0702**

**ORGANIC CHEMISTRY -III**

**(REACTIVITY AND MECHANISMS)**

**Credit 4** **64 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Review different bonding models with emphasis on understanding three dimensional structures of molecules. | Analyze |
| C.O. 2:<br>Study Qualitative Molecular Orbital Theory and group orbital concepts to sketch MO's of common organic structures, functional groups etc. | Evaluate |
| C.O. 3:<br>Apply the concepts of Frontier orbital theory in the study of ionic, radical and pericyclic reactions. | Analyze |
| C.O. 4:<br>Interpret structure and stability of reactive intermediates. | Evaluate |
| C.O. 5:<br>Apply methods and techniques to study mechanisms of organic reactions. | Apply |
| C.O. 6:<br>Predict the reactivity of an organic compound from its structure and based on the reaction conditions. | Evaluate |
| C.O. 7:<br>Propose a reasonable mechanism for a given organic reaction. | Evaluate |
| C.O. 8:<br>Predict the products in a particular reaction considering the stereochemical aspect. | Evaluate |
| C.O. 9:<br>Illustrate the mechanistic pathway of different rearrangement reactions and identify the products. | Analyze |
| C.O. 10:<br>Identify the mechanism and the product in a given reaction under photochemical condition. | Analyze |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | x | x | | | x | | | x | | |
| C.O. 2 | x | x | | | x | | | x | | |
| C.O. 3 | x | x | | | x | | | x | | |
| C.O. 4 | x | x | | | x | | | x | | |
| C.O. 5 | x | x | | | | | | x | | |
| C.O. 6 | x | x | | | x | | | x | | |
| C.O. 7 | x | x | | | x | | | x | | |
| C.O. 8 | x | x | | | x | | | x | | |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| C.O. 9 | x | x | | | x | | | x | | |
| C.O. 10 | x | x | | | x | | | x | | |

| **UNIT I** | **10 hrs** |
|---|---|
| Study of Structure and Models of bonding: VB and MO models of bonding, Structure and Stability of Reactive intermediates: Carbocations, Carbanions, Carbenes, Nitrenes, and Radicals. Bonding Weaker than Covalent Bonds. Solvent and solution properties, solvent scales. Acid – Base properties in non-aqueous systems, acidity scales, Applications of Molecular Orbital Theory in Understanding reactions and Mechanisms. Qualitative MO theory. Group orbitals. Frontier Orbitals, Substituent effects on frontier orbitals, HSAB concept, Nucleophiles and Electrophiles, Perturbation theory of reactivity. Application of Frontier Orbital theory in studying ionic and radical reactions, Ambident electrophiles, α-effect. | |
| **UNIT II** | **10 hrs** |
| The study of reactions and the methods of studying reaction mechanisms.<br>Classification of reactions according to IUPAC conventions. Reaction mechanism: guidelines on Pushing of electrons. Reactive intermediates: Formation, stability and general reactivity. Methods of determining reaction mechanisms (kinetic and non kinetic methods): The Hammond postulate, reactivity vs selectivity principle, the Curtin-Hammett principle, microscopic reversibility, kinetic vs thermodynamic control. Isotope effects: Primary, secondary and Equilibrium isotope effects, Tunneling effects, solvent isotope effects and heavy atom Isotope effects.<br>Linear free energy relationships: Hammett and Taft parameters, Solvent effects (Grunwald-Winstein plots and Schleyer adaptation), nucleophilicity and nucleofugality. Isokinetic and Isoequilibrium temperature, Enthalpy – entropy compensation. Experimental techniques to determine reaction mechanisms: identification of intermediates by trapping and competition experiments, cross - over experiments, isotope scrambling, radical clocks and traps, matrix isolation. | |
| **UNIT III** | **14 hrs** |
| Substitutions on Aliphatic carbon – saturated and unsaturated systems – Mechanism of nucleophilic substitution – SN2, SN1 – ion pairs, SET, Neighbouring group participation – non classical carbocations, SNi, Tetrahedral mechanism. Electrophilic substitution – SE2, SEi, SE1. Free radical substitution.<br>Reactivity – Effect of substrate structure, nature of reagents, solvents and stereochemistry on the outcome of these reactions. Ambident nucleophiles and substrates. Typical reactions involving substitution.<br>Substitutions on aromatic carbon: Mechanism of electrophilic, nucleophilic and free radical substitutions – orientation and reactivity. Typical reactions involving aromatic substitution. | |
| **UNIT IV** | **16 hrs** |
| Mechanisms of polar addition – electrophilic, nucleophilic and free radical addition. Nonpolar additions (excluding pericyclic reactions) - Reactivity and orientation. Eliminations - E2, E1 and | |

| | |
|---|---|
| E1CB mechanisms, reactivity and orientation. Pyrolytic syn eliminations, α - eliminations, elimination vs. substitution. Typical reactions involving addition and elimination.<br>Rearrangements involving electron deficient carbon and nitrogen. Mechanism of the following rearrangements: Wagner-Meerwein, Pinacol, Demyanov, dienone-phenol, Favorskii, Wolff, Hofmann, Curtius, Lossen, Schmidt, Beckmann, benzidine, and Hofmann-Loffler, Fries, Baeyer-Villiger rearrangements. Fritsch-Buttenberg-Wiechell rearrangement, Corey-Fuchs reaction, Seyferth-Gilbert homologation, Grubbs catalysts and olefin metathesis. | |
| **UNIT V** | **14 hrs** |
| Pericyclic reactions: study of the principle of conservation of orbital symmetry: Orbital symmetry diagrams for cycloaddition and electrocyclic reactions.<br>Aromatic Transition State Theory and The Generalized Woodward – Hoffmann rule applied to cycloaddtions, Electrocyclic reactions, Sigmatropic rearrangements and Chelotropic reactions.<br>Pericyclic Reactions in Organic Synthesis: Stereochemistry and Regiochemistry of Cycloaddtions. Substituent and medium effects, Secondary Orbital Interactions in [4+2] cycloadditions, Intramolecular Diels–Alder reactions. Stereochemistry of Electrocyclic Reactions and Sigmatropic rearrangements. Cope rearrangement, Claisen rearrangement and ene-reaction.<br>1,3-dipolar cycloaddition reactions, Photochromism and thermochromism, Pericyclic reactions in Organic synthesis – case studies.<br>Photochemistry: Unimolecular and bimolecular processes in the excited states, mechanism of important photochemical reactions, Paterno-Buchi reaction, Norrish Type I and Type II fragmentation, di-pimethane rearrangement, Barton reaction, photochemistry of olefins, arenes, cyclohexadienones; photoreduction and photo-oxygenation. | |

**Recommended References:**


1. J. March, Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th ed., Wiley, 2013.
2. T. H. Lowry, K. S. Richardson, Mechanism and Theory in Organic Chemistry, 3rd ed., Benjamin-Cummings Publishing Company, 1997.
3. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry (parts A and B), 5$^{th}$ ed., Springer, 2008.
4. E. V. Anslyn, D. A. Dougherty, Modern Physical Organic Chemistry. University Science Books, 2006.
5. F. A. Carroll, Perspectives on structure and mechanism in organic chemistry, Wiley, 2011.
6. N. S. Issacs, Physical Organic Chemistry, 2nd Edition, Prentice Hall, 1995.
7. A. Pross, Theoretical and Physical Principles of Organic Chemistry, 1st ed., Wiley, 1995.
8. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2nd ed., Oxford University Press, 2012.

9. I. Flemming: Molecular orbitals and organic chemical reactions, student ed., Wiley, 2009.
10. J. McMurry, Organic Chemistry, 5th ed., Brooks/Cole, 2000.
11. R. Bruckner, Advanced organic chemistry: Reaction Mechanisms. Academic Press, 2001.
12. P. Sykes, Guidebook to Mechanism in Organic Chemistry, 6th ed., Prentice Hall, 1986.
13. N. J. Turro, Modern Molecular Photochemistry, University Science Books, 1996.
14. N. J. Turro, J. C. Scaiano, V. Ramamurthy, Modern Molecular Photochemistry of Organic Molecules, 1st ed., University Science Books, 2010.

**CORE**

**25-802-0703**

**THEORETICAL CHEMISTRY-I**

**(QUANTUM CHEMISTRY)**

**Credit 3** **48 hours**

| **Course Outcome**<br>After the completion of the course the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Account for the basic principles and concepts of quantum mechanics. | Analyze |
| C.O. 2:<br>Apply the postulates of quantum mechanics to simple systems of chemical interest, such as the particle-in-a-box, harmonic oscillator, rigid rotor, and hydrogenic atoms. | Apply |
| C.O. 3:<br>Derive the variational principle, use it to calculate properties for simple systems of chemical interest. | Analyze |
| C.O. 4:<br>Use perturbation theory to calculate properties for simple systems of chemical interest. | Analyze |
| C.O. 5:<br>Define and explain the Hartree-Fock self-consistent field method. | Understand |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | x | x | | | | | | x | | |
| C.O. 2 | x | x | | | x | | | x | | |
| C.O. 3 | x | x | | | x | | | x | | |
| C.O. 4 | x | x | | | x | | | x | | |
| C.O. 5 | x | x | | | | | | x | | |

**UNIT I** **10 hrs**

Wave-particle duality, uncertainty principle, postulates of quantum mechanics, Schrödinger equation, Time dependent and time independent Schrodinger wave equation. Its application on some model systems viz., free particle, particle in one, two and three-dimensional box (rectangular and cubical), separation of variables, concept of degeneracy, introduction to quantum mechanical tunneling.

**UNIT II** **10 hrs**

Vibrational motion, Harmonic oscillator, Method of power series, Hermite equation and Hermite Polynomials, Recursion formula, wave function and energy. Rigid rotator, Wave function in spherical polar coordinates, Planar rotator, phi equation, theta equation and solutions Lagendre equation and Lagendre polynomials, Spherical harmonics, Angular momentum operator L2 and Lz, Space quantization.

| UNIT III | 10 hrs |
|---|---|
| H atom, separation into three equations and solutions, Laguerre equation and Laguerre polynomials wave equation and energy of H like systems, quantum numbers and their importance, Radial wave function and radial distribution functions, angular wave function, Shapes of s, p, d and f atomic orbitals. Postulate of electron spin-orbital and spin functions. Zeeman effect. | |
| **UNIT IV** | **12 hrs** |
| Many electron atoms. Approximate methods in quantum mechanics: The variation theorem, linear variation principle and perturbation theory (first order and nondegenerate), application of variation method and perturbation theory to the Helium atom, antisymmetry, Pauli exclusion principle, Slatter determinantal wave functions. Electron spin. | |
| **UNIT V** | **6 hrs** |
| Hartree-Fock Self Consistent Field method, The Coulomb and Exchange Operators, The Fock Operator, Koopmans' theorem, Brillouin's theorem, The Roothaan Equations, Slater's treatment of complex atoms, Slater orbitals. Pauli principle, Slater determinant and wave function. | |

**Recommended Text Books:**


1. D. A. McQuarrie, Quantum Chemistry, 3rd ed., Univ. Sci. Books, Mill Valley, California, 1983.
2. I. N. Levine, Quantum Chemistry, 6th ed., Pearson Education, London, 2008.
3. P. W. Atkins, R.S Friedman, Molecular Quantum Mechanics, 5th ed., OUP, Oxford, 2012.
4. J. P. Lowe, Quantum Chemistry 3rd ed., Academic Press, New York, 2008.
5. A. Szabo, N. S. Ostlund, Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory, Dover Book ed., Mc.Graw-Hill, New York, 1982.
6. P.W. Atkins, Physical Chemistry, 8th ed., Wiley, New York, 2006.
7. R. K. Prasad, Quantum Chemistry, 3rd ed., New Age International, 2006.
8. D. J. Griffiths, Introduction to Quantum Mechanics, 2nd ed., 2004.
9. J. J. Sakurai, Modern Quantum Mechanics, 2nd ed., 2010

**CORE**

**25-802-0704**

**THEORETICAL CHEMISTRY – II**

**(GROUP THEORY AND SPECTROSCOPY)**

**Credit 4** **64 hours**

| **Course Outcome** After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1: Analyze the symmetry of any given molecule and assign the point group | Analyze |
| C.O. 2: Apply the principles of symmetry and group theory in structure, bonding and spectral characteristics of molecules | Apply |
| C.O. 3: Explain the factors affecting the intensity and broadening of lines in spectra and methods to enhance the sensitivity | Understand |
| C.O. 4: Explain the principles of rotational, vibrational, Raman, electronic, fluorescence and NMR spectroscopy | Understand |
| C.O. 5: Solve problems based on rotational, vibrational, Raman electronic, fluorescence and NMR spectroscopy | Apply |
| C.O. 6: Apply various theoretical aspects to various spectroscopic techniques for prediction of different spectroscopic observations | Analyze |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | x | x | | | x | | | | | |
| C.O. 2 | x | x | | | x | | | | | |
| C.O. 3 | x | x | | | x | x | x | | x | |
| C.O. 4 | x | x | | | x | x | x | | x | |
| C.O. 5 | x | x | | | x | x | x | | x | |
| C.O. 6 | x | x | | | x | x | x | | x | |

| **UNIT I** | **18 hrs** |
|---|---|
| Matrix representation of symmetry operations, similarity transformation and classes, Symmetry classification of molecules into point groups (Schoenflies symbol)- Application of symmetry to predict polar and chiral compounds. Reducible and Irreducible representations - Great Orthogonality theorem and its consequences (statement only, proof not needed), Character tables, Reduction formula, construction of character tables for point groups with order ≤6-, Interpretation of character tables. Wave functions as bases for irreducible representations, Direct product. | |

| UNIT II | 12 hrs |
|---|---|
| Application of symmetry to predict polar and chiral compounds. Application of Group theory to Hybridization of atomic orbitals: Construction of hybrid orbitals for AB3(planar), AB4(Td), AB5(D3h) and AB6(Oh) type of molecules.<br>Application of group theory to Molecular Orbital Theory: LCAO and Huckel approximations. Symmetry adapted linear combinations, Projection operators, Application of projection operators to pi-bonding in ethylene, cyclopropenyl systems, benzene and naphthalene. Application of projection operators to sigma bonding in ethylene and PtCl4<br>2-. Molecular orbitals for tetrahedral and octahedral molecules.. | |
| **UNIT III** | **12 hrs** |
| Spectroscopy and its importance in chemistry. Link between spectroscopy and quantum chemistry, Energy levels in molecules, Born-Oppenheimer approximation,<br>Absorption and emission of radiation, Intensity and width of spectral lines, Beer lambert's law, Integrated absorption coefficient, Line width – natural line broadening, Doppler broadening, minimisation of line broadening, Induced and spontaneous transitions, correlation to the Einstein coefficients of absorption and emission, Basis of selection rules Fermi golden rule, lasers. | |
| **UNIT IV** | **12 hrs** |
| Rotational spectroscopy: Rotation of rigid bodies, moment of inertia, linear molecules, spherical, symmetric and asymmetric tops, Schrödinger equation of a rigid rotator and brief discussion of its results, Quantization of rotational energy levels, selection rules, rotational spectra and line intensities, structure determination from rotational constants, isotopic effects.<br>Vibrational Motion: Schrödinger equation of a linear harmonic oscillator and brief discussion of its results, concept of zero-point energy. Quantization of vibrational energy levels. Selection rules, IR spectra of diatomic molecules.<br>Structural information derived from vibrational spectra, dissociation energies, vibration-rotation transitions in diatomics, harmonic oscillator, anharmonicity, centrifugal distortion, Vibration of polyatomic molecules, normal modes, combination, difference and hot bands, Fermi Resonance, Group frequencies. Effect of hydrogen bonding (inter- and intramolecular) on vibrational frequencies.<br>Raman spectroscopy: Light scattering and Raman effect, classical and quantum models for scattering, Stokes and anti-Stokes lines; their intensity difference, polarizability, selection rules, group theoretical treatment of vibrations, Effect of nuclear spin, Vibrational Raman spectra, rule of mutual exclusion for centrosymmetric molecules, polarized and depolarized Raman lines, resonance Raman scattering.<br>Applications of Group theory for molecular vibration, symmetry of group vibrations. Selection rules and applications to IR and Raman spectra. | |

| **UNIT V** | **10 hrs** |
|---|---|
| Electronic Spectroscopy of molecules: Molecular orbitals and states, terms ymbols, selection rules, vibrational and rotational structures, Free Electron model, its application to electronic spectra of polyenes. Frank-Condon principle, electronic transitions, Beer Lambert's Law, dissociation and predissociation, photoelectron spectroscopy, dissociation and predissociation, calculation of heat of dissociation, Birge Sponer method, electronic spectroscopy of polyatomic molecules Singlet and triplet states, Jablonski diagram, fluorescence and phosphorescence, Solvent and environmental effects, Fluorescence quenching, energy transfer and electron transfer, time domain lifetime measurements.<br>NMR: Expression for Hamiltonian/Energy - Zeeman interaction, torque exerted by a magnetic field on spins, equation, its solution and the physical picture of precession. Thermal equilibrium, Relaxation, chemical shift, shielding and deshielding, Karplus relationships, Bloch equations, the rotating frame, pulsed experiments, NOE, double irradiation, selective decoupling, double resonance, Polarisation transfer, Two-dimensional NMR, Solid state NMR, NQR, MRI. | |

**Recommended Text Books:**


1. F. A. Cotton, Chemical Applications of Group theory, Wiley Eastern, Singapore, 2nd ed., 1992.
2. V. Ramakrishnan, M. S. Gopinathan, Group theory in Chemistry, Vishal Pub. New Delhi, 1996.
3. Alan Vincent, Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications, 2nd ed., Wiley, 2013.
4. Robert L. Carter, Molecular Symmetry and Group Theory, Wiley, 2009.
5. G. M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, New York, 1962.
6. C. N. Banwell, Fundamentals of Molecular Spectroscopy, 4th ed., Tata McGraw Hill, 1996.
7. A. E. Derome, Modern NMR Techniques for Chemical Research, Pergamon Press, 1987.
8. D. H. Williams, I. Flemming, Spectroscopic Methods in Organic Chemistry, 4th ed., McGraw-Hill, 1985.
9. H. Gunther, NMR Spectroscopy, 2nd ed., John Wiley, 2005.
10. N. B. Colthup, L. H. Daly, S. E. Wiberley, Introduction to Infrared and Raman Spectroscopy, 3rd ed., 1982.
11. R. A. Alberty, Physical Chemistry 8th ed., Wiley, New York, 1994.
12. P. W. Atkins, Physical Chemistry 8th ed., W. H. Freeman, New York, 2006.
13. I. N. Levine, Molecular Spectroscopy, John Wiley & Sons.
14. J. M. Hollas, Modern Spectroscopy, John Wiley & Sons.
15. P. F. Bernath, Spectra of Atoms and Molecules, III Edn, Oxford University Press.
16. J. L. McHale Molecular Spectroscopy, Pearson Education.
17. W. W. Parson, Modern Optical Spectroscopy, Springer-Verlag.

18. Jack D. Graybeal, Molecular Spectroscopy, Mc Graw Hill International Editions
19. M.H. Levitt, Spin Dynamics, II edn.Wiley
20. James Keeler, Understanding NMR spectroscopy, II edn. Wiley
21. Joseph R. Lakowicz, Principles of Fluorescence Spectroscopy, 3rd Ed., Plenum Press, 2010.

**CORE/LAB**

**25-802-0705**

**ADVANCED CHEMICAL SYNTHESIS AND SEPARATION LAB**

**Credit 2** **96 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Acquire knowledge on safe laboratory practices of handling laboratory glassware, equipment and chemical reagents. | Knowledge |
| C.O. 2:<br>Plan and perform synthetic procedures, chromatographic separation and purification of organic compounds. | Understand |
| C.O. 3:<br>Separate organic compounds from the organic binary mixture and identify the functional group(s) present. | Analyze |
| C.O. 4:<br>Use software to Draw the structures and schemes of organic molecules and reactions. | Apply |
| C.O. 5:<br>Use Chemical Abstracts, Scopus, Organic Synthesis collective volumes on web etc. to search, analyse and collect chemical information. | Apply |
| C.O. 6:<br>Identify the cations in a mixture of unknown salts. | Analyze |
| C.O. 7<br>Estimate the amount of a given metal ion by complexometric and cerimetric reactions. | Analyze |
| C.O. 8<br>Synthesise metal complexes and characterize them by various physicochemical methods. | Apply |
| C.O. 9<br>Record and interpret electronic spectrum of different metal complexes. | Apply |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | X | X | | | | X | | X | X | |
| C.O. 2 | X | X | X | | X | X | | X | X | |
| C.O. 3 | X | X | | X | | X | | X | X | |
| C.O. 4 | X | X | | | | X | X | X | X | |
| C.O. 5 | X | X | | | X | X | | X | X | |
| C.O. 6 | X | X | | | | | | X | X | |
| C.O.7 | X | X | | X | | | | X | X | |
| C.O. 8 | X | X | X | | | X | | X | X | |
| C.O. 9 | X | X | | | | X | X | X | X | |

**UNIT I** **48 hrs**

**Part I:** General methods of separation and purification of Organic compounds such as 1) Solvent extraction 2) Thin layer chromatography and paper chromatography 3) column chromatography

**Part II:** Separation and identification of the components of organic binary mixtures.

**Part III:** Preparation of Organic compounds by multistep reactions, purification of products and characterisation using UV-Vis, FTIR and NMR.*

**Part IV:** Drawing the structures of organic molecules and reaction schemes by Proprietary and open source computer software. Use Chemical Abstracts, Scopus, Organic Synthesis collective volumes on web etc., to search, analyse and collect chemical information.

*Progress of the reactions should be followed by spectroscopic and chromatographic methods (UV-Vis, TLC, GC, HPLC, etc)

**UNIT II** **48 hrs**

Reactions of titanium, vanadium, chromium, manganese, iron, cobalt, nickel and copper ions. Reactions of some less common metal ions (Tl, W, Mo, V, Zr, Th, U). The spot test technique for metal ions. Semimicro qualitative analysis of common and rare cations in a mixture.

Estimation of metal ions by complexometric and cerimetric titrations. Estimation of Mg, Ca, Mn, hardness of water.

Synthesis of inorganic complexes and their characterization by various physicochemical methods, such as IR, UV, Visible, NMR, magnetic susceptibility etc. Selection can be made from the following or any other complexes for which references are available in the literature.

Tris(oxalato)manganese(III)

Tetrapyridinesilver(II)peroxidisulphate

Tris(acetylacetonato) iron(III)

Bis(N,N-diethyldithiocarbamato)nitrosyliron(I)

Optical isomers of tris(ethylenediamine)cobalt(III)chloride

Nitropentamminecobalt(III) chloride

Tri(acetylacetonato)manganese(III)

Tris(thiourea) copper(I) sulphate

Phenyl lithium

Tetraphenyl lead

Ferrocene

Phosphonitrilic chloride

Anhydrous copper(II) nitrate

Interpretation of its electronic spectrum and calculation of Dq values.

Determination of crystal field splitting energy for certain ligands and construction of a part of the spectrochemical series.

**Recommended Text Books:**


1. A. I. Vogel, A. R. Tatchell, B. S. Furnis, A. J. Hannaford, P. W. G. Smith, Vogel's Textbook of Practical Organic Chemistry, 5th ed., John Wiley, 1989.
2. D. L. Pavia, G. M. Lampman, G. S. Kriz, Introduction to Organic laboratory Techniques, 3rd ed., Saunders Golden Sunburst Series.
3. 3. L. W. Harwood, C. J. Moody, Experimental Organic Chemistry-Principles and
4. Practice, Blackwell Science Publications.
5. 4. G. Pass, H. Sutcliffe. Practical Inorganic Chemistry 2nd ed., Chapman & Hill. 1974.
6. 5. G. Marr, B. W. Rockett, Practical Inorganic Chemistry, Van Nostrand, 1972.

**CORE/LAB**

**25-802-0706**

**OPEN ENDED LAB-III**

**Credit 2** **96 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Design experiments and validate the hypothesis of an independent research problem. | Evaluate |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | x | x | | | | x | x | x | x | |

| **UNIT I** | **96 hrs** |
|---|---|
| The students shall perform literature review/ experiments/analysis for validating the hypothesis.<br>The students shall submit a project progress report | |

**ELECTIVE**

**25-802-0707**

**SUPRAMOLECULAR CHEMISTRY**

**Credit 3** **48 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Explain the structural features of any given supramolecular system | Analyze |
| C.O. 2:<br>Analyze the type of possible interactions in any given host guest assembly | Analyze |
| C.O. 3:<br>Predict the photochemical and Photophysical behavior in constrained media | Analyze |
| C.O. 4:<br>Analyze the change in electronic structure of the supramolecular systems based on the interaction with the host | Evaluate |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | X | | | | | | | | | |
| C.O. 2 | X | X | | | | | | | | |
| C.O. 3 | | X | | | X | | | | | |
| C.O. 4 | | | | | X | | X | | | |

| **UNIT I** | **10 hrs** |
|---|---|
| Structure, Preparation and Properties of: crown ethers, cryptates, cryptands, carcerands, calixarenes, cyclodextrins, fullerenes, dendrimers, rotaxanes, cucurbiturils, COF, MOF. | |
| **UNIT II** | **10 hrs** |
| Noncovalent Interactions –Hydrogen bonding, π Effects, dipole interactions, Induced dipole interactions, Hydrophobic interactions. Solvent Effects, Thermodynamics of binding phenomena. | |
| **UNIT III** | **10 hrs** |
| Molecular Recognition – Host guest interactions, Complementarity and Reorganization, large ion pairing component, hydrophobic component, hydrogen bond, π-component. Complex Architectures – Self-assembly, coordination, hydrogen bonding. | |
| **UNIT IV** | **10 hrs** |
| Photochemistry in constrained media- photophysical, photochemical processes, energy transfer, electron transfer. Effect of structural features and interactions on energy levels. | |
| **UNIT V** | **8 hrs** |
| Applications – photocatalysis, water splitting, solar cell, $CO_2$ reduction, drug delivery, sensors, gas separation and storage. | |

**Recommended Text Books:**


1. Jonathan W. Steed, Jerry L. Atwood, Supramolecular Chemistry, Wiley, 2013.
2. J. M. Lehn, Supramolecular Chemistry: Concepts and Perspectives, Wiley, 1995
3. E.V. Ansyln, D. A. Dougherty, Modern Physical Organic Chemistry, University Press, 2006.
4. P. Klan and J. Wirz, Photochemistry of Organic Compounds,
5. Modern Molecular Photochemistry of Organic Molecules, Nicholas J. Turro, V. Ramamurthy, J.C. Scaiano,
6. Christian S. Diercks, Markus J. Kalmutzki, and Omar M. Yaghi, Introduction to Reticular Chemistry: Metal-Organic Frameworks and Covalent Organic Frameworks, Wiley, 2019.
7. Shengqian Ma, Jason A Perman, Elaboration and Applications of Metal-organic Frameworks, World Press, 2018.

**ELECTIVE**

**25-802-0708**

**GREEN CHEMISTRY**

**Credit 3** **48 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Apply the concepts of green chemistry for a given chemical process | Analyze |
| C.O. 2:<br>Describe the various green materials which can be used as alternatives | Understand |
| C.O. 3:<br>Describe the various green technologies which can be used as alternatives | Understand |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | X | | X | | | | | | | |
| C.O. 2 | X | | X | | | | | | | X |
| C.O. 3 | X | | X | | | | | | | X |

| **UNIT I** | **10 hrs** |
|---|---|
| Green Chemistry and industry, waste minimization, E factor and atom economy, Reduction of-material use, energy, risk and hazards. Sustainable use of- chemical feedstocks, water, energy. LCA methodology, Renewables as Chemical Feedstocks and Biocatalysis, Process Intensification for Green Chemistry. | |
| **UNIT II** | **10 hrs** |
| Catalysis in green chemistry – Homogenous catalysis, Heterogeneous catalysis, metal catalysts, metal oxide catalyst, metal complexes, Solid Acid Catalysts - Concepts and applications, Zeolite, Heteropolyacid, Ion-exchange resins as solid acid catalysts, Kvaerner Process, Nafion /silica nanocomposites, Haldor–Topsoe alkylation process to high-octane fuels. Micelle-templated Silica as Catalysts in Green Chemistry - Synthesis of micelle templated materials, Catalytic Applications - Oxidation catalysis, Base catalysis, Enantioselective catalysis. | |
| **UNIT III** | **10 hrs** |
| Phase-transfer Catalysis(PTC) - Classical PTC Reactions, Nucleophilic aliphatic and aromatic Substitutions, Phase-transfer catalysis elimination and isomerisation reactions, Base-promoted alkylation and arylation, Inverse PTC, Phase-transfer Catalysis in Polymerisation, Applications of PTC in Analytical Chemistry. Biocatalysis - antibody catalysts, Enzyme Catalysts, Biomimetic catalysts, Chemical Production by Biocatalysis, Bulk chemicals, Pharmaceuticals, Flavour and | |

| | |
|---|---|
| fragrance compounds, Carbohydrates, Polymers, Biocatalysis in supercritical $CO_2$, Biocatalysis in waste treatment. | |
| **UNIT IV** | **10 hrs** |
| Specific green technologies - hydrogen peroxide in waste minimization, waste minimization in pharmaceutical process development, supercritical carbon dioxide as an environmentally benign reaction medium for chemical synthesis, reduction of volatile organic compound emission during spray painting. Extraction of natural product with super-heated water, Synthesis at organic – water interface, Envirocats, applications of microwaves for environmentally benign organic chemistry, Sonochemistry – Concept, application in chemical synthesis. | |
| **UNIT V** | **8 hrs** |
| Photochemistry - Photons as Clean Reagents, Reduced usage of reagents, Lower reaction temperatures, Control of selectivity, Photochemical reactions for industry, General Problems with Photochemical Processes, Specialized photochemical reactors and process technology, Photochemical reactors, Light sources, Artificial Photosynthesis for small molecule conversions. Green Nanoscience - Photocatalysis by Nanostructured $TiO_2$-based Semiconductors, Formation of Nanoparticles Assisted by Ionic Liquids, Nanoencapsulation for Process Intensification, Nanophase Inorganic Materials, Nanomaterials from Biobased Amphiphiles. | |

**Recommended References:**


1. Paul T. Anastas and John C. Warner, Green Chemistry: Theory and Practice, Oxford University Press, 1998.
2. J. Clark, D. Mcquarrie, Hand Book of green Chemistry and technology, Blackwell science, 2002.
3. Mike Lancaster, Green Chemistry: An Introductory Text, RSC, 2007.
4. P. T. Anastas, T. C. Williamsons, Green Chemistry – Designing Chemistry for the Environment, ACS, 1994.
5. V. K. Ahluwalia, M. Kidwai, New Trends in Green Chemistry, 2nd edition, Anamaya Publishers, 2006.
6. V. K. Ahluwalia, Green Chemistry, Narosa Publishing House, 2011.
7. Alvise Perosa, Maurizio Selva, Handbook of Green Chemistry- Volume 8-Green Nanoscience, Wiley-VCH, 2012.
8. Allen J. Bard, Larry R. Faulkner, Electrochemical Methods-Fundamentals and Applications, John Wiley & Sons, New York, 1980

**ELECTIVE**

**25-802-0709**

**POLYMER CHEMISTRY**

**Credit 3** **48 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Recognise the concept of macromolecules and describe the classification, synthesis and process technologies involved inco mmon polymers. | Understand |
| C.O. 2:<br>Analyse the kinetics and mechanism involved in different types of polymerization | Analyze |
| C.O. 3:<br>Apply the concepts of stereochemical aspects and analyse the conformation and configuration of polymers | Analyze |
| C.O. 4:<br>Apply different characterisation techniques to identify polymers. | Apply |
| C.O. 5:<br>Explain the synthesis, structure and applications of industrial polymers. | Understand |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | X | | X | | | | | | X | |
| C.O. 2 | | | | | X | | | | | |
| C.O. 3 | X | X | | | | | | | X | X |
| C.O. 4 | | | | | | X | X | | | |
| C.O. 5 | | | | | | X | X | | | |

| **UNIT I** | **10 hrs** |
|---|---|
| History of Polymer Science. Concept of macromolecules, Principle of duality, Integration of molecular character and material character. Molecular design, synthesis and process technologies. Nomenclature and Classification. Raw Material sources of polymers. Natural gas, coal and petroleum. Monomers and polymers derived from natural gas. Petroleum and petrochemicals. Monomers and polymers derived from ethylene and propylene. Monomers and polymers derived from C4 and C5 Systems and BTX fraction. Acetylene as a source of monomers. | |
| **UNIT II** | **10 hrs** |
| Polymerization processes. Free radical addition polymerization. Kinetics and mechanism. Chain transfer. Molecular weight distribution and molecular weight control. Cationic and anionic polymerization. Polymerization without termination. Living polymers. Step Growth polymerization. Kinetics and mechanism. Linear Vs cyclic polymerization, Group Transfer, metathesis and ring | |

| | |
|---|---|
| opening polymerization. Copolymerization. The copolymerization equation, Q-e scheme, Gelation and Crosslinking. Copolymer composition drift. Polymerization techniques. Bulk Solution, melt, suspension, emulsion and dispersion techniques. | |
| **UNIT III** | **10 hrs** |
| Polymer Stereochemistry. Organizational features of polymer chains. Configuration and conformation, Tacticity, Repeating units with more than one asymmetric center. Chiral polymers – main chain and side chain. Stereoregular polymers. Manipulation of polymerization processes. Zeigler-Natta and Kaminsky routes. Coordination polymerization. Metallocene and Metal oxide catalysts. | |
| **UNIT IV** | **10 hrs** |
| Polymer Characterization. Molecular weights. Concept of average molecular weights, Determination of molecular weights. GPC and Light scattering techniques. Molecular weight distribution. Crystalline and amorphous states. Glassy and Rubbery States. Glass transition and crystalline melting. Spherullites and Lammellae. Degree of Crystallinity, Thermal analysis of polymers. TG/DTG, DTA/DSC, Spectroscopy of polymers. Microstructure determination by IR, Raman, UV, NMR and MS techniques. Solid State NMR and polymer stereochemistry. | |
| **UNIT V** | **8 hrs** |
| Industrial polymers. Synthesis, Structure and applications. Polyethylene, polypropylene, polystyrene. PVC, PVA, PAN, PA. Poly(vinyl carbazole), poly(vinyl imidazole). PMMA and related polymers. Flourine containing polymers. Reaction polymers. Polyamides, polyesters. Epoxides, polyurethanes, polycarbonates, phenolics, PEEK, Silicone polymers. Reactions of polymers. Polymers as aids in Organic Synthesis. Polymeric Reagents, Catalysts, Substrates, Liquid Crystalline polymers. Main chain and side chain liquid crystalline polymers. | |

**Recommended Text Books:**


1. Billmayer, F.W. Textbook of Polymer Science. 3rd Ed., Wiley. N.Y.1991.
2. Cowie, J.M.G. Polymers: Physics and Chemistry of Modern Materials. Blackie. London,1992.
3. Young, R.J. Principles of Polymer Science, 3rd Ed., Chapman and Hall. N.Y.1991.
4. Flory, P.J. A Text Book of Polymer Science. Cornell University Press. Ithacka, 1953.
5. Ullrich, F. Industrial Polymers, Kluwer, N.Y.1993.
6. Elias, H.G. Macromolecules, Vol. I & II, Academic, N.Y.1991.
7. Brydson, J.A. Polymer chemistry of Plastics and Rubbers, ILIFFE Books Ltd., London,1966.

**MOOC ELECTIVE**

**25-802-0710**

**BONDS AND BANDS IN SOLIDS**

**Credit 2** **32 hours**

| **Course Outcome**<br>After the completion of the course the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Describe the theoretical aspects of solid state structure | Understand |
| C.O. 2:<br>Correlate the structural aspects to electronic properties | Apply |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | X | X | | | | | | | | |
| C.O. 2 | X | X | | | | | | | | |

| **UNIT I** | **6 hrs** |
|---|---|
| One-electron Hamiltonian after B.O and SCF approx., Bonding in Hn System, n=2,3….N | |
| **UNIT II** | **6 hrs** |
| Bloch’s theorem, Energy bands, Metal, Insulator, Semi-conductors; Brillouin Zones, Different Schemes, Density of States, Extension to p-orbitals, square lattices etc | |
| **UNIT III** | **6 hrs** |
| Peiperl’s instability, Nearly Free Electron Model, Fermi Surface, Density of States, Effective Mass etc.,, Failures of MO and Band Theories, Beyond energy band, Interacting electron models and Kinetic exchange | |
| **UNIT IV** | **6 hrs** |
| Energy levels in interacting models, Excitons; Lattice, vibrations, Acoustic modes, optic modes etc., | |
| **UNIT V** | **8 hrs** |
| Phonon Photon interaction, thermal properties of insulators | |

**Recommended Text Books:**


1. C. Kittel, “Introduction to Solid State Physics”
2. J. M. Ziman, “Principles of the Theory of Solids”
3. N.W. Ashcroft and N.D. Mermin, “Solid State Physics”.


SWAYAM

Prof. S. Ramashesha

IISc, Bangalore

**AUDIT**

**25-802-0711**

**PROFESSIONAL AND CAREER DEVELOPMENT IN CHEMISTRY**

**Credit 0** **32 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Skills on subject specific pedagogy, soft skills, ICT tools, research proposal writing, finding scholarships and software for chemistry | Create |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | | | | | | | | | x | x |

| **UNIT I** | **32 hrs** |
|---|---|
| Soft Skills – Powerpoint, Word, Exel, Reference management software- Mendeley, Origin, Veusz, Research Proposal Writing – Literature review, Components of proposals, ICT – Google Classroom, Moodle, Class Recording, Teach Infinity, OBS, edmondo, QUIZZ Quiz, Document scanner., Subject specific pedagogy – Molecular model kit, ChemDraw, ChemSketch, Finding International Scholarships- MEXT, DAAD, EURAXESS, J-Rec, Funding through embassy<br>Lab safety, research ethics, research methodology. | |

**Recommended Text Books:**


1. John M. Swales & Christine B. Feak, Academic Writing for Graduate Students 3rd Edition, Michigan Publishing, 2012
2. Stephen Bailey, Academic Writing, A Handbook for International Student, 5th Edition, Routledge, Taylor & Francis, 2018.

**CORE**

**25-802-0801**

**Inorganic Chemistry – IV**

**(CHEMISTRY OF d- AND f-BLOCK ELEMENTS)**

**Credit 3** **48 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Describe and explain the structure, bonding and magnetism in metal complexes using crystal field theory. | Analyze |
| C.O. 2:<br>Describe various metal-ligand interactions in terms of sigma- and pi-bonding. | Analyze |
| C.O. 3:<br>Identify various d-d transitions and interpret the electronic spectra of any given transition metal complex. | Evaluate |
| C.O. 4:<br>Interpret the ESR spectra of any given transition metal complex. | Evaluate |
| C.O. 5:<br>Explain the stability of metal complexes, their reactivity, and the mechanisms of ligand substitution and redox reactions. | Evaluate |
| C. O. 6:<br>Interpret the Mossbauer spectra of iron complexes. | Apply |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | X | X | | | | | | X | | |
| C.O. 2 | X | X | | | X | | | X | | |
| C.O. 3 | X | X | | | | X | | X | | |
| C.O. 4 | X | X | | | | X | | X | | |
| C.O. 5 | X | X | | | X | | | X | | |
| C.O. 6 | X | X | | | | X | | X | | |

| **UNIT I** | **6 hrs** |
|---|---|
| Crystal-field theory, d-orbital splitting in octahedral, tetrahedral, square planar, trigonal bipyramidal, trigonal planar and linear geometries, crystal field stabilization energy, effect of pairing energy. Molecular Orbital Theory: construction of molecular orbital diagrams using group theory, qualitative MO diagrams for octahedral, tetrahedral and square planar complexes, effect of $\pi$-bonding, experimental evidence for $\pi$-bonding, spectrochemical series. | |
| **UNIT II** | **10 hrs** |
| Microstates, Atomic term symbols Free ion terms for dn configuration, Splitting of terms in octahedral and tetrahedral octahedral fields, Correlation diagram for $d^2$ configuration in octahedral geometry, d-d transitions, Selection rules for electronic transitions. | |

| | |
|---|---|
| Orgel diagram – splittings for $d^1$, $d^9$, high spin $d^4$, $d^6$, splittings for high spin $d^2$, $d^3$, $d^8$ and $d^7$<br>Calculation of Dq, B and β<br>Tanabe Sugano diagrams – splittings for low spin $d^n$ systems Electronic Spectral interpretation of some coordination compounds<br>Consequence of Jahn Teller effect on the electronic spectra of coordination compounds<br>Charge transfer spectra, Electronic spectra of lanthanide and actinide complexes | |
| **UNIT III** | **6 hrs** |
| Magnetism: brief review of different types of magnetic behaviours, spin-orbit coupling, quenching of orbital angular moments in crystal field, spin-only formula, correlation of μs and μeff values, magnetic moments of T terms and A, E terms, temperature independence paramagnetism, magnetic properties of lanthanides and actinides. | |
| **UNIT IV** | **12 hrs** |
| Electronic paramagnetic resonance spectroscopy: Electronic Zeeman effect, Zeeman Hamiltonian and EPR transition energy. Presentation of spectra. The effects of electron Zeeman, nuclear Zeeman and electron nuclear hyperfine terms in the Hamiltonian on the energy of the hydrogen atom. Second order effect. Hyperfine splittings in isotropic systems, spin polarization mechanism and McConnell's relations Anisotropy in g-value, EPR of triplet states, zero field splitting, Kramer's rule, survey of EPR spectra of first row transition metal ion complexes.<br>Mossbauer spectroscopy- Principles and applications to coordination compounds. | |
| **UNIT V** | **14 hrs** |
| Reaction Mechanism: Thermodynamic and kinetic consideration, formation constant and rate constant, inert and labile complexes, factors affecting the stability and lability of complexes.<br>Ligand substitution in octahedral complexes, mechanism of substitution reactions in octahedral complexes, dissociative, associative and interchange mechanism, energy profile of reactions, acid and base hydrolysis, factors affecting the rate of substitution reactions in octahedral complexes.<br>Ligand substitution in square planar complexes, mechanism of substitution reactions in square planar complexes, energy profile of reactions, the trans effect and its applications, theories for explaining trans effect, factors affecting the rate of substitution reactions in square planar complexes.<br>Electron Transfer Reactions: inner sphere and outer sphere mechanism, Marcus theory, photochemical reactions | |

**Recommended Text Books:**


1. G.L. Miessler, P.J. Fischer, D.A. Tarr, Inorganic Chemistry, 5th ed., Pearson, 2014.
2. F. A. Cotton, G. Wilkinson, C. A, Murillo, M. Bochmann Advanced Inorganic Chemistry, 6th ed., Wiley-Interscience: New York, 1999.

3. J.E. Huheey, E. A. Keiter, R. L. Keiter, Inorganic Chemistry: Principles of structure and Reactivity, 4th ed., Harper Collin College Publishers, 1993.
4. J. W. Steed, J. L. Atwood, Supramolecular Chemistry, 2nd ed., John Wiley & Sons Ltd., 2009.
5. D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, 3rd ed., ELBS, 1999.
6. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd ed., John Wiley and Sons, 1994.
7. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2nd ed., BH, 1997.
8. R. S.Drago, Physical Methods for Chemists, 2nd ed., Saunders College Publishing, 1992.
9. C. E. Housecroft, A. G. Sharpe, Inorganic Chemistry, 5th ed., Pearson, 2018.
10. W. L. Jolly, Modern Inorganic Chemistry, 2nd ed., McGraw-Hill, New York, 1991.
11. Elements of Chemical Thermodynamics, Addison Wesley, 2nd Edn, 2013.

**CORE**

**25-802-0802**

**ORGANIC CHEMISTRY -IV**

**(REACTIONS, REAGENTS AND SYNTHESIS)**

**Credit 4** **64 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Interpret the differences in reactivity of various reducing and oxidizing agents with mechanistic illustrations. | Apply |
| C.O. 2:<br>Analyse the reagents and conditions for the synthesis of specific target molecules. | Analyze |
| C.O. 3:<br>Describe strategies for the stereospecific/stereo selective organic transformations towards chiral target molecules. | Apply |
| C.O. 4:<br>Construct a synthetic pathway for simple to complex organic molecules by retrosynthetic approach. | Apply |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | X | | | | | | | | | |
| C.O. 2 | | | X | | | | | X | | |
| C.O. 3 | | | X | | | | | X | | |
| C.O. 4 | | | X | | | | | X | | |

| **UNIT I** | **14 hrs** |
|---|---|
| Reagents for oxidation and reduction: Chromium reagents, activated DMSO, osmium tetroxide, selenium dioxide, singlet oxygen, peracids, hydrogen peroxide, periodic acid, lead tetraacetate, ozonolysis, Woodward and Prevost hydroxylation, Wacker process, Oppenauer oxidation, Sharpless, Shi and Jacobsen asymmetric epoxidations. Catalytic hydrogenations (heterogeneous- Palladium/Platinum/Rhodium and Nickel, homogeneous-Wilkinson), metal hydride reduction- $LiAlH_4$, DIBAL-H, Red-Al, $NaBH_4$ and $NaCNBH_3$. Selectrides, trialkylsilanes and trialkyl stannane. Birch reduction, hydrazine and diimide reduction. Meerwein-Ponndorf-Verley reaction, Enzymatic reduction using Baker's yeast. | |
| **UNIT II** | **12 hrs** |
| Synthetic applications of organometallic and organo-nonmetallic reagents: Hydorboration reactions, Sakurai allylation, Gilman's reagent, Ullmann and Glaser coupling reactions. Suzuki coupling, Sonogashira coupling, Heck reaction, Buchwald–Hartwig coupling, Negishi coupling and Stille | |

| | |
|---|---|
| coupling. Metathesis processes of electrophilic carbene complexes (first- and second-generation Grubbs catalyst), ROMP, Dötz reaction and methylenation of carbonyls. Reagents such as NBS, DCC, DMAP, DEAD, DDQ. Phase transfer catalysts. Chemistry of Nucleophilic Heterocyclic Carbenes (NHCs), multicomponent reactions such as Ugi reaction, Passerini reaction, Biginelli reaction. Click reaction. | |
| **UNIT III** | **12 hrs** |
| Chemistry of carbonyl compounds: Reactivity of carbonyl groups in aldehydes, ketones, carboxylic acids, esters, acyl halides and amides. Substitution at carbonyl carbon, mechanisms of ester hydrolysis, substitution at α-carbon, aldol and related reactions. Grignard reaction, Reformatsky reaction, Claisen, Darzen, Dieckmann, Knoevenagel and Stobbe condensations. Perkin, Prins, Mannich, Stork-enamine reactions. Conjugate additions, Michael additions and Robinson annulation. Favorskii reaction, Julia olefination, Peterson olefination. Reaction with phosphorous and sulfur ylides. | |
| **UNIT IV** | **12 hrs** |
| Asymmetric Synthesis: Introduction to asymmetric synthesis, principle, general strategies, chiral pool strategy, chiral auxiliaries, chiral reagents – Binol derivatives of $LiAlH_4$, chiral catalysts – CBS catalyst. Stereospecific and stereoselective synthesis, determination of enantiomeric and diastereomeric excess.<br>Stereoselective nucleophilic additions to acyclic carbonyl groups-Cram's Rule, Felkin-Ahn Model, Effect of chelation on selectivity. | |
| **UNIT V** | **14 hrs** |
| Synthesis planning and analysis: Convergent, divergent and parallel synthesis. Protecting groups-protection and deprotection of hydroxyl, carboxylic acids, carbonyls in aldehydes and ketones, amines, alkenes and alkynes. Chemo- & regioselective protection and deprotection. Functional group equivalents, reversal of reactivity (Umpolung). Disconnection approach-introduction to retrosynthesis, basic principles, synthons, and synthetic equivalents. Monofunctional and bifunctional disconnection, One group C-X and two group C-X disconnections, one group C-C and two group C-C disconnections. Retrosynthesis of longifoline, Corey lactone, Djerassi - Prelog lactone and Dluciferin. | |

**Recommended References:**


1. M. B. Smith, Organic Synthesis, 2nd ed., McGraw-Hill, 2000.
2. M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th ed., Wiley, 2013.
3. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry (parts A and B), 5$^{th}$ ed., Springer, 2008.
4. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2nd ed., Oxford University Press, 2012.

5. P. S. Kalsi, Stereochemistry, Conformation and Mechanism, 9th ed., New Age Publications, 2017.
6. T. Tsuji, Transition Metal Reagents and Catalysts: Innovations in Organic Synthesis, John Wiley & Sons, 2000.
7. S. Warren, Organic Synthesis: The Disconnection Approach, 2nd ed., John Wiley, 2008.
8. E. Robert, Gawley, J. Aube, Principles of Asymmetric Synthesis, 2nd ed., Elsevier, 2012.
9. G. L. D. Krupadanam, Fundamentals of Asymmetric Synthesis, 1st ed., CRC press, 2014.
10. T.W. Greene, P. G. M. Wuts, Protecting Groups in Organic Synthesis, 2nd ed., John Wiley, 1991.
11. H. R. Crabtree, The Organometallic Chemistry of the Transition Metals, 6th ed., John Wiley & Sons, 2014.
12. S. D. Burke, R. L. Danheiser, Handbook of Reagents for Organic Synthesis, John Wiley & Sons, 1999.

**CORE**

**25-802-0803**

**ORGANIC CHEMISTRY -V**

**(SPECTROSCOPY OF ORGANIC COMPOUNDS)**

**Credit 3** **48 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Identify structures of unknown organic compounds using hyphenated techniques and spectral library matching. | Evaluate |
| C.O. 2:<br>Identify structures of unknown organic compounds based on the data from UV-Vis, IR, Mass Spectrometry $^{1}$HNMR and $^{13}$CNMR spectroscopy. | |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | X | X | | | | | | X | X | |
| C.O. 2 | X | X | | | | | | X | X | |

| **UNIT I** | **10 hrs** |
|---|---|
| Study of Mass Spectrometry applied to organic molecular systems Elemental analysis, empirical formula, molecular formula, Molecular mass, nominal mass, Exact mass, Index of hydrogen deficiency. The technique of Mass Spectrometry: Molecular ion, ion production methods (EI). Soft ionization methods: FAB, CA, MALDI, PD, Field desorption electrospray ionization, HRMS and formula mass, LC-MS, GC-MS. MS- MS Mass spectra of chemical classes and its correlation with structure: Fragmentation patterns, nitrogen and ring rules, Rule of thirteen, McLafferty rearrangement. | |
| **UNIT II** | **10 hrs** |
| Study of Ultraviolet-Visible Absorption and Emission and Chirooptical Spectroscopy applied to organic molecular systems<br>Energy levels and selection rules, Woodward-Fieser and Fieser-Kuhn rules, estimation of λmax of substituted aromatic ketones, aldehydes and acids. Spectral correlation with structure: Influence of substituents, conjugation, Intramolecular Charge transfer, Solvent effect<br>Fluorescence Spectroscopy. Excitation and Emission Spectra. Fluorescence Quantum Yield and Lifetime. Spectral correlation with structure: Influence of substituents, ring size, strain and conjugation, Intramolecular Charge transfer, Intramolecular proton transfer, Solvent effect<br>Chirooptical Spectroscopy: Introduction and applications of ORD, CD, Octant rule, axial haloketone rule, Cotton effect. | |

| UNIT III | 8 hrs |
|---|---|
| Study of Infrared Spectroscopy applied to organic molecular systems<br>Fundamental vibrations, overtones, Fermi Resonance, Hot bands, combination bands<br>Spectral correlation with structure: Characteristic regions of the spectrum.<br>Influence of substituents, ring size, hydrogen bonding, vibrational coupling, hybridization and field effect on frequency.<br>IR spectra of chemical classes including amino acids and its correlation with structure. | |
| **UNIT IV** | **10 hrs** |
| Study of NMR spectroscopy applied to organic molecular systems<br>The NMR instrumentation and Experiment: Magnetic nuclei with special reference to $^{1}H$ and $^{13}C$ nuclei. Chemical shift and shielding/deshielding, relaxation processes, chemical and magnetic non-equivalence, local diamagnetic shielding and magnetic anisotropy. Proton and $^{13}C$ NMR scales, characteristics of 13C as a nucleus.<br>Spin-spin splitting, AX, AX2, AX3, A2X3, AB, ABC, AMX type coupling, First order and non-first order spectra, Pascal's triangle, coupling constant, mechanism of coupling, Karplus curve, quadrupole broadening and decoupling, diastereomeric protons, virtual coupling, long range coupling effects, NOE, coupling with other nuclei.<br>Simplification non-first order spectra to first order spectra, shift reagents mechanism of action, spin decoupling and double resonance, Chemical shifts and homonuclear/heteronuclear couplings, the basis of heteronuclear decoupling.<br>Polarization transfer. Selective Population Inversion (qualitative description only), DEPT, sensitivity enhancement and spectral editing. 2D NMR and COSY, HMQC, HMBC. | |
| **UNIT V** | **10 hrs** |
| Identification of structures of unknown organic compounds using hyphenated techniques and Spectral library matching.<br>Identification of structures of unknown organic compounds based on the data from UV-Vis, IR, Mass, $^{1}$HNMR and $^{13}$CNMR spectroscopy. | |

**Recommended Text Books:**


1. D. L. Pavia, G. M. Lampman, G. S. Kriz, J. R. Vyvyan, Introduction to Spectroscopy: A Guide for Students of Organic Chemistry, Indian ed., Brooks/Cole Cengage Learning, 2007.
2. Atta-Ur-Rahman, M. I. Choudhary, Solving Problems with NMR Spectroscopy, Academic Press, New York, 1996.
3. L. D. Field; S. Sternhell, J. R. Kalman; Organic Structures from Spectra, 4th ed., Wiley 2008.
4. R. S. Drago, Physical Methods for Chemist, Saunders,1992.

5. C. N. Banwell, E. M. McCash, Fundamentals of Molecular Spectroscopy, $4^{th}$ ed., McGrawHill, 1994.
6. D. F. Taber, Organic Spectroscopic Structure Determination, A Problem Based Learning Approach, Oxford University Press, 2009.
7. R. M. Silverstein, G. C. Bassler, T. C. Morril, Spectroscopic Identification of Organic Compounds, John Wiley, 1991.
8. D. H. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, Tata McGraw Hill, 1988.
9. W. Kemp, Organic Spectroscopy, 2nd ed., ELBS-Macmillan, 1987.
10. F. Bernath, Spectra of Atoms and Molecules, 2nd ed., Oxford University Press, 2005.
11. E. B. Wilson, Jr., J. C. Decius, P. C. Cross, Molecular Vibrations: The Theory of Infrared and Raman Spectra, Dover Publications, 1980.
12. A. Weil, J. R. Bolton, Electron Paramagnetic Resonance: Elementary Theory and Practical Applications, 2nd ed., Wiley Interscience, John Wiley & Sons, Inc.,2007.
13. C. P. Slichter, Principles of Magnetic Resonance, 3rd ed., Springer-Verlag, 1990.
14. H. Gunther, NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry, 3rd ed., Wiley- VCH, 2013.
15. Spectral data bases (RIO DB of AIST, for example).

**CORE**

**25-802-0804**

**PHYSICAL CHEMISTRY- III**

**(STATISTICAL AND NON-EQUILIBRIUM THERMODYNAMICS)**

**Credit 3** **48 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Explain the different types of statistics and calculate the thermodynamic probability of any given thermodynamic system. | Analyze |
| C.O. 2:<br>Calculate the partition function and thermodynamic properties from spectroscopic data. | Apply |
| C.O. 3:<br>Apply the principles of statistical thermodynamics to ideal gases, solids and metals. | Apply |
| C.O. 4:<br>Explain the basics of transport phenomena's viz., Osmosis, biological motors and electro kinetic effects. | Understand |
| C.O. 5:<br>Derive expression for entropy production for physical and chemical processes | Apply |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | X | X | | | X | | | | | |
| C.O. 2 | X | X | | | X | | | | | |
| C.O. 3 | X | X | | | X | | | | | |
| C.O. 4 | X | X | | | X | | | | | |
| C.O. 5 | X | X | | | X | | | | | |

| **UNIT I** | **8 hrs** |
|---|---|
| Kinetic Theory of gases, Maxwell Distribution of velocity, Boltzmann distribution, Types of molecular velocities- r.m.s, most probable and mean velocity, Molecular Collisions, Mean free path, Transport properties- Diffusion, effusion, Viscosity, Thermal conductivity.<br>Thermodynamic probability, microstate and macrostate, entropy and probability, most probable distribution, residual entropy and its calculation. Ensembles, Maxwell - Boltzmann statistics. | |
| **UNIT II** | **10 hrs** |
| Partition function and its relation to thermodynamic properties, Translational, rotational and Vibrational partition function. Molecular partition function for delocalized systems, calculation of equilibrium constant using partition functions. | |

| | |
|---|---|
| Heat capacity of gases, Anomalous heat capacity of $H_2$, Heat capacity of solids: Dulong - Petits law, Einstein's theory and its modification, Debye's theory of heat capacity of solids. | |
| **UNIT III** | **10 hrs** |
| Quantum statistics, Bose - Einstein statistics, Fermi - Dirac statistics, Comparison of Maxell - Boltzman, Bose=- Einstein and Fermi - Dirac Statistics, Dilute Systems. Application of Bose - Einstein Statistics, Gas degeneration, Application to liquid helium, Bose Einstein Condensation. Application of Fermi -Dirac Statistics to electrons in metals, Extreme Gas Degeneration, Electron gas in metals and its contribution to pressure and heat capacity. | |
| **UNIT IV** | **10 hrs** |
| Partition function for systems of dependent particles, Configurational integral and configurational partition function. Imperfect gas, van der Waals equation and Virial equation of state, Evaluation of the first virial coefficient. Condensed state, Cluster integrals, Communal entropy. | |
| **UNIT V** | **10 hrs** |
| Linear Non-equilibrium thermodynamics- General theory, Local entropy production, balance equation for concentration. Energy conservation in open systems. Entropy balance equation. Forces and Fluxes, Steady state and local equilibrium conditions. Linear phenomenological laws. Phenomenological coefficient, Systems with heat, matter and electrical transport, Onsager Reciprocal relation, Application to Diffusion -Thermal diffusion, Thermal Osmosis and electrokinetic effects, Soret Coefficient, Seebeck effect. | |

**Recommended Text Books:**


1. F.W. Sears, Introductions to Thermodynamics, Kinetic Theory of Gases and Statistical Mechanics, Addision Wesley Pub. Cambridge, 1998.
2. F.C. Andrews, Equilibrium to Statistical Mechanics, John Wiley, New York, 2002.
3. L.K. Nash, Statistical Thermodynamics, Addison Wesley, New York, 1999.
4. P. W. Atkins, J. de Paula, Physical Chemistry 8th ed., 9th edn. Wiley, New York, 2006
5. D. A. McQuarrie, Physical Chemistry- A Molecular Approach, South Asian Edn., 2008.
6. M. Dole, Introduction to Statistical Thermodynamics, Prentice Hall, London, 1997.
7. J. Kestin, J.R. Dorfman, A Course in Statistical Thermodynamics, Academic press, 1971.
8. D. A. McQuarrie, Statistical Thermodynamics, South Asian Edn., 2008.
9. I. Prigogine, Introduction to Thermodynamic Irreversible Processes, 3rd ed., Wiley Interscience, 1968.
10. S. R. de Groot, P. Mazur, Non-equilibrium Thermodynamics, Dover Publications, 2011.
11. G. Lebon, D. Jou, J. Casas, Understanding Non-equilibrium Thermodynamics, Springer. 2008.
12. S. Kjelstrup, D. Bedeaux, E. Johannessen, J. Gross, Non-Equilibrium Thermodynamics for Engineers: Second Edition, World Scientific Publishing Company, 2017.

13. D. Kondepudi and I. Prigogine, Modern Thermodynamics: From Heat Engines to dissipative Structures, Wiley, New York.

**CORE**

**25-802-0805**

**THEORETICAL CHEMISTRY-III**

**(CHEMICAL BONDING AND COMPUTATIONAL CHEMISTRY)**

**Credit 3** **48 hours**

| **Course Outcome**<br>After the completion of the course, the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Explain the quantum mechanical nature of the chemical bond. | Understand |
| C.O. 2:<br>Account for the basic principles and concepts of molecular orbital theory and valence bond theory using quantum mechanical principles. | Apply |
| C.O. 3:<br>Describe quantum mechanically the chemical bonding of any given di and tri- atomic molecules with molecular orbital theory and valence bond theory. | Analyze |
| C.O. 4:<br>Describe the main similarities and differences between theoretical approaches and identify advantages and disadvantages for modelling various chemical problems. | Apply |
| C.O. 5:<br>Use computational chemistry software to perform and interpret electronic structure calculations. | Evaluate |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | X | X | | | | | | X | | |
| C.O. 2 | X | X | | | | | | X | | |
| C.O. 3 | X | X | | | | | | X | | |
| C.O. 4 | X | X | | | X | X | X | X | | |
| C.O. 5 | X | X | | | X | | X | X | X | |

| **UNIT I** | **12 hrs** |
|---|---|
| Chemical bonding, Born Oppenheimer approximation, Valence bond method. Comparison of VB and MO method, LCAO approximation, calculation of energy. levels from wave functions, application to diatomic molecules such as, $H_2^+$, $H_2$.<br>Concept of σ, σ*, π, π* orbitals and their characteristics, hybrid orbitals, calculation of coefficients of AO used in sp, $sp^2$ and $sp^3$ hybrid orbitals, interpretation of geometry, Valence bond model of $H_2$, Hybridisation of $H_2O$, $BF_3$, $NH_3$ and $CH_4$. | |
| **UNIT II** | **8 hrs** |
| Pi bonding in simple molecules, HMO method for linear conjugated hydrocarbons, linear, cyclic, polycyclic, heterocyclic; ethylene, 1,3- butadiene,allyl radical, cation and anion, aromatic | |

| | |
|---|---|
| hydrocarbons, cyclopropenyl systems, cyclobutadiene, benzene, naphthalene and other conjugated systems. calculation of charge distribution, bond orders and reactivity. QMOT: Applications of Molecular Orbital Theory in Understanding reactions and Mechanisms. Qualitative MO theory. Group orbitals. Frontier Orbitals, Substituent effects on frontier orbitals, HSAB concept, Nucleophiles and Electrophiles, Perturbation theory of reactivity. Application of Frontier Orbital theory in studying ionic and radical reactions, Ambident electrophiles, α-effect. | |
| **UNIT III** | **8 hrs** |
| Tools and philosophy of computational chemistry. potential energy surface – local minima, global minima, saddle point and transition states, geometry optimization-stationary points. | |
| **UNIT IV** | **8 hrs** |
| Basis sets, Slater and Gaussian functions, classification of basis sets – minima l,double zeta, triple zeta, split valence, polarization and diffuse basis sets, contracted basis sets, Pople style basis sets and their nomenclature, correlation consistent basis sets.<br>SCF methods, semiempirical, ab initio, electron correlations, post-Hartree-Fock methods and density functional theory. | |
| **UNIT V** | **12 hrs** |
| Molecular structure, internal coordinates, Cartesian coordinates, geometry optimization, frequency analysis, partial charge, MO, Computational calculations listed below using available Molecular orbital theory suite of programme package: Constructing molecular structures or models; Molecular geometry optimization; Conformational analysis; Thermodynamic and spectroscopic properties; Molecular orbital analysis; Electron density and electrostatic potential map. | |

**Recommended Text Books:**


1. J. P. Lowe, Quantum Chemistry, 3rd ed., Academic Press, New York, 2008.
2. F. Jensen, Introduction to Computational Chemistry, 2nd ed., Wiley, New York, 2009.
3. R. Leach, Molecular Modeling, Principles and Applications, 2nd ed., Pearson Education, London, 2001.
4. A. K. Chandra, Introduction to Quantum Chemistry, 4th ed., Tata McGraw-Hill, 1994.
5. L. Pauling, E. B. Wilson, Introduction to Quantum Mechanics, McGraw-Hill, 1935.
6. A. Szabo, N. S. Ostlund, Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory, Dover Book ed., Mc.Graw-Hill, New York, 1982.
7. T. A. Albright, J. K. Burdett, M.-H. Whangbo, Orbital Interactions in Chemistry, 2nd ed., John Wiley and Sons, Inc., Hoboken, New Jersey, 2013.

**CORE/LAB**

**25-802-0806**

**ADVANCED PHYSICAL CHEMISTRY LAB-II**

**Credit 2** **96 hours**

| **Course Outcome**<br>After the completion of the course the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Operate various sophisticated instruments. | Apply |
| C.O. 2:<br>Perform experiments based on various laws of physical chemistry. | Apply |
| C.O. 3:<br>Analyze the results obtained from various experiments. | Analyze |
| C.O. 4:<br>Calculate the unknown concentration of the given solution based on the results obtained from the experiment. | Evaluate |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | X | X | | | | X | X | X | X | |
| C.O. 2 | X | X | | | | X | | X | X | |
| C.O. 3 | X | X | | | | X | | X | X | |
| C.O. 4 | X | X | | X | | | | X | X | |

**UNIT I** **96 hrs**

i. Molecular weight determination by cryoscopic methods, Formula of complexes.

ii. Phase diagrams: Two component liquid–liquid and solid-liquid systems. Three component liquid-liquid systems.

iii. Determination of transition temperature, molecular weight determination.

iv. Refractometry: Variation of refractive index with composition, formula of complexes.

v. Chemical Kinetics: Acid and base catalysed hydrolysis of esters,

vi. Dependence of temperature and ionic strength on the rate of reactions, Hydrolysis of p-nitrophenyl acetate using spectrophotometry.

vii. Ostwald Viscometer: Viscosity of liquid and liquid mixtures.

viii. Conductometry: Cell constant, conductivity of a weak-acid, solubility of a sparingly soluble salt, conductometric titrations. Determination of critical micelle concentration of colloids.

ix. Poteniometry: Measurement of electrode potentials, activity coefficients and potentiometric titrations, pH metric titrations.

x. Adsorption: Checking the validity of Freundlich and Langmuir adsorption and determination of unknown concentration.

| | |
|---|---|
| xi. | Spectrophotometry: Checking the validity of beer Lambert's law and determination of unknown concentration. |
| xii. | Demonstration of instrumentation of AAS, Flame photometry, Fluorescence spectrometer, GPC, Electrochemical work station etc. |

**Recommended Textbooks:**


1. A. Findlay, Practical Physical Chemistry, 9th ed., Longman, 1973.
2. D. P. Shoemaker, C.W. Garland, J.W, Nibler, Experiments in Physical Chemistry, 5th ed., McGraw Hill, 1989.
3. J. B. Yadav, Advanced Practical Physical Chemistry, 36th ed., KrishnaPrakashan Media (P) Ltd, 2016.
4. J. N. Gurtu, A.N. Gurtu, Advanced Physical Chemistry Experiments, 6th ed., Pragati, 2014..

**CORE/LAB**

**25-802-0807**

**OPEN ENDED LAB-IV**

**Credit 2** **96 hours**

| **Course Outcome**<br>After the completion of the course the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Design experiments and validate the hypothesis of an independent research problem. | Evaluate |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | x | x | | | | x | x | x | x | |

| **UNIT I** | **96 hrs** |
|---|---|
| The students shall perform literature review/ experiments/analysis for validating the hypothesis.<br>The students shall submit a project report and appear for viva-voce. | |

**ELECTVE**

**25-802-0808**

**BIOANALYTICAL CHEMISTRY**

**Credit 2** **32 hours**

| **Course Outcome**<br>After the completion of the course the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Demonstrate key features and characteristics of major biomolecules. | Understand |
| C.O. 2:<br>Describe and explain the principles and applications of MRI and NMR for bioanalysis. | Understand |
| C.O. 3:<br>Outline the principles and theory of major types of electrophoresis and electrophoretic separation. | Apply |
| C.O. 4:<br>Explain the theory and applications of biochemical analysis like RIA, ELISA. | Analyze |
| C.O. 5:<br>Appreciate the variety of popular methods to separate and isolate biomolecules. | Evaluate |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | X | X | | | | | | X | | |
| C.O. 2 | X | X | | | | X | | X | | |
| C.O. 3 | X | X | | | | X | | X | | |
| C.O. 4 | X | X | | | | X | | X | | |
| C.O. 5 | X | X | | | | X | | X | | |

| **UNIT I** | **10 hrs** |
|---|---|
| Biomolecules- amino acid, protein, nucleic acid –structures, physical and chemical properties, features and characteristics of major biomolecules, structure function relationship, significance. Different methods for the estimation of protein. Transition metals in health and disease - Importance of transition metals in physiological processes, Therapeutic implications of transition metals. | |
| **UNIT II** | **8 hrs** |
| Transmission electron Microscopy (TEM), Scanning electron Microscopy (SEM) – Instrumentation and its biological applications. Nuclear magnetic resonance (NMR) and magnetic resonance imaging (MRI) technologies: key tools for the life and health sciences. Principles of NMR and the importance of this biomolecular analytical technique. Established and emerging applications of NMR.<br>Principles and uses of MRI. MRI as a principal diagnostic and research tool. | |
| **UNIT III** | **4 hrs** |
| Electrophoretic techniques – Principles of electrophoretic separation. Types of electrophoresis | |

| | |
|---|---|
| including paper, gel. Electroporation, Pulse field gel electrophoresis- applications in life and health science. | |
| **UNIT IV** | **4 hrs** |
| Radio immune assay (RIA) - principle and applications. Enzyme linked immune sorbent assay (ELISA) principle and applications. Biosensors-applications. | |
| **UNIT V** | **6 hrs** |
| Principle of centrifugation, concept of RCF, features and component of major types of centrifuge, preparative, differential and density gradient centrifugation, analytical ultra-centrifugation, centrifugation. Flow cytometry: principles and applications of this core method of separation. | |

**Recommended Text Books:**


1. V. A. Gault, N. H. Mcclenaghan, Understanding bio analytical chemistry - principle and applications, John Wiley and Sons, Ltd Publications, 2009.
2. A. Manz, N. Pamme, D. Iossifidis, Bio-analytical Chemistry, 2004
3. S. R. Mikkelsen, E. Corton, Bio Analytical Chemistry, John Wiley and Sons, Ltd Publications, 2004.
4. K. Wilson, J. Walker, Practical Biochemistry-Principles and techniques, 5th ed., Cambridge University press, 2000.

**ELECTIVE**

**25-802-0809**

**ADVANCED PHOTOCHEMISTRY**

**Credit 2** **32 hours**

| **Course Outcome**<br>After the completion of the course the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Describe various photochemical and photophysical processes and apply established experimental methods for the investigation of these processes. | Apply |
| C.O. 2:<br>Explain theories of photoinduced electron transfer and reactivity of excited states and their significance in different fields including biomedical applications and photosynthesis. | Evaluate |
| C.O. 3:<br>Apply the knowledge of photochemistry of semiconductors and advanced materials for various applications involving photochemical energy conversions. | Apply |
| C.O. 4:<br>Explain theory and application of photocatalysis and explain the environmental impact of atmospheric photochemistry. | Evaluate |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | X | X | | | | | | X | | |
| C.O. 2 | X | X | | | | | | X | | |
| C.O. 3 | X | X | | | X | | | X | | |
| C.O. 4 | X | X | X | | X | | | X | | |

| **UNIT I** | **8 hrs** |
|---|---|
| Energy Transfer-Theories of Energy Transfer – Photosensitization of Organic and Inorganic Molecules – Singlet Oxygen – Methods of singlet oxygen generation and Detection – Chemistry of Singlet Oxygen – Photodynamic Therapy of Cancer. | |
| **UNIT II** | **8 hrs** |
| Photoinduced Electron Transfer – Theory of Electron transfer – Circumventing Back Electron transfer – Photoinduced Electron transfer reactions of Organic and Inorganic Molecules – Photosynthesis. | |
| **UNIT III** | **4 hrs** |
| Photochemistry and Photophysics of Semiconductors – Semiconductor Photocatalysis and applications. Atmospheric photochemistry Electrical and optical properties. Nano domains of Carbon-fullerenes, carbon nanostructures, graphene, graphene quantum dots. | |

| UNIT IV | 6 hrs |
|---|---|
| Photochemistry and Advanced Materials - Artificial Solar Energy Harvesting – Photochemical Splitting of Water – Dye sensitized solar cells - Grätzel Cell – Bulk heterojunction devices for solar energy harvesting - Organic light emitting devices. Photoresists – Photolithography – Photochromism – Photonic Materials and Lasers. | |

| UNIT V | 6 hrs |
|---|---|
| Photochemistry in Practice – Radiometry and Actinometry – Principles of Radiometry and radiometers – Actinometry – Quantum Yields – Light Sources – Optical Materials and Filters – Photochemical Reactors. | |

**Recommended Text Books:**


1. N. J. Turro, V. Ramamurthy, J. C. Scaiano, Modern Molecular Photochemistry of Organic Molecules, University Science Books, 2010.
2. C.E. Wayne, Photochemistry (Oxford Chemistry Primers), Oxford University Press; 1st ed., 1996.
3. J. R. Lakowicz, Principles of Fluorescence Spectroscopy, Plenum Press, 3rd ed., 2010.
4. A. M. Braun, M.-T. Maurette, Esther Oliveros, Photochemical Technology, John Wiley & Sons, 1991.
5. M. A. Fox, M. Chanon, Photoinduced Electron Transfer Part A, B. C and D, Elsevier Science Publishing Company, 1988.
6. J. Mattay Ed., Photoinduced Electron Transfer 1-5 (Topics in Current Chemistry), Springer, 1st ed., 1990-1993.
7. G. J. Kavarnos, Fundamentals of Photoinduced Electron Transfer, 1st ed., Wiley-VCH, 1993.
8. V. Ramamurthy, K. Schanze, Molecular and Supramolecular Photochemistry, Volume 10, Semiconductor Photochemistry and Photophysics, Marcel Dekker, New York, 2003.
9. V. Ramamurthy, Photochemistry in Organized and Confined Media, VCH Publishers, New York, 1991.

**ELECTIVE**

**25-802-0810**

## THEORY OF ORBITAL INTERACTIONS IN CHEMISTRY

**Credit 2** **32 hours**

| **Course Outcome**<br>After the completion of the course the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Examine the physical properties associated with molecules and the pathways taken by chemical reactions. | Analyze |
| C.O. 2:<br>Correlate qualitatively the shape and energy of orbitals and the chemical reaction exhibited by any molecule. | Apply |
| C.O. 3:<br>Explore the effects of symmetry, overlap, and electronegativity in the molecular orbital in case of chemical reaction. | Evaluate |
| C.O. 4:<br>Explore the structures and reactivity relationships associated with any molecule. | Evaluate |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | X | X | | | X | | | X | | |
| C.O. 2 | X | X | | | X | | | X | | |
| C.O. 3 | X | X | | | X | | | X | | |
| C.O. 4 | X | X | | | X | | | X | | |

| **UNIT I** | **6 hrs** |
|---|---|
| Atomic and Molecular Orbitals, Concepts of Bonding and Orbital Interaction, Orbital Interaction Energy, Molecular Orbital Coefficients, Electron Density Distribution, Perturbational Molecular Orbital Theory, Linear $H_3$, HF, and the Three-Orbital Problem. | |
| **UNIT II** | **10 hrs** |
| Molecular Orbital Construction from Fragment Orbitals, Triangular $H_3$, Rectangular and Square Planar $H_4$, Tetrahedral and Linear $H_4$, Pentagonal $H_5$ and Hexagonal $H_6$, Molecular Orbitals of Diatomic Molecules and Electronegativity Perturbation, Geometrical Perturbation of Molecular orbitals, Molecular Orbitals of $AH_2$, Walsh Diagrams, Jahn–Teller Distortions. | |
| **UNIT III** | **6 hrs** |
| Molecular Orbitals of Small Building Blocks, AH System, $AH_3$ Systems, pi-Bonding Effects of Ligands, $AH_4$ System, Molecules with Two Heavy Atoms, $A_2H_6$ Systems, Orbital Interactions through Space and through Bonds. | |
| **UNIT IV** | **4 hrs** |
| Polyenes and Conjugated Systems, Acyclic Polyenes, Huckel Theory, Cyclic Systems, Conjugation | |

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| in Three Dimensions, Solids, Energy Bands, Hypervalent Molecules. |
| **UNIT V** **6 hrs** |
| Transition Metal Complexes. Octahedral $ML_6$, pi-Effects in an Octahedron, Distortions from an Octahedral Geometry, Square Planar, Tetrahedral $ML_4$ Complexes, Five Coordination, Square Pyramidal $ML_5$ Fragment, $ML_3$ Fragment, $ML_2$ and $ML_4$ Fragments, $M_2L_8$ Dimers, CpM and $Cp_2M$, Isolobal Analogy. |

**Recommended Text Books:**


1. T. A. Albright, J. K. Burdett, M.-H. Whangbo, Orbital Interactions in Chemistry, 2nd ed., John Wiley and Sons, Inc., Hoboken, New Jersey, 2013.
2. I. Flemming, Molecular Orbitals and Organic Chemical Reactions, Students ed., Wiley, 2009.
3. A. Rauk, Orbital Interaction Theory of Organic Chemistry, 2nd ed., Wiley- Blackwell, 2000.
4. W. L. Jorgensen, L. Salem, The Organic Chemist's Book of Orbitals, Academic Press, 1973.

**ELECTIVE**

**25-802-0811**

**MATERIALS CHEMISTRY**

**Credit 4** **75 hours**

| **Course Outcome**<br>After the completion of the course the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>To acquire basic knowledge on various types of materials | Understand |
| C.O. 2:<br>To gain insight on the structure – property relationship of different materials | Understand |
| C.O. 3:<br>To get an idea about the materials in advanced technological applications | Analyze |
| C.O. 4:<br>To get hands on experience on the synthesis and characterization of various classes of materials | Apply |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | X | | | | | | | | | |
| C.O. 2 | X | | | | | | | | | |
| C.O. 3 | X | | | | | | | | | |
| C.O. 4 | | | X | | | | | X | | |

| **UNIT I** | **12 hrs** |
|---|---|
| Chemistry of Materials. Ionic and covalent solids. Molecular and metallic solids. Amorphous and crystalline materials. Crystalline state. Structural organization of crystalline solids-theories of bonding. Crystal structures. Imperfections in crystal structures.<br>Semiconductor materials- properties and types of semiconductors. Structure and Bonding of semiconductor materials. Silicon based semiconductors. II-VI (wide band gap) and III-V (narrow band gap) compound semiconductors. Electrical, optical and magnetic properties of semiconductor materials. Preparation and properties of ZnO, ZnS, CdS, CdTe, Ga-As, In-S, Cu-In-S. Application in photovoltaic devices. | |
| **UNIT II** | **10 hrs** |
| Polymer Materials- classification and nomenclature of polymers. Methods of Polymerization. Structure–property relationships. Plastics and elastomers. Viscoelastic behaviour. Rubber like elasticity. Crystalline and amorphous polymers. Glass transition temperature and crystalline melting. Functional Polymers. | |
| **UNIT III** | **12 hrs** |
| Nanomaterials. Materials in the nanodomain. Zero, one- and two-dimensional materials. Particle size | |

| | |
|---|---|
| dependent change in properties of materials. Metals in the nanodomain. Gold and silver nanoparticles. Preparation, properties and applications. Core shell structures. Semiconductor nanoparticles. Quantum dots. ZnO, ZnS, CdS and CdSe quantum dots.<br>Electrical and optical properties. Nano domains of Carbon-fullerenes, carbon nanostructures, graphene, graphene quantum dots. | |
| **UNIT IV** | **14 hrs** |
| Materials in Advanced Technology. Organic Polymer Semiconductors, Solid ionic conductors - Advanced materials for energy generation and energy storage. Porous membranes. Optical and photonic materials. | |
| **UNIT V** | **15 hrs** |
| Synthesis and characterization of various classes of materials — including semiconductors, polymers, nanomaterials and 2D materials. | |

**Recommended Text Books:**


1. B. D. Fahlman, Materials Chemistry, 2nd ed. Springer, Heidelberg, 2011.
2. Harry R. Allcock, Introduction to Material Chemistry, John Wiley & Sons, Inc., New Jersy, 2008
3. R. Zallen, Physics of Amorphous Solids, Wiley, New York, 1983.
4. R. J. Borg, G. J. Dienes, The Physical Chemistry of Solids, Academic Press, Boston, 1993.
5. D. Kingery, H. K. Bowen, D. R. Uhlmann, Introduction to Ceramics, 2nd ed., Wiley, New York, 1992.
6. J. M. J. Cowie, Polymers. Physics and Chemistry of Modern Materials, 3rd ed., CRC Press, Boca Raton, 2007.
7. S. O. Kasap, Principles of Electronic Materials and Devices, Mc Graw Hill, 2006.

**CORE**

**25-802-0910**

**ANALYTICAL CHEMSITRY-II**

**(ADVANCED ANALYTICAL TECHNIQUES AND INSTRUMENTAL METHODS)**

**Credit 4** **64 hours**

| **Course Outcome**<br>After the completion of the course the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Explain the theory, instrumentation and applications of various electroanalytical techniques, chromatographic, thermal and surface analysis | Apply |
| C.O. 2:<br>Predict appropriate chromatographic methodology for separation of a given mixture | Analyze |
| C.O.3:<br>Perform separation of components in a mixture using GC-MS and HPLC | Evaluate |
| C.O. 4:<br>Perform individual and simultaneous voltammetric analysis of samples | Evaluate |
| C.O. 5:<br>Analyse the surface of various samples using SEM, AFM, TEM | Analyze |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | X | | | | | | | | | |
| C.O. 2 | X | X | | | | | | | | |
| C.O. 3 | X | X | X | X | | X | X | | X | |
| C.O. 4 | X | X | X | X | | X | X | | X | |
| C.O. 5 | X | X | X | X | | | | | | |

**UNIT I** **18 hrs**

Potentiometry: different types of indicator electrodes, limitations of glass electrode, applications in pH measurements, other types of ion selective electrodes, solid, liquid, gas sensing and specific types of electrodes, biomembrane, biological and biocatalytic electrodes as biosensors, importance of selectivity coefficients. CHEMFETS- importance of specially designed amplifier systems for ion selective electrode systems. Potentiometric titrations- types and applications.

Electrogravimetry- electrogravimetry without potential control, controlled potential electrogravimetry, applications

Coulometry- constant current and constant potential coulometry, applications primary and secondary coulometry, advantages of coulometric titrations

Conductance measurement – conductometric titrations

| | |
|---|---|
| Polarography – current – voltage curve, DME-components of polarographic current, supporting electrolyte, polarographic maxima. Half-wave potential, Applications of Polarography<br>Voltammetry - different types, Theory and applications Stripping analysis. Amperometric titrations – Different types and Applications<br>Impedance spectroscopy, Voltammetric sensors – individual and simultaneous analysis-Case study | |
| **UNIT II** | **12 hrs** |
| Gas chromatography – basic instrumental set up-inlets, carriers, columns, detectors and comparative study of TCD, FID, ECD, NPD and MS. Qualitative and quantitative studies using GC, Preparation of GC columns, packet columns and capillary columns, selection of stationary phases of GLC, Choosing the parameters- Temperature, Length of the column, Sample size, Flow rate<br>CHN analysis by GC, Case study<br>GC Capillary electrophoresis-migration rates and plate heights, instrumentation, sample introduction, detection methods, applications. Capillary gel electrophoresis.<br>Capillary isotachophoresis. Isoelectric focusing.<br>Capillary electro chromatography-packed columns. Micellar electro kinetic chromatography. and GC-MS applications | |
| **UNIT III** | **12 hrs** |
| HPLC – Separation process, Eddy diffusion, Mass transfer, Longitudinal diffusion, Retention parameters in HPLC-Capacity factor, Retention time, Retention volume, Peak width, Total number of theoretical plates, Height equivalent of a theoretical plate, Resolution and retention time, Solvent delivery systems, Detectors<br>Instrumentation and functioning of HPLC, Types of HPLC - Modes of separation in HPLC-adsorption chromatography, reversed phase chromatography, ion pair chromatography, ion exchange chromatography Solubility and retention in HPLC<br>Method development in HPLC - Selection of mobile phase and optimization, Preparation of sample, Selection of column and solvent<br>HPLC method validation, HPLC Analysis -Case study Dos and Don'ts in HPLC - Troubleshooting in HPLC | |
| **UNIT IV** | **12 hrs** |
| Measurement of alpha, beta, and gamma radiations, neutron activation analysis and its applications. Principle and applications of isotope dilution methods,<br>Radioimmunoassay (RIA), Immunoradiometric assay (IRMA), Enzyme linked immunosorbent assay (ELISA)-Principles and practical aspects<br>Thermal methods of Analysis TG, DTA and DSC - Instrumentation and Theory – Factors affecting TGA - effect of atmosphere on DTA. TG of copper sulphate pentahydrate and calcium oxalate monohydrate. Application of thermal methods for identification of substances. | |

| UNIT V | 10 hrs |
|---|---|
| Chemical Analysis of surfaces: Surface preparations-ion scattering spectrometry secondary ion scattering microscopy (SIMS)-Auger election spectroscopy-ESCA instrumentation and application. Principle, instrumentation and applications of SEM, TEM and AFM, Case study | |

**Recommended Text Books:**


1. J.M. Mermet, M. Otto, R. Kellner, Analytical Chemistry, Wiley-VCH, 2004.
2. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Saunders College Pub., 2007.
3. J.G. Dick, Analytical Chemistry, R.E. Krieger Pub., 1978.
4. J.H. Kennedy, Analytical Chemistry: Principles, Saunders College Pub., 1990.
5. G.H. Jeffery, J. Bassett, J. Mendham, R.C. Denney, Vogel's Text Book of Quantitative Chemical Analysis, 5th Edn., John Wiley& sons,1989.
6. C.L. Wilson, D.W. Wilson, Comprehensive Analytical Chemistry, Elsevier, 1982.
7. G.D. Christian, J.E. O'Reilly, Instrumental Analysis, Allyn & Bacon, 1986.
8. R.A. Day, A.L. Underwood, Quantitative Analysis, Prentice Hall, 1967.
9. H.A. Laitinen, W.E. Harris, Chemical Analysis, McGraw Hill, 1975.
10. F.W. Fifield, D. Kealey, Principles and Practice of Analytical Chemistry, Blackwell Science, 2000.
11. Contemporary Instrumental Analysis, Kenneth A. Rubinson, Judith F. Rubinson, Prentice Hall, New Jersey, 2000.
12. Wilson & Wilson's, Comprehensive Analytical Chemistry, Volume 47, Modern Instrumental Analysis, Edited by S. Ahuja, N. Jespersen, Reed Elsevier India Private Ltd., Noida, 2006.
13. Journal of Chromatography Library, Volume 3, Liquid Column Chromatography- A Survey of Modern Techniques and Applications, Edited by Z. Deyl, K. Macek, J. Janak, Elsevier Scientific Publishing Company, Amsterdam, 1975.
14. Gas Chromatography, John Willett, John Wiley & Sons, Singapore, 1991.
15. Fundamentals of Analytical Chemistry, Doughlas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, 9th Ed., Cengage Learning, 2014.
16. Allen J. Bard, Larry R. Faulkner, Electrochemical Methods-Fundamentals and Applications, John Wiley & Sons, New York, 1980.

**CORE**

**25-802-0902**

**Inorganic Chemistry – V**

**(ORGANOMETALLIC AND BIOINORGANIC CHEMISTRY**

**Credit 3** **48 hours**

| **Course Outcome**<br>After the completion of the course the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Distinguish the different types of ligands with respect to the type of interaction with the metal. | Analyze |
| C.O. 2:<br>Evaluate the structure, bonding and reactions of organometallic compounds and metal clusters. | Evaluate |
| C.O. 3:<br>Predict the stability of organometallic compounds and metal clusters. | Apply |
| C.O. 4:<br>Explain the application of reactions of organometallic complexes in homogeneous catalytic processes. | Apply |
| C.O. 5:<br>Identify the role of metals in biological systems. | Apply |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | X | X | | | | | | X | | |
| C.O. 2 | X | X | | | X | | | X | | |
| C.O. 3 | X | X | | | X | | | X | | |
| C.O. 4 | X | X | | | X | | | X | | |
| C.O. 5 | X | X | | | | | | X | | |

**UNIT I** **8 hrs**

Compounds with transition metal to carbon bonds: eighteen electron rule; classification of ligands, nomenclature, σ donor ligands – metal alkyl, aryl complexes; σ donor/π acceptor ligands, – metal alkenyls, alkynyls, carbenes, carbynes, carbonyls, isocyanide, fluxionality of ligands – structure, bonding, spectra, preparation and reactions.

**UNIT II** **8 hrs**

σ, π donor/π acceptor ligands – olefin complexes, alkyne, allyl, enyl complexes, metallocene-ferrocene, titanocene, zircanocene, arene complexes, cycloheptatriene, cyclooctatetraene, cyclobutadiene complexes, fluxionality of ligands – structure, bonding, preparation, reactions and spectroscopy.

| UNIT III | 8 hrs |
|---|---|
| Metal–Metal bonds and Transition metal clusters; preparation, properties and spectroscopy. Parallels with nonmetal chemistry- isolobal analogy. Application of Wade-Mingos-Lauher rules in predicting thestructure of organometallic clusters. | |
| **UNIT IV** | **12 hrs** |
| Reactions of organometallic complexes – Ligand cone angle, oxidative addition, reductive elimination, insertion, nucleophilic and electrophilic attack of coordinated ligands. Homogeneous catalysis using organometallic compounds: olefin hydrogenation, hydroformylation, Wacker process, Ziegler-Natta polymerisation, cyclo oligomerisation, olefin isomerisation, olefin metathesis, Monsanto acetic acid synthesis, Fischer-Tropsch process, hydrosilylation, coupling reactions in organic chemistry. | |
| **UNIT V** | **12 hrs** |
| Metal ions in biological systems: Heme proteins – hemoglobin, myoglobin Non-Heme Iron Proteins: Iron storage and transfer – ferritin, transferrin; electron transfer (Iron-sulfur protein) – rubredoxin, ferredoxin; $O_2$ transport – hemerythrin Copper proteins and Enzymes – Hemocyanin, superoxide dismutase, ceruloplasmin, cytochrome coxidase; Zinc and Cobalt enzymes – carbonic anhydrase, carboxypeptidase, interchangeability of zinc and cobaltenzymes; Vitamin B12 and B12 Photosynthesis and $N_2$ fixation Metals in medicines and therapy | |

**Recommended Text Books**


1. Ch. Elschenbroich, A. Salzer, Organometallics – A Concise Introduction, VCH Publishers, 1989.
2. B. D. Gupta, A. J. Elias, “Basic Organometallic Chemistry”, University Press, 2010.
3. P. Powell, Principles of Organometallic Chemistry, 2nd ed., ELBS, 1991.
4. J. E. Huheey, E. A. Keiter, R. L. Keiter, Inorganic Chemistry: Principles of structure and Reactivity, 4th ed., Harper Collin College Publishers, 1993.
5. E.-I. Ochiai. Bioinorganic Chemistry – An Introduction, Allyn and Bacon Inc., 1977.
6. N. Kaim, B. Schwederski. Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, John Wiley, 1994.
7. Bertini, H. B. Gray, S. J. Lippard, J. S. Valentine, Bioinorganic Chemistry, Viva Books, 1998.
8. R. W. Hay, Bio Inorganic Chemistry, Ellis Horwood, 1987.
9. J. A. Cowan, Inorganic Biochemistry – An Introduction, 2nd ed., VCH, 1997.
10. N. S. Hosmane (Ed) Boron Science: New Technologies and Applications, CRC Press, 2011.
11. S. J. Lippard, J. M. Berg. Principles of Bioorganic Chemistry, Panima Publ. Corpn. 2005.
12. M. N. Hughes, The Inorganic Chemistry of Biological Processes, Wiley, 1981.

**CORE**

**25-802-0903**

**ORGANIC CHEMISTRY-VI**

**(CHEMISTRY OF NATURAL PRODUCTS)**

**Credit 3** **48 hours**

| **Course Outcome**<br>After the completion of the course the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Device synthesis scheme for heterocyclic aromatic and nonaromatic organic compounds. | Analyze |
| C.O. 2:<br>Elucidate structure and device synthesis for important natural products. | Apply |
| C.O. 3:<br>Describe molecular structure of carbohydrates, proteins, DNA, RNA and synthesis of vitamin C and shikimic acid. | Understand |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | X | X | X | | | | | X | | |
| C.O. 2 | X | X | X | | | | | X | | |
| C.O. 3 | X | X | X | | | | | X | | |

| **UNIT I** | **6 hrs** |
|---|---|
| Nomenclature and general characteristics of heterocyclic compounds. Structure, properties, synthesis and reactivity of three and four-membered ring heterocycles containing one heteroatom. | |
| **UNIT II** | **10 hrs** |
| Heteroaromatic compounds (five and six-membered rings) containing one or two heteroatoms. Fused ring compounds: Synthesis and properties of indole, quinoline, isoquinoline, coumarin, flavone, purine and pyrimidine bases present in nucleosides. | |
| **UNIT III** | **12 hrs** |
| Terpenoids: Classification, biosynthesis. Structure elucidation and synthesis of abietic acid. Steroids: classification, biosynthesis. Structure elucidation of cholesterol, conversion of cholesterol to progesterone, androsterone and testosterone. Fatty acids: structure, biosynthesis. Prostaglandins-classification, structure, biosynthesis and synthesis. Alkaloids: Classification, isolation, structure elucidation based on degradative reactions (quinine and atropine). Biosynthesis of quinine and papaverine. | |
| **UNIT IV** | **10 hrs** |
| Carbohydrates: Structure of ribose, glucose, fructose, maltose, sucrose, lactose, starch cellulose and cyclodextrins. Preparation of alditols, glycosides (O, C, and N), deoxysugars. Synthesis of Vitamin | |

| |
|---|
| C from glucose. Nucleic acids: Structure and synthesis, genetic code, recombinant DNA, biosynthesis of shikimic acid. |
| **UNIT V** **10 hrs** |
| Aminoacids, peptides and enzymes: Synthesis of aminoacids – Strecker and azalactone synthesis, enantioselective synthesis of aminoacids, reactions of aminoacids. Structure of proteins, introduction to enzymes and coenzymes with special reference to the function of chymotrypsin, NAD, thiamine, pyridoxal. In vitro and in vivo synthesis of peptides, solid phase synthesis. |

**Recommended Text Books:**


1. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry (parts A and B), 5$^{th}$ ed., Springer, 2008.
2. I. L. Finar, Organic Chemistry Volumes 1 & 2, 6th ed., Pearson Education Asia, 2004.
3. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2nd ed., Oxford University Press, 2012.
4. N. R. Krishnaswamy, Chemistry of Natural Products; A Unified Approach, Universities Press, 1999.
5. R. J. Simmonds, Chemistry of Biomolecules: An Introduction, RSC, 1992.
6. R. O. C. Norman, Principles of Organic Synthesis, 2nd ed., Chapman and Hall, 1978.
7. J. A. Joule, K. Mills, Heterocyclic Chemistry, 5th ed., Wiley, 1998.
8. J. J. Li, E. J. Corey, Total Synthesis of Natural Products: At the Frontiers of Organic Chemistry, Springer, 2012.
9. T. Eicher, S. Hauptmann, The Chemistry of Heterocycles, 2nd ed., Wiley, 2003.
10. K. C. Nicolaou, S. A. Snyder, Classics in Total Synthesis II: More Targets, Strategies, Methods, Wiley, 2003.

**CORE**

**25-802-0904**

**PHYSICAL CHEMISTRY-IV**

**(CHEMICAL KINETICS, REACTION DYNAMICS, CATALYSIS AND SURFACE CHEMISTRY)**

**Credit 3** **48 hours**

| **Course Outcome**<br>After the completion of the course the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Interpret the basic reaction dynamics and obtain the rate constants for reactions in gaseous state and solutions. | Analyze |
| C.O. 2:<br>Calculate thermodynamic parameters from kinetic data. | Apply |
| C.O. 3:<br>Interpret the kinetics of unimolecular, termolecular and fast reactions. | Apply |
| C.O. 4:<br>Identify isotope effects in reactions | Analyze |
| C.O. 5:<br>Apply the principles of acid-base and enzyme catalysis to solve any given kinetic data. | Analyze |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | X | X | | | X | | | | | |
| C.O. 2 | X | X | | | X | | | | | |
| C.O. 3 | X | X | | | X | | | | | |
| C.O. 4 | X | X | | | X | | | | | |
| C.O. 5 | X | X | | | X | | | | | |

| **UNIT I** | **8 hrs** |
|---|---|
| Complex Reactions- Parallel, Consecutive and Opposing reactions, Steady state Approximation, Kinetics of chain reactions - Photochemical reactions $H_2$-$Cl_2$ and $H_2$-$Br_2$ reaction, Organic decomposition reactions-Rice Herzfield mechanism (acetaldehyde and ethane), Branched Chain Reactions, Explosions-Semenov Hinshelwood mechanism ($H_2$-$O_2$ reaction), Fast Reactions-Relaxation methods- Perturbations, Flash photolysis and Pulse radiolysis | |
| **UNIT II** | **10 hrs** |
| Molecular reaction dynamics: Reactive encounters, Theories of reaction rates-Collision Theory. Collision and reaction cross section. Activated Complex Theory- PES, Erying equation, Comparative evaluation of collision and transition state theory, Thermodynamic treatment of reaction rates. Theory of unimolecular reactions- Lindemann Mechanism, Modifications to Lindemann mechanism- | |

| | |
|---|---|
| Hinshelwood, RRK and RRKM model. Termolecular reactions. Molecular beam methods, Stripping and rebound mechanism | |
| **UNIT III** | **10 hrs** |
| Reactions in Solutions – Cage effect, Transition state theory for reactions in solutions, Effect of ionic strength, dielectric constant and Internal pressure. Primary and secondary salt effect. Solute-solvent interactions. Ion dipole and dipole-dipole reactions. Diffusion controlled reactions. Isotope effects: Equilibrium isotope effects. Primary and Secondary kinetic isotope effects. | |
| **UNIT IV** | **10 hrs** |
| Surfaces and interfaces: Surface free energy and Surface tension, Contact angles and Wetting, Surface films. capillarity, vapour pressure of droplets- Kelvin equation. pressure difference across curved surface -Laplace equation, Surface wetting- hydrophilicity and hydrophobicity. Physical and chemical adsorption. Adsorption isotherms- Langmuir (kinetic and statistical derivation), Freundlich and BET (derivation) isotherms, Determination of surface area using Langmuir and BET isotherms, Isosteric heat of adsorption. Thermodynamics of adsorption- Gibbs adsorption isotherm. | |
| **UNIT V** | **10 hrs** |
| Catalysis and Inhibition, heterogeneous Catalysis – Transition state theory, General mechanism. General Mechanism of homogeneous catalysis- Arrhenius and vant Hoff intermediates, Acid base catalysis- specific and general acid catalysis, Enzyme catalysis- Michaelis-Menten Mechanism, Competitive and non competitive inhibition. Unimolecular and bimolecular Surface reactions- Kinetics of adsorption- Langmuir Hinshelwood mechanism and Rideal-Eley mechanism.<br>Autocatalysis- Oscillatory reactions- Lotka- Volterra, Oregonator, Brussellator. | |

**Recommended Text Books:**


1. W. J. Moore and R. G. Pearson, Kinetics and Mechanism, Wiley, New York.
2. K. J. Laidler, Chemical-Kinetics, McGraw Hill, New York.
3. M. R. Wright, An Introduction to Chemical Kinetics, Wiley, 2004.
4. Richard Masel, Chemical kinetics and Catalysis, Wiley Interscience.
5. P. W. Atkins, Physical Chemistry 8th Edn., Wiley, New York.
6. Christian Reichardt, Solvents and Solvent effects in Organic Chemistry, Wiley VCH 2003.
7. A. W. Adamson, The Physical Chemistry of Surfaces, 2nd Edn., Wiley. New York.
8. W. J. Moore and R. G. Pearson, Kinetics and Mechanism, Wiley, New York.
9. K. J. Laidler, Chemical-Kinetics, McGraw Hill, New York.
10. M. R. Wright, An Introduction to Chemical Kinetics, Wiley, 2004.
11. A. Somorjai, Chemistry of Surfaces, 3rd Edn. Wiley, New York.
12. Clark, “Theory of adsorption and catalysis”, Academic Press, 1970.
13. J.M. Thomas & W.J. Thomas, “Introduction to principles of heterogeneous catalysis”, Academic Press, New York, 1967.

14. R.H.P. Gasser, "An introduction to chemisorption and catalysis by metals", Oxford, 1985.
15. D.K Chakraborthy, "Adsorption and catalysis by solids", Wiley Eastern Ltd. 1990.

**CORE**

**25-802-0905**

**PHYSICAL CHEMISTRY-V**

**ADVANCED ELECTROCHEMISTRY**

**Credit 3** **48 hours**

| **Course Outcome**<br>After the completion of the course the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Describe the theories effecting ionic conductance and apply the concepts to calculate conductance behaviour of a given system. | Apply |
| C.O. 2:<br>Describe the electronic conductance behaviour in charged interfaces and analyse the catalytic behaviour of a system. | Analyze |
| C.O. 3:<br>Learn the working principle and advancement in futuristic electrochemical devices. | Understand |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | X | X | | | | | | X | | |
| C.O. 2 | X | X | | | | | | X | | |
| C.O. 3 | X | X | | | | X | | X | | |

| **UNIT I** | **8 hrs** |
|---|---|
| Review of basic concepts, Ionic Conductance, Ion Solvent Interactions, Ion-Water Interactions, Coordination Number, Solvation numbers, Hydration of simple cation, anion, and transition metal ion. Ion-Ion Interaction, Debye-Huckel Theory, Ionic Atmosphere, time of Relaxation, Mechanism of Electrolytic Conductance, Linearized P-B equation, Activity and Activity Coefficient of Electrolytes, Validity of Deby-Huckel theory, Debye-Hückel limiting law, Debye-Hückel-Bronsted Equation. | |
| **UNIT II** | **12 hrs** |
| Ion transport, Fick's law of diffusion, Diffusion Coefficient, Ionic drift in presence of electric field, drift velocity, transport number, Debye-Huckel-Onsager Equation, Relaxation effect, time of relaxation, Determination of degree of dissociation, Debye-Falkenhagen Effect, Wien Effect. Ionic liquids, Limiting case of zero solvent-pure electrolyte, features of ionic liquid, diffusion in IL, ionic conductance IL, liquid oxide electrolytes. | |
| **UNIT III** | **12 hrs** |

| | |
|---|---|
| Electrodics, Charged Interfaces, Electrode Potential, Factors Influencing electrode potential, Band Bending, electrolytic polarization, dissolution and decomposition potential, concentration polarization. Concentration cells.<br>Structure of electrified interfaces, liquid junction potential, the electrode double layer, electrode-electrolyte interface, different models of double layer, theory of multilayer capacity, electrocapillary, Lippmann equation, membrane potential. | |
| **UNIT IV** | **8 hrs** |
| Electrode kinetics, Ion adsorption, Electron Transfer Under an Interfacial Electric Field, Overvoltage, theories of overvoltage, Tafel equation, Butler-Volmer equation. Electrocatalyst- Homogeneous, heterogeneous, Randles-Sevcik Equations, Pourbiax diagrams, PCET. | |
| **UNIT V** | **8 hrs** |
| Semiconductor electrode interface. Band bending, photoelectrochemistry, fuel cells, battery-metal – ion, metal-air battery, Corrosion, Bioelectrochemistry – nervous system, enzyme as electrodes. | |

**Recommended Text Books:**


1. J. Bockris, A. K. N. Reddy, Modern Electrochemistry-1 Ionics, 2nd ed., Springer Science & Business Media, 2018.
2. J. Bockris, A. K. N. Reddy, M. E. Gamboa-Aldeco, Modern Electrochemistry-2A: Fundamentals of Electrodics, 2nd ed., Springer Science & Business Media, 2018.
3. J. Bockris, A. K. N. Reddy, Modern Electrochemistry 2B: Electrodics in Chemistry, Engineering, Biology and Environmental Science, 2nd ed., Springer Science & Business Media, 2018.
4. R. Crow, Principles and Applications of Electrochemistry, 4th ed., 1994.
5. S. Glasstone, An Introduction to Electrochemistry, Paperback ed., 2007.

**ELECTIVE**

**25-802-0906**

## TRANSITION METALS: CHEMISTRY AND APPLICATIONS IN ORGANIC SYNTHESIS

**Credit 3** **48 hours**

| **Course Outcome**<br>After the completion of the course the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Describe the structure, bonding and properties of transition metal complexes. | Understand |
| C.O. 2:<br>Predict and explain the principle and mechanism involved in transition metal-mediated transformations. | Apply |
| C.O. 3:<br>Construct organic molecules for various applications using palladium reagents. | Apply |
| C.O. 4:<br>Predict the structure and reactions of various metal-carbene Complexes. | Apply |
| C.O. 5:<br>Apply transition metal complexes for various asymmetric transformations | Apply |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | X | X | | | | | | | | X |
| C.O. 2 | X | X | | | | | | | | X |
| C.O. 3 | | X | X | | | | | X | | X |
| C.O. 4 | | X | | | | | | | | X |
| C.O. 5 | | X | X | | | | | | X | X |

| **UNIT I** | **10 hrs** |
|---|---|
| Basic concepts in organometallic chemistry: Introduction, 18 electron rule and its limitations, electron counting with examples, oxidation state, types of ligands, bonding, back-bonding. Formation of transition metal complexes, coordination number and geometry. σ-Bonded and π-bonded organometallic compounds. | |
| **UNIT II** | **12 hrs** |
| Mechanisms involved in transition metal chemistry: Oxidative addition, reductive elimination, transmetallation, migrative insertion, β-hydride elimination, nucleophilic and electrophilic attack on transition metal complexes. C-H activation. Catalytic mechanism of hydrogenation and hydroformylation. Single electron transfer and radical reactions. Homogeneous and heterogeneous catalysis. | |

| UNIT III | 12 hrs |
|---|---|
| Reactions mediated by palladium-based reagents: Characteristics of organopalladium compounds, catalysts and precursors, mechanistic features of cross- coupling reactions, reactivity of substrates, selectivity. Palladium catalysed coupling reactions: Corriu-Kumada reaction, Hiyama reaction, Suzuki coupling, Sonogashira coupling, Heck reaction, Buchwald–Hartwig coupling, Negishi coupling, Stille coupling. Miscellaneous reactions catalysed by palladium- Direct arylation, cyanation, carbonylation, Tsuji-Trost allylic substitution, α-allylic alkylation and α-fluorination. | |
| **UNIT IV** | **10 hrs** |
| Transition metal carbene complexes: Structure and properties. Fischer carbene complexes-preparation and reactions. Schrock carbene complexes-preparation and reactions. Non-stabilised carbene complexes. Metathesis process of carbene complexes. | |
| **UNIT V** | **10 hrs** |
| Transition metals in asymmetric catalysis: Asymmetric catalysis in metathesis, epoxidation, allylation, hydroformylation, isomerisation of allylic amines, hydrocyanation, hydrogenation, Heck reaction and Pauson–Khand reaction. | |

**Recommended Text Books:**


1. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals, 6th Edn., John Wiley & Sons, 2014.
2. L. S. Hegedus, B. C. G. Soderberg, Transition Metal in the Synthesis of Complex Organic Molecules, 3rd Edn., University of Science Books, 2010.
3. D. Astruc, Organometallic Chemistry and Catalysis, Springer, 2007.
4. J. Tsuji, Transition Metal Reagents and Catalysts: Innovations in Organic Synthesis, John Wiley & Sons, 2002.
5. I. Omae, Applications of Organometallic Compounds, John Wiley & Sons, 1998
6. R. Bates, Organic Synthesis Using Transition Metals, 2nd Edn., John Wiley & Sons, 2012.
7. B. Gabriele, Organic Synthesis via Transition Metal-Catalysis, MDPI, 2022.
8. K. Grela, Olefin Metathesis, John Wiley & Sons, 2014.

**ELECTIVE**

**25-802-0907**

**SPECTROSCOPIC TECHNIQUES**

**Credit 3** **48 hours**

| **Course Outcome**<br>After the completion of the course the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Explain the fundamentals of spectroscopy. | Understand |
| C.O. 2:<br>Correlate the structure of molecule with UV-Visible and IR spectral data. | Apply |
| C.O. 3:<br>Interpret first order NMR spectra. | Analyze |
| C.O. 4:<br>Determine the primary structure of peptides based on mass spectra. | Analyze |
| C.O. 5:<br>Examine secondary structure of peptides based on IR, NMR and mass spectral data. | Evaluate |
| C.O. 6:<br>Explain the applications of X ray and microscopic techniques. | Understand |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | X | X | | | | | | | | |
| C.O. 2 | X | X | X | | | X | | | X | X |
| C.O. 3 | X | X | X | | | X | | | X | X |
| C.O. 4 | X | X | | | | X | | | X | X |
| C.O. 5 | X | X | | | | X | | | X | X |
| C.O. 6 | X | X | | | | X | | | X | X |

**UNIT I** **8 hrs**

Different regions of electromagnetic spectrum and energy associated with a particular frequency, Types of spectroscopic techniques, Energy levels in molecules. Population of energy levels, basics of light absorption, factors affecting sensitivity, intensity and width of spectral lines, absorption characteristics, structural information based on absorption characteristics

**UNIT II** **10 hrs**

UV-visible spectroscopy – Principle, allowed and forbidden transitions, chromophores, auxochromes, effect of structure on absorption characteristics

Basics of ORD and CD and emission spectroscopy.

IR spectroscopy –Principle, intra and intermolecular hydrogen bonding, effect of concentration and temperature, Fourier transform IR, group frequencies, fundamental frequencies, overtones, Fermi Resonance.

| | |
|---|---|
| **UNIT III** | **10 hrs** |
| Experimental aspects of FT NMR, factors influencing sensitivity and resolution, Proton NMR, Chemical shift, Applications of chemical shift, spin-spin coupling, Analysis of spin systems, factors affecting coupling constants, NMR of Carbon-13, DEPT analysis and brief introduction to correlation spectroscopy (COSY, HMBC and HSQC). Brief introduction to NMR of other biologically relevant nuclei such as $^{15}N$, $^{2}D$ and $^{31}P$. | |
| **UNIT IV** | **12 hrs** |
| Mass spectrometry - high resolution mass spectrometry, soft ionization techniques, MS/MS data, application of GC-MS and LC-MS data, introduction to fragmentation modes and determination of primary structure of peptides on the basis of mass spectral data.<br>Problems based on combined application of various spectroscopic techniques to examine secondary structure of peptides. | |
| **UNIT V** | **14 hrs** |
| Introduction to microscopic and X-ray techniques. Confocal micros copy,fluorescence and radioisotope labeling as diagnostic tools. Basic introduction to Electron microscopy: types, sample preparation and analysis. Powder XRD and single crystal XRD | |

**Recommended Text Books:**


1. D. L. Pavia, G. M. Lampman, G. S. Kriz, Introduction to Spectroscopy, A Guide for Students of Organic Chemistry, 3rd ed., Thomson. 2004.
2. Atta-Ur-Rahman, M. I. Choudhary, Solving Problems with NMR Specroscopy, Academic Press, New York, 1996.
3. L. D. Field, S. Sternhell, J. R. Kalman, Organic Structures from Spectra, 4th ed., Wiley, 2008.
4. R. S. Drago, Physical Methods for Chemist, Saunders, 1992.
5. C. N. Banwell, E. M. McCash, Fundamentals of Molecular Spectroscopy, 4$^{th}$ ed., McGrawHill, 1994.
6. D. F. Taber, Organic Spectroscopic Structure Determination, A Problem Based Learning Approach, Oxford University Press, 2009.
7. H. Gunther, NMR Spectroscopy, 2nd ed., John Wiley and Sons, 1995.
8. R. M. Silverstein, G. C. Bassler, T. C. Morril, Spectroscopic identification of organic compounds, John Wiley, 1991.
9. D. H. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, Tata McGraw Hill. 1988.
10. W. Kemp, Organic Spectroscopy, 2nd ed., ELBS Macmillan, 1987.
11. F. Bernath, Spectra of Atoms and Molecules, 2nd ed., Oxford University Press, 2005.
12. E. B. Wilson, Jr., J. C. Decius, P. C. Cross, Molecular Vibrations: The Theory of Infrared and Raman Spectra, Dover Publications, 1980.
13. A. Weil, J. R. Bolton, Electron Paramagnetic Resonance: Elementary Theory and Practical Applications, 2nd ed., Wiley Inter Science, John Wiley & Sons, Inc., 2007.
14. C. P. Slichter, Principles of Magnetic Resonance, 3rd ed., Springer-Verlag, 1990.

15. H. Gunther, NMR Spectroscopy: Basic principles, Concepts, and Applications in Chemistry, 2nd ed., Wiley 1997.
16. Spectral data bases (RIO DB of AIST, for example).

**ELECTIVE**

**25-802-0908**

## NEW METHODS AND STRATEGIES IN ORGANIC SYNTHESIS AND DYNAMIC STEREOCHEMISTRY

**Credit 3** **64 hours**

| **Course Outcome**<br>After the completion of the course the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>To learn various organic reactions and reagents used in them as tools applied in the art of organic synthesis. | Apply |
| C.O. 2:<br>Analyze the reagents and conditions for the synthesis of specific target molecules. | Analyze |
| C.O. 3:<br>To learn and apply various concepts such as stereochemistry and fundamental principles of stereoselectivity in organic chemistry. | Apply |
| C.O. 4:<br>Analyze the effect of molecular conformation in the outcome of a reaction | Analyze |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | X | X | | | | | | X | | |
| C.O. 2 | X | | X | | | | | X | | |
| C.O. 3 | X | | X | | | | | X | | |
| C.O. 4 | X | | X | | | | | X | | |

| **UNIT I** | **14 hrs** |
|---|---|
| Chemo-, regio- and stereoselective functional groups interconversions; oxidation and reduction processes and their synthetic utility; metal-free oxidation (boron-, peroxide-, sulfur-, iodine-based) and metal-based (Ru-, Cr-, Mn-, Os-, Pd-) reagents; transfer hydrogenation; enantioselective oxidation and reduction processes. | |
| **UNIT II** | **12 hrs** |
| Strategic carbon-carbon and carbon-heteroatom bonds formation; carbon-carbon multiple bonds construction processes and corresponding named reactions; functional group transposition; conjunctive reagents; construction of cyclic frameworks; fused and spirocyclic systems. | |
| **UNIT III** | **12 hrs** |

| | |
|---|---|
| Domino/Cascade reactions: principles and advantages; rationalization with examples of radical, anionic, cationic, and pericyclic domino/cascade processes. | |
| **UNIT IV** | **13 hrs** |
| Stereoselectivity in cyclic molecules: Introduction; Stereochemical control in six membered rings; Reactions on small rings; Regiochemical control in cyclohexene epoxides; Stereoselectivity in bicyclic compounds; Fused bicyclic compounds; Spirocyclic compounds; Reactions with cyclic intermediates or cyclic transition states. | |
| **UNIT V** | **13 hrs** |
| Diastereoselectivity: Prochirality; Diastereoselective additions to carbonyl groups without rings; Stereoselective reactions of acyclic alkenes; Stereoselective Aldol reactions; Single enantiomers from diastereoselective reactions. | |

**Recommended Text Books:**


1. W. Carruthers, Modern Methods of Organic Synthesis, Cambridge University Press, 1996
2. L. Kuerti and B. Czako, Strategic Applications of named Reactions in Organic Synthesis, Elsevier Academic Press, 2005
3. F. A. Cary and R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5$^{th}$ Edition, Springer, 2009
4. J. Clayden, N. Greeves, and S. Warren, Organic Chemistry, Oxford University Press, 2nd Edition, 2012
5. L. F. Tietze, G. Brasche, and K. Gericke, Domino Reactions in Organic Synthesis, Wiley, 2006
6. Roderick Bates, Organic Synthesis using Transition Metals, 2nd Edition, Wiley, 2012.
7. George S. Zweifel and Michael H. Nantz, Modern Organic Synthesis: An Introduction, W. H. Freeman Publisher, 2007.
8. P.S.Kalsi: Stereochemistry, Conformation and Mechanism, 3rd edn., New Age Publications
9. Peter Sykes, A Guide Book to Mechanism in Organic Chemistry, Pearson Education, New Delhi.
10. Bruckner, R. Advanced Organic Chemistry: Reaction Mechanisms, 1st edn., Academic Press, 2001.

**ELECTIVE**

**25-802-0909**

## ADVANCED TECHNIQUES IN ORGANIC SYNTHESIS: THEORY AND PRACTICE

**Credit 3** **48 hours**

| **Course Outcome**<br>After the completion of the course the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Independently organizing and carrying out the most sophisticated and widely used organic transformations in a safe lab setting. | Apply |
| C.O. 2:<br>Characterize simple to complex molecules using spectroscopic methods. | Apply |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | X | X | | | | | | X | | |
| C.O. 2 | X | | X | | | | | X | | |
| C.O. 3 | X | | X | | | | | X | | |
| C.O. 4 | X | | X | | | | | X | | |

| **UNIT I** | **9 hrs** |
|---|---|
| General methods in organic synthesis: Condensation, substitution, cycloaddition, oxidation, and reduction. Methods for heterocycles and their important reactions. | |
| **UNIT II** | **9 hrs** |
| Advanced organic reactions: Multicomponent reactions, organo-catalysed reactions, click reactions. Cross-coupling reactions, metathesis reactions, and application in the synthesis of functional molecules and drugs. | |
| **UNIT III** | **24 hrs** |
| Practice : General methods of separation and purification of organic compounds such as 1) solvent extraction 2) thin layer chromatography and paper chromatography 3) column chromatography.<br>Drawing the structures of organic molecules and reaction schemes by Proprietary and open source computer software. Use Chemical Abstracts, Scopus, Scifinder etc., to search, analyse and collect chemical information. | |
| **UNIT IV** | **24 hrs** |
| Practice: Hands-on training in conducting reactions under an inert atmosphere and usage of Schlenk line techniques. Drying of solvents like THF, methanol and toluene. Handling of the Glove box. Green strategies such as microwave, sonochemistry, electrochemical and photochemical reactions. Training in cross-coupling reactions and olefin metathesis. | |
| **UNIT V** | **13 hrs** |
| Practice: Characterization of synthesized molecules using GC, LCMS, IR, NMR and | |

| |
|---|
| HPLC techniques. Determination of specific rotation of enantiopure molecules. |

**Recommended Text Books:**


1. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2nd ed., Oxford University Press, 2012.
2. A. I. Vogel, A. R. Tatchell, B. S. Furnis, A. J. Hannaford, P. W. G. Smith, Vogel's Textbook of Practical Organic Chemistry, 5th ed., John Wiley, 1989.
3. P. S. Kalsi, Stereochemistry, Conformation and Mechanism, 10th ed., New Age Publications, 2019.
4. T. Tsuji, Transition Metal Reagents and Catalysts: Innovations in Organic Synthesis, John Wiley & Sons, 2000.
5. D. L. Pavia, G. M. Lampman, G. S. Kriz, Introduction to Spectroscopy, A Guide for Students of Organic Chemistry, 3rd ed., Thomson. 2004.
6. J. R. Mohrig, D. G. Alberg, G. E. Hofmeister, P. F. Schatz, C. N. Hammond, Laboratory Techniques in Organic Chemistry, 4th ed., W. H. Freeman and Company, 2014.

**CORE/LAB**

**25-802-1001**

**PROJECT DISSERTATION**

**Credit 16**

| **Course Outcome**<br>After the completion of the course the student will be able to | **Cognitive Level** |
|---|---|
| C.O. 1:<br>Identify and hypothesise an advanced level research problem. | Create |
| C.O. 2:<br>Design experiments and validate the hypothesis of an advanced level research problem. | Create |

| Course Outcome | Program Outcomes | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | P.O. 1 | P.O. 2 | P.O. 3 | P.O. 4 | P.O. 5 | P.O. 6 | P.O. 7 | P.O. 8 | P.O. 9 | P.O. 10 |
| C.O. 1 | X | X | X | X | X | X | | X | X | |
| C.O. 2 | X | X | X | X | X | X | X | X | X | |

| **UNIT I** |
|---|
| The students shall carry out research project in reputed research laboratory for the entire semester.<br>The students shall submit a project report on the research work carried out.<br>The students will have to present the results of the research project in a seminar and appear for a comprehensive viva-voce. |

# Guidelines for setting up Question Papers in Theory Courses

1. The entire syllabus must be covered in the question paper.
2. Each question must be mapped to a specific C.O.
3. All the C.O.s must be reflected in the question paper.
4. The question paper may consist of questions at different cognitive levels such that, 20% of "remember" level, 40% of "understand" level and 40% of "apply and higher" level.

***END***