

**Course Structure and Detailed Syllabi for Integrated M.  
Sc. (Chemistry)**

***Starting Year: 2018, Autumn Semester***

***(Revised)***

(Approved in 38<sup>th</sup> Academic Council 02.09.2020)

**Department of Chemical Sciences  
(DST-FIST and UGC-SAP DRS-II SUPPORTED)**



**TEZPUR UNIVERSITY**

## Preamble

The Department of Chemical Sciences, Tezpur University started the Integrated M.Sc. in chemistry programme in the year 2009. The programme would allow students to grow fundamental knowledge of chemical sciences and specialize them for careers in chemistry with high scientific depth and temperament. Upon successful completion of the entire programme, student shall be awarded with degree as Integrated M.Sc. in Chemistry. However, student can choose for lateral exit with the Bachelor's Degree with Honours in Chemistry. The department has adopted choice based credit system in the integrated M.Sc. programme in autumn semester, 2018 which is a Learning Outcome-based curriculum framework (LOCF). The Choice Based Credit System (CBCS) adopts an interdisciplinary approach in learning and enables students to learn at their own pace to complete a programme of study, choose electives from a wide range of courses across departments/centres/institutions, study add on courses and acquire more than required number of credits. In CBCS system the courses are divided into three main categories viz. Core Courses, Elective Courses and Ability Enhancement Courses. Each course is assigned with a fixed number of credits based on the contents to be learned. The number of credits earned by the student reflects the knowledge or skill acquired by them. The Learning outcome based curricular framework (LOCF) gives a broad structural framework that can include the recent curricular needs as well as provide sufficient flexibility to inculcate changes in content that is important for advancement of chemistry education. For assessment of students continuous comprehensive evaluation shall be followed to reduce the weightage on the semester-end examination so that students enjoy a de-stressed learning environment. The grade points earned for each course reflects the student's proficiency in that course. This curriculum for the Integrated M.Sc. in Chemistry will make students skilled and knowledgeable enough in making right decision regarding the goals they wish to pursue their educational career and in life.

## 1. Introduction

The main objectives of the programme are to impart the key knowledge of chemical sciences and laboratory resources to prepare students for choosing careers in chemistry and related areas with strong scientific depth and temperament. The eligibility criteria for enrolment in the Integrated M.Sc. in Chemistry programme is 10+2 Standard passes with minimum 60% aggregate marks in Physics, Chemistry and Mathematics. The curriculum for the Integrated M.Sc. in Chemistry programme is based on Choice Based Credit System (CBCS) and learning outcome based curriculum framework (LOCF). The CBCS provides an opportunity to a student to choose any elective courses from the syllabus comprising of different elective courses. The syllabus offers a flexibility of programme structure while ensuring that students get a strong foundation and gains in-depth knowledge in chemistry. The LOCF strategy gives students a clear view to focus their learning effort and enable them to make a choice of the elective courses they prefer to study. The Integrated M.Sc. in chemistry programme comprises ten semesters course spread over five academic years. The total credit requirement to acquire the Integrated M.Sc. degree is 210 credits. The details of the courses and credit system are explained in the annexure. The syllabus fulfils the current needs to acquire a good chemistry degree and to secure a good choice in higher education in chemistry and the area of their interest as well as employment.

## 2. Qualification descriptors for the graduates

### Knowledge & Understanding:

- Gains comprehensive knowledge and understanding on fundamental principles and concepts chemical sciences that covers the sub-disciplines (Physical, Inorganic, Organic) as well as advanced and emerging topics.
- Able to apply underlying ideas and principles outside the context in which they were first studied and in interdisciplinary problems and circumstances.

### Skills and Techniques:

- Exhibition of skills required for conducting the documented laboratory procedure as well as developed skills for the planning new experiments, data analysis and

presentation of quantitative and/or qualitative data or information, ideas, concepts etc.

- Acquisition of skills in the handling of chemicals and operation of standard instruments.
- Development of information searching and management skills

#### **Competence:**

- Acquisition of competence in the use of routine materials, techniques and practices of chemistry
- Development of competence in intellectual, practical, IT skills and Communication skills necessary for employment as professional chemist.
- Development of responsibilities of the uses of chemistry in everyday life.

### **3. Graduate Attributes**

- Students will have in-depth knowledge and understandings of the fundamentals knowledge of current chemical and basic sciences.
- Students will develop analytical/ critical thinking, learn application of modern tools and develop mutual and multidisciplinary competence
- Students will be able to clearly communicate the results of scientific work in oral, written and ICT formats to both science community and society.
- . Students will be able to demonstrate knowledge and skills in analysing and identifying entrepreneur opportunities.

### **4. Program Outcomes**

**P01.** Students will have a firm foundation in the fundamentals and application of current chemical and basic science including those in Physical, Organic, Inorganic, Analytical and Biochemistry.

**P02.** Students will be able to seek new knowledge, skills and manage relevant information from various sources.

**P03.** Students will be trained to work effectively and safely in the laboratory environment independently as well as in teams.

**P04.** Students will be able to design and carry out scientific experiments as well as accurately draw logical inferences from the results of such experiments.

**P05.** Students will be able to explain why chemistry is an integral activity for addressing social, economic, and environmental problems

## 5. Programme structure

**Total Credit for the programme: (UG + PG): 130 + 80 =210**

**Structure of the curriculum:**

Course category	No of courses	Credits per course	Total Credits
I. Core courses	40	3/4/6/8	135
II. Elective courses			
Generic elective (GE) courses	10	3	30
Discipline Specific Elective (DSE) Courses	9	3	27
III. Ability Enhancement Compulsory (AEC) Courses	3	3/4	10
IV. Skill Enhancement Course (SEC)	3	2/3	8
Total Credits			210

## 6. SEMESTER-WISE SCHEDULE

### SEMESTER I

Course type	Course title	Lecture (L)	Tutorial (T)	Practical (P)	Contact Hours (CH)	Credits
Core	CI 101: Chemistry-I	3	0	0	3	3
	CI 105: Chemistry Laboratory- I	0	0	3	6	3
Generic	PI 101: Physics-I	3	0	0	3	3
Elective	BI 101: Biology-I	3	0	0	3	3
	MI 101: Mathematics-I	3	0	0	3	3
	PI 197: Physics laboratory	0	0	3	6	3
	CI 107: Chemistry Laboratory (for Math)	0	0	3	6	3
Ability Enhancement Compulsory	EG:101: Communicative English (Language Proficiency)	3	0	0	3	3

### SEMESTER II

Course type	Course title	Lecture (L)	Tutorial (T)	Practical (P)	Contact Hours (CH)	Credits
Core	CI 102: Chemistry-II	3	0	0	3	3
	CI 106: Chemistry Laboratory- II	0	0	3	6	3
Generic	PI 102: Physics-II	3	0	0	3	3
Elective	BI 102: Biology-II	3	0	0	3	3
	MI 102: Mathematics-II	2	1	0	3	3

	BI 107: Biology Laboratory	0	0	3	6	3
	CI 107: Chemistry Laboratory (For Bio and Phys)	0	0	3	6	3
Ability Enhancement Compulsory	ES 103: Environmental Studies	4	0	0	4	4

### SEMESTER III

Course type	Course title	Lecture (L)	Tutorial (T)	Practical (P)	Contact Hours	Credits
Core	CI 203: Physical Chemistry-I	3	0	0	3	3
	CI 205: Organic Chemistry-I	3	0	0	3	3
	CI 207: Inorganic Chemistry-I	3	0	0	3	3
	CI209: Chemistry Laboratory -III	0	0	3	6	3
Generic Elective	PI 201: Physics-III	3	0	0	3	3
	MI 219: Mathematics-III	3	0	0	3	3
	CI 201: Chemistry-III (For non-major)	3	0	0	3	3
Ability Enhancement Compulsory	CS 535: Introduction to Scientific Computing	3	0	0	3	3
Skill Enhancement	NS 201: NSS	0	0	1	2	2

### SEMESTER IV

Course type	Course title	Lecture (L)	Tutorial (T)	Practical (P)	Contact Hours (CH)	Credits
Core	CI 204: Physical Chemistry-II	3	0	0	3	3
	CI 206: Organic Chemistry-II	3	0	0	3	3
	CI 208: Inorganic Chemistry-II	3	0	0	3	3
	CI212: Chemistry Laboratory -IV	0	0	4	8	4
Discipline Specific Elective	CI 216: Basic Analytical Chemistry	3	0	0	3	3
Skill Enhancement Course	CI 214: IT Skills for Chemists	3	0	0	3	3
	DM101: Disaster Management	2	1	0	3	3

### SEMESTER V

Course type	Course title	Lecture (L)	Tutorial (T)	Practical (P)	Contact Hours (CH)	Credits
Core	CI 301: Physical Chemistry-III	3	0	0	3	3
	CI 303: Organic Chemistry-III	3	0	0	3	3
	CI 305: Inorganic Chemistry-III	3	0	0	3	3
	CI 307: Quantum Chemistry	3	0	0	3	3
	CI 309: Chemistry Laboratory -V	0	0	4	8	4
Discipline Specific Elective	CI 311: Green Methods in Chemistry	3	0	0	3	3
	CI313: Industrial Chemistry	3	0	0	3	3



## SEMESTER VI

Course type	Course title	Lecture (L)	Tutorial (T)	Practical (P)	Contact Hours (CH)	Credits
Core	CI 302: Physical Chemistry-IV	3	0	0	3	3
	CI 304: Organic Chemistry-IV	3	0	0	3	3
	CI 306: Inorganic Chemistry-IV	3	0	0	3	3
	CI 308: Principles of Spectroscopy	3	0	0	3	3
	CI 310: Chemistry Laboratory -VI	0	0	4	8	4
	CI 314: Seminar	1	0	0	0	0
Discipline Specific Elective	CI 312: Introduction to Polymer Chemistry	3	0	0	3	3

## SEMESTER VII

Course type	Course title	Lecture (L)	Tutorial (T)	Practical (P)	Contact Hour (CH)	Credits
Core	CI 401: Principles of Inorganic Chemistry	3	0	0	3	3
	CI403:Chemical and Statistical Thermodynamics	3	0	0	3	3
	CI 407: Principles of Organic Chemistry	3	0	0	3	3
	CI 409: Quantum Chemistry and Chemical Bonding-I	3	0	0	3	3
	CI 411: Principles and Applications of Spectroscopy	3	0	0	3	3
	CI 405: Laboratory Course in Organic Chemistry	0	0	6	12	6

### SEMESTER VIII

Course type	Course title	Lecture (L)	Tutorial (T)	Practical (P)	Contact Hour (CH)	Credits
Core	CI 408: Chemistry of Transition Elements	3	0	0	3	3
	CI 410: Chemical Dynamics and Electrochemistry	3	0	0	3	3
	CI 414: Quantum Chemistry and Chemical Bonding-II	3	0	0	3	3
	CI 412: Laboratory Course in Inorganic Chemistry	0	0	6	12	6
	CI 418: Organic Reactions and Mechanism	3	0	0	3	3
Discipline Specific Elective	CI 416: History of Chemistry	3	0	0	3	3

### SEMESTER IX

Course type	Course title	Lecture (L)	Tutorial (T)	Practical (P)	Contact Hour (CH)	Credits
Core	CI 501: Bio-Organic Chemistry	3	0	0	3	3
	CI 519: Physical Chemistry of Surface and Condensed Systems	3	0	0	3	3
	CI 521: Analytical Methods in Chemistry	3	0	0	3	3
	CI 525: Organometallic Chemistry	3	0	0	3	3
	CI505: Laboratory Course in Physical	0	0	6	12	6

	Chemistry					
Discipline Specific Elective	CI 523: Chemical Technology and Society	3	0	0	0	3

### SEMESTER X

Course type	Course title	Lecture (L)	Tutorial (T)	Practical (P)	Contact Hour (CH)	Credits
<b>Core</b>	CI 530: Project Work*	0	0	8	16	8
<b>Elective I</b> (Discipline Specific Elective)	CI 506: Catalysis / CH508: Methods in Organic Synthesis / CI528: Special Topics in Inorganic Chemistry / CI532: Chemistry of Paints and Surface Coating	3	0	0	3	3
<b>Elective II</b> (Discipline Specific Elective)	CI 514: Biomolecular Chemistry/ CI516: Computational Chemistry and Numerical Analysis / CI518: Organic Solid States Chemistry / CI520: Environmental and Green Chemistry / CI534: Industrial Polymer	3	0	0	3	3
<b>Elective III</b> (Discipline Specific Elective)	CI522: Polymer Chemistry / CI524:Heterocyclic Compounds and Medicinal Applications / CI526:Bio-inorganic Chemistry / CI536: Chemistry of Materials	3	0	0	3	3

**\* To be carried out in the Department under the guidance of an assigned faculty member of the Department.**

**Elective I: Any one from the following group**

CI 506 Catalysis

CI 508 Methods in Organic Synthesis

CI 528 Special Topics in Inorganic Chemistry

CI 532: Chemistry of Paints and Surface Coating

**Elective II: Any ONE from the following group**

CI 514 Biomolecular Chemistry

CI 516 Computational Chemistry and Numerical Analysis

CI 518 Organic Solid States Chemistry

CI 520 Environmental and Green Chemistry

CI 534 Industrial Polymer

**Elective III: Any ONE from the following group**

CI 522 Polymer Chemistry

CI 524 Heterocyclic Compounds and Medicinal Applications

CI 526 Bio-inorganic Chemistry

CI 536 Chemistry of Materials

**7. Mapping of course with program outcomes (POs)**

Course title	P01	P02	P03	P04	P05
CI 101: Chemistry-I	✓	✓			✓
CI 105: Chemistry Laboratory- I	✓	✓	✓	✓	✓
PI 101: Physics-I	✓	✓			✓
BI 101: Biology-I	✓	✓			✓
MI 101: Mathematics-I	✓	✓			✓
PI 197: Physics laboratory	✓	✓	✓	✓	✓
CI 107: Chemistry Laboratory (for Math)	✓	✓	✓	✓	✓

EG:101: Communicative English (Language Proficiency)		✓			✓
CI 102: Chemistry-II	✓	✓			✓
CI 106: Chemistry Laboratory- II	✓	✓	✓	✓	✓
PI 102: Physics-II	✓	✓			✓
BI 102: Biology-II	✓	✓			✓
MI 102: Mathematics-II	✓	✓			✓
BI 107: Biology Laboratory	✓	✓	✓	✓	✓
CI 107: Chemistry Laboratory (For Bio and Phys)	✓	✓	✓	✓	✓
ES 103: Environmental Studies	✓	✓			✓
CI 203: Physical Chemistry-I	✓	✓			✓
CI 205: Organic Chemistry-I	✓	✓			✓
CI 207: Inorganic Chemistry-I	✓	✓			✓
CI209: Chemistry Laboratory -III	✓	✓	✓	✓	✓
PI 201: Physics-III	✓	✓			✓
MI 219: Mathematics-III	✓	✓			✓
CI 201: Chemistry-III (For non-major)	✓	✓			✓
CS 535: Introduction to Scientific Computing	✓	✓	✓		✓
NS 201: NSS			✓		
CI 204: Physical Chemistry-II	✓	✓			✓
CI 206: Organic Chemistry-II	✓	✓			✓
CI 208: Inorganic Chemistry-II	✓	✓			✓
CI212: Chemistry Laboratory -IV	✓	✓	✓	✓	✓
CI 214: IT Skills for Chemists	✓	✓		✓	✓
CI 216: Basic Analytical Chemistry	✓	✓		✓	✓
DM101: Disaster Management		✓	✓		
CI 301: Physical Chemistry-III	✓	✓			✓
CI 303: Organic Chemistry-III	✓	✓			✓
CI 305: Inorganic Chemistry-III	✓	✓			✓

CI 307: Quantum Chemistry	✓	✓			✓
CI 309: Chemistry Laboratory -V	✓	✓	✓	✓	✓
CI 311: Green Methods in Chemistry	✓	✓			✓
CI313: Industrial Chemistry	✓	✓		✓	✓
CI 302: Physical Chemistry-IV	✓	✓			✓
CI 304: Organic Chemistry-IV	✓	✓			✓
CI 306: Inorganic Chemistry-IV	✓	✓			✓
CI 308: Principles of Spectroscopy	✓	✓			✓
CI 310: Chemistry Laboratory -VI	✓	✓	✓	✓	✓
CI 312: Introduction to Polymer Chemistry	✓	✓			✓
CI 314: Seminar		✓		✓	✓
CI 401: Principles of Inorganic Chemistry	✓	✓	✓		✓
CI 403: Chemical and Statistical Thermodynamics	✓	✓	✓		✓
CI 407: Principles of Organic Chemistry	✓	✓	✓		✓
CI 409: Quantum Chemistry and Chemical Bonding-I	✓	✓	✓		✓
CI 411: Principles and Applications of Spectroscopy	✓	✓	✓		✓
CI 405: Laboratory Course in Organic Chemistry	✓	✓	✓	✓	✓
CI 408: Chemistry of Transition Elements	✓	✓	✓		✓
CI 410: Chemical Dynamics and Electrochemistry	✓	✓	✓		✓
CI 414: Quantum Chemistry and Chemical Bonding-II	✓	✓	✓		✓
CI 412: Laboratory Course in Inorganic Chemistry	✓	✓	✓	✓	✓
CI 418: Organic Reactions and Mechanism	✓	✓	✓		✓
CI 416: History of Chemistry	✓	✓	✓		✓
CI 501: Bio-Organic Chemistry	✓	✓	✓		✓
CI 519: Physical Chemistry of Surface and Condensed Systems	✓	✓	✓		✓
CI 521: Analytical Methods in Chemistry	✓	✓	✓	✓	✓
CI 525: Organometallic Chemistry	✓	✓	✓		✓
CI 505: Laboratory Course in Physical Chemistry	✓	✓	✓	✓	✓

CI 530: Project Work		✓	✓	✓	✓
CI 523: Chemical Technology and Society	✓	✓	✓		✓
CI 506: Catalysis Synthesis	✓	✓	✓		✓
CI508: Methods in Organic	✓	✓	✓		✓
CI528: Special Topics in Inorganic Chemistry	✓	✓	✓		✓
CI532: Chemistry of Paints and Surface Coating	✓	✓	✓		✓
CI514: Biomolecular Chemistry	✓	✓	✓		✓
CI516: Computational Chemistry and Numerical Analysis	✓	✓	✓	✓	✓
CI518: Organic Solid States Chemistry	✓	✓	✓		✓
CI520:Environmental and Green Chemistry	✓	✓	✓	✓	✓
CI534: Industrial Polymer	✓	✓	✓	✓	✓
CI 522: Polymer Chemistry	✓	✓	✓		✓
CI524:Heterocyclic Compounds and Medicinal Applications	✓	✓	✓		✓
CI526:Bio-inorganic Chemistry	✓	✓	✓		✓
CI536: Chemistry of Materials	✓	✓	✓		✓

## 8. Evaluation plan

Students shall be evaluated separately in each course through a Continuous Comprehensive Evaluation (CCE) system as mentioned in the academic guideline of Tezpur University.

## 9. DETAILED SYLLABUS

### SEMESTER I

CI 101

Chemistry-I

L 3 T 0 P 0 CR 3

#### Course outcomes:

On completion of this course, the students will be able to understand:

CO1 : Atomic theory and its evolution

CO2: Periodic properties of elements

CO3: Basic of organic molecules, structure, bonding and organic reaction mechanisms

CO4: Synthesis of hydrocarbons

CO5: Basics of Chemical thermodynamics and thermodynamic laws, Fundamentals of solution and colligative properties

#### Course Content:

##### Unit 1

[3 Lectures]

Structure of atom, Hund's rule, Aufbau principle, Pauli's exclusion principle.

##### Unit 2

[4 Lectures]

Periodic Properties: Periodicity of the elements, shielding, effective nuclear charge, Slater's rule, the size of the atoms, atomic, covalent and van der Waals radii, ionization energy, electron affinity, electronegativity.

##### Unit 3

[5 Lectures]

Basics of organic chemistry-1 : Bonding, structure and physical properties of organic compounds: Valence bond theory: Concept of hybridization of organic compounds and shapes of molecules; MO theory: Acyclic  $\pi$  orbital system and cyclic  $\pi$  orbital systems; Physical properties: Melting point, boiling point, solubility, dipole moment.



**Unit 4****[3 Lectures]**

Basics of organic chemistry-2: Electronic and steric effects: Inductive effect, resonance, hyperconjugation, steric effect, steric inhibition of resonance.

**Unit 5****[3 Lectures]**

Basics of organic chemistry-3: Thermodynamics and kinetics of organic reactions: Free energy and equilibrium, enthalpy and entropy factor, intermolecular & intramolecular reactions, rate constant and free energy of activation, free energy profiles for one step and multi-step reactions, catalyzed reactions, kinetic control and thermodynamic control, kinetic isotopic effect, principle of microscopic reversibility, Hammond postulate.

**Unit 6****[3 Lectures]**

Alkanes: Synthesis by: Decarboxylation, reduction of alkyl halides and tosylates, Kolbe electrolysis, Wurtz reaction, Corey-House synthesis; Reactions of alkanes: Halogenation, nitration, sulphonation, oxidation and cracking of alkanes.

**Unit 7****[3 Lectures]**

Alkenes and alkynes: Synthesis, Dehydration of alcohols, pyrolysis of esters, Cope reaction, Elimination of alkyl halides, geminal- and vicinal dihalides, Hofmann elimination; Reactions: Addition of  $X_2$  ( $X = \text{halogen}$ ),  $H-X$ ,  $HO-X$ , interhalogens, water, Oxymercuration-demercuration, hydroboration-oxidation, ozonolysis, catalytic reduction, dihydroxylation, epoxidation, polymerization, alkylation of alkynes, oxidation of alkynes to 1,2-diketones, allylic and benzylic halogenation of alkenes mediated by radicals.

**Unit 8****[4 Lectures]**

First Law of Thermodynamics: Thermodynamics terms, state and path functions, concept of heat and work, internal energy, enthalpy, first law of thermodynamics;  $w$ ,  $q$ ,  $\Delta U$  and  $\Delta H$  for expansion and compression of ideal gases, heat capacities, physical

change, standard enthalpies of physical and chemical changes, Hess's law, Kirchhoff's law.

### **Unit 9**

**[4 Lectures]**

Second Law of Thermodynamics: Spontaneous processes, Carnot cycle, entropy, criteria of spontaneity, statements of the second law of thermodynamics, entropy changes, Clausius inequality, Gibbs energy, Helmholtz energy, Third law of thermodynamics.

### **Unit 10**

**[2 Lectures]**

Solutions: Ideal and non-ideal solutions

### **Unit 11**

**[2 Lectures]**

Colligative properties

### **Text Book(s)**

1. Lee, J. D. *Concise Inorganic Chemistry*, 5<sup>th</sup> Edn., (Chapman & Hall, 2002).
2. Atkins, P. and Paula, J. de. *Atkins' Physical Chemistry*, 10<sup>th</sup> Edn., (Oxford University Press, 2014).
3. Clayden, J., Greeves, N., Warren, S., Wothers, P. *Organic Chemistry*, 2<sup>nd</sup> Edn., (Oxford University Press, 2012).
4. Finar, I. L., *Organic Chemistry* (Volume 1), 6<sup>th</sup> Edn., (Pearson Education, 2002).

### **Reference Book(s)**

1. Levine, I. N., *Physical Chemistry*, 6<sup>th</sup> Edn., (McGraw Higher Edn., 2008).
2. Carey, F. A., Sundberg, R. J. *Advanced Organic Chemistry, Part A: Structure and Mechanisms*, 5<sup>th</sup> Edn., (Springer, New York, 2007).
3. March, J., Smith, M. B. *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, 6<sup>th</sup> Edn., (Wiley, 2007).

**Course Content:**

1. Qualitative Analysis of Inorganic Mixtures (excluding interfering radicals)
2. Preparation of Mohrs salt
3. Estimation of Glucose
4. Nitration of organic compounds
5. Reduction of functional groups
3. Preparation of buffer solution and measurement of pH
4. Viscosity measurement of solution
5. Conductometric acid-base titration
6. Measurement surface tension of liquid by stalagmometer
7. Verification of Beer-Lamberts law
8. Titration of a mixture of AcOH, HCl and CuSO<sub>4</sub> by conductometric method

**Text Book(s)**

1. Furniss, B. S., Ford, A. J. H., Smith, P. W. H., Tatchell, A. R. *Vogel's Textbook of Practical Organic Chemistry*, 5<sup>th</sup> Edn., (Wiley, 1989).
2. Jadav, J. B. *Advanced Practical Physical Chemistry*, (Krishna Prakashan, 2015).
3. Mendham, J., Danney, R. C., Barnes, J. D., Thomas, M. *Vogel's Textbook of Quantitative Chemical Analysis*, 6<sup>th</sup> Edn., (Prentice Hall, 2009).
4. Gurdeep, R. *Advanced Practical Inorganic Chemistry*, (Krishna Prakashan, 2013).

**Course Content:**

1. Qualitative Analysis of Inorganic Mixtures (excluding interfering radicals)
2. Preparation of Mohrs salt
3. Estimation of Glucose
4. Nitration of organic compounds
5. Reduction of functional groups
3. Preparation of buffer solution and measurement of pH.
4. Viscosity measurement of solution
5. Conductometric acid-base titration
6. Measurement surface tension of liquid by stalagmometer
7. Verification of Beer-Lamberts law
8. Titration of a mixture of AcOH, HCl and CuSO<sub>4</sub> by conductometric method and CuSO<sub>4</sub> by conductometric method

**Text Book(s)**

1. Furniss, B. S., Ford, A. J. H., Smith, P. W. H., Tatchell, A. R. *Vogel's Textbook of Practical Organic Chemistry*, 5<sup>th</sup> Edn., (Wiley, 1989).
2. Jadav, J. B. *Advanced Practical Physical Chemistry*, (Krishna Prakashan, 2015).
3. Mendham, J., Danney, R. C., Barnes, J. D., Thomas, M. *Vogel's Textbook of Quantitative Chemical Analysis*, 6<sup>th</sup> Edn., (Prentice Hall, 2009).
4. Gurdeep, R. *Advanced Practical Inorganic Chemistry*, (Krishna Prakashan, 2013).

## SEMESTER II

**CI 102**

**Chemistry-II**

**L 3 T 0 P 0 CR 3**

### **Course outcomes:**

On completion of this course, the students will be able to understand:

CO1: Structure and bonding of homonuclear diatomic molecule, Polarizability of ions

CO2: Stereochemistry of organic molecules – conformation and configuration, Asymmetric molecules and nomenclature, Aromatic compound and arom

CO3: Organic Intermediates, their generation and reactivity

CO4: Thermodynamic properties of gases and liquids, fundamentals of electrochemistry

CO5: Kinetics of simple reactions, Factors affecting the rate of the reaction

### **Course Content:**

#### **Unit 1**

**[8 Lectures]**

Structure and Bonding: Valence Bond and LCAO-MO theory, bonding in homonuclear diatomic molecules (e.g.: H<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub>, F<sub>2</sub>), covalent and ionic bonding, bond order, resonance, formal charge, VSEPR model, Polarizability of cations and anions, Fajan's rules.

#### **Unit 2**

**[4 Lectures]**

Basics organic chemistry-4: Nucleophiles, electrophiles, keto-enol tautomerism, acidity and basicity of organic compounds, Frost diagram, Hückel's rules for aromaticity, antiaromaticity, homoaromaticity.

#### **Unit 3**

**[6 Lectures]**

Stereochemistry-1: Representation of organic molecules in Fischer, saw horse, Newman, and flying-wedge, projection formulae and their interconversion, symmetry elements, molecular chirality, optical activity, optical purity, meso compounds, racemic mixture,

resolution, enantiomers, diastereomers, epimers, anomers, atropisomers, basic concepts of stereochemical nomenclatures: *threo/erythro*, *syn/anti*, *R/S*, *cis/trans* and *E/Z*).

#### **Unit 4**

**[4 Lectures]**

Reactive intermediates: Carbocation, carbanion, carbene, nitrene, free radical and benzyne: Generation, stability and reactions.

#### **Unit 5**

**[4 Lectures]**

Properties of gases and liquids: Equations of state, kinetic model of gases, collision theory, real gases, Maxwell distribution of molecular speeds, qualitative description of the structure of liquids, surface tension and viscosity.

#### **Unit 6**

**[6 Lectures]**

Electrochemistry: Conduction in electrolyte solutions, ionic mobility, Kohlrausch law, Ostwald's dilution law, transport number, Debye-Huckel Limiting Law, electrochemical cells, EMF, Nernst equation.

#### **Unit 7**

**[4 Lectures]**

Rate of reactions: Rate equations of zero, first, second, pseudo 1<sup>st</sup> order reactions, determination of order of a reaction, activation energy, activated complex theory, collision theory.

#### **Text Book(s)**

1. Atkins, P., Paula, J. de. *Atkins' Physical Chemistry*, 10<sup>th</sup> Edn., (Oxford University Press, 2014).
2. Overton, T., Armstrong, F., Rourke, J., Weller, M. *Inorganic Chemistry*, 6<sup>th</sup> Edn., (Oxford University Press, 2015).
3. Clayden, J., Greeves, N., Warren, S., Wothers, P. *Organic Chemistry*, 2<sup>nd</sup> Edn., (Oxford University Press, 2012).
4. Sengupta, S. *Basic Stereochemistry of Organic Molecules*, 1<sup>st</sup> Edn., (Oxford University Press, 2014).

## Reference Book(s)

1. Laidler, K. J., Meiser, J. H., Sanctuary, B. C., *Physical Chemistry*, 4<sup>th</sup> Edn., (Brooks Cole, 2002).
2. Carey, F. A., Sundberg, R. J. *Advanced Organic Chemistry, Part B: Reactions and Synthesis*, 5<sup>th</sup> Edn., (Springer, New York, 2007).
3. March, J., Smith, M. B. *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, 6<sup>th</sup> Edn., (Wiley, 2007).
4. Eliel, E. L., Wilen, S. H., Doyle, M. P. *Basic Organic Stereochemistry*, 1<sup>st</sup> Edn., (Wiley-Interscience, 2001).

CI 106

Chemistry Laboratory-II

L O T O P 3 CR 3

### Course Content:

#### Section A: Inorganic Chemistry

1. Estimation of sodium carbonate and sodium hydrogen carbonate present in a mixture
2. Estimation of oxalic acid by titrating with  $\text{KMnO}_4$
3. Estimation of water of crystallization in Mohr's salt by titrating with  $\text{KMnO}_4$
4. Estimation of Fe (II) ions by titrating with  $\text{K}_2\text{Cr}_2\text{O}_7$  using internal indicator
5. Estimation of Cu (II) ions iodometrically using  $\text{Na}_2\text{S}_2\text{O}_3$

#### Section B: Organic Chemistry

1. Detection of extra elements (N, S, Cl, Br, I) in organic compounds (containing upto two extra elements)
2. Separation of mixtures by Chromatography: Measure the  $R_f$  value in each case (combination of two compounds to be given)
  - (a) Identify and separate the components of a given mixture of  $\alpha$ -amino acids (glycine, aspartic acid, glutamic acid, tyrosine or any other amino acid) by paper chromatography
  - (b) Identify and separate the sugars present in the given mixture by paper chromatography.

### **Text Book(s)**

1. Svehla, G., Sivasankar, B. *Vogel's Qualitative Inorganic Analysis*, 7<sup>th</sup> Edn., (Pearson Education, 2012).
2. Mendham, J., Denney, R. C., Barnes, J. D., Thomas, M., Sivasankar, B. *Vogel's Quantitative Chemical Analysis*, 6<sup>th</sup> Edn., (Pearson Education, 2009).
3. Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A. J., Smith, P. W. G., *Textbook of Practical Organic Chemistry*, 5<sup>th</sup> Edn., (Prentice-Hall, 1996).
4. Mann, F.G., Saunders, B.C. *Practical Organic Chemistry*, (Orient-Longman, 1960).

### **CI 107 Chemistry Laboratory (for MBBT and Physics) L O T O P 3 CR 3**

#### **Course Content:**

1. Qualitative Analysis of Inorganic Mixtures (excluding interfering radicals)
2. Preparation of Mohrs salt
3. Estimation of Glucose
4. Nitration of organic compounds
5. Reduction of functional groups
3. Preparation of buffer solution and measurement of pH
4. Viscosity measurement of solution
5. Conductometric acid-base titration
6. Measurement surface tension of liquid by stalagmometer
7. Verification of Beer-Lamberts law
8. Titration of a mixture of AcOH, HCl and CuSO<sub>4</sub> by conductometric method

### **Text Book(s)**

1. Furniss, B. S., Ford, A. J. H., Smith, P. W. H., Tatchell, A. R. *Vogel's Textbook of Practical*, 5<sup>th</sup> Edn., (Wiley, 1989).
2. Jadav, J. B. *Advanced Practical Physical Chemistry*, (Krishna Prakashan, 2015).



3. Mendham, J., Denney, R. C., Barnes, J. D., Thomas, M., Sivasankar, B. *Vogel's Quantitative Chemical Analysis*, 6<sup>th</sup> Edn., (Pearson Education, 2009).
4. Gurdeep, R. *Advanced Practical Inorganic Chemistry*, (Krishna Prakashan, 2013).

### **SEMESTER III**

#### **CI 201 Chemistry-III (For non-major)**

**L O T O P 3 CR 3**

#### **Course outcomes:**

On completion of this course, the students will be able to understand:

CO1: Concepts of acids and bases, and their strength

CO2: Fundamentals of coordination chemistry

CO3: Aromatic compounds and aromaticity

CO4: Synthesis and properties of hydrocarbons

CO5: Weak electrolyte and ionic equilibrium

#### **Course Content:**

##### **Unit 1**

**[5 Lectures]**

Acid -Base concept: Arrhenius concept, Brønsted-Lowry acids and bases, Lewis acids and bases, Hard Soft acids - bases and HSAB principle, Acid and base strength, levelling effect.

##### **Unit 2**

**[5 Lectures]**

Coordination chemistry: Werner's theory, classification of ligands, coordination number, nomenclature of coordination compounds, isomerism.

##### **Unit 3**

**[6 Lectures]**

Aromaticity and Hückel Rule, Orientation of substituents, Directive influence of substituents, o/p ration, kinetically and thermodynamically controlled reactions.

##### **Unit 4**

Alkynes: Preparation, properties and reactions.

**[5 Lectures]**

## Unit 5

Alkyl halides: Preparation, properties and reactions.

[5 Lectures]

## Unit 6

[10 Lectures]

Ionic equilibrium: Arrhenius theory of electrolytic dissociation, Ostwald dilution law, Dissociation constant of weak acids and bases, Ionization of water,  $pK_w$  and pH, Salt effect, pH expressions for various neutralization reaction, Henderson- Hasselbalch equation, solubility product, common ion effect, Buffer solutions, theory of acid base indicators, acid base titration curves (pH variation).

### Text Book(s)

1. Huheey, J. E., Keiter, E. A., Keiter, R. L. and Medhi, O. K. *Inorganic Chemistry: Principles of Structure and Reactivity*, 4<sup>th</sup> Edn., (Pearson Education, 2006).
2. Barrow, G. M. *Physical Chemistry*, 5<sup>th</sup> Edn., (McGraw Hill, 2007).
3. Finar, I. L. *Organic Chemistry (Volume 1)*, 6<sup>th</sup> Edn., (Pearson Education, 2002).
4. Ghosh, S. K., *Advanced General Organic Chemistry*, 3<sup>rd</sup> Edn., (New Central Book Agency (P) Ltd., 2008).

### Reference Book(s)

1. Smith, M. B., March, J. *March's Advanced Organic Chemistry, Reaction Mechanism and Structure* 6<sup>th</sup> Edn., (Wiley, 2007).
2. Clayden, J., Greeves, N., Warren, S., Wothers, P. *Organic Chemistry*, 2<sup>nd</sup> Edn., (Oxford University Press, 2012).

CI 203      Physical Chemistry-I

L 3 T 0 P 0 CR 3

### Course outcomes:

After completion of the course, the learner shall be able to :

CO1: Understand the concept of system, variables, heat, work, and laws of thermodynamics.

CO2: Understand the concept of heat of reactions and use of equations in calculations of bond energy, enthalpy, etc.

C03: Understand the concept of entropy; reversible, irreversible processes.

C04: Calculation of entropy using 3<sup>rd</sup> law of thermodynamics.

C05: Understand the structure and thermodynamics of the three states of matters viz. solid, liquid, gas.

### **Course Content:**

#### **Unit 1**

Chemical Thermodynamics: The basic concepts, thermodynamics terms, concept of system and surroundings, type of systems, concept of boundary or wall, steady state and equilibrium state, thermodynamic coordinates, state of a system, equation of state, state and path functions, exact and inexact differential, Euler's theorem, concept of intensive and extensive variables, Partial derivatives and cyclic rule, reversible and irreversible process, concept of heat, work and energy (IUPAC convention), general expressions of work, graphical explanation of work done during expansion and compression of an ideal gas, Reversible and irreversible processes and work done.

**[3 Lectures]**

Zeroth and First law of Thermodynamics: Concept of thermal equilibrium and the zeroth-law of thermodynamics, First law of thermodynamics, internal energy (U) as a state function. Enthalpy as a state function, heat changes at constant volume and constant pressure; heat capacity, relation between  $C_P$  and  $C_V$  using ideal gas and van der Waals equations, the work of adiabatic changes, heat capacity ratio and adiabats, Joule's experiment and its consequence, Joule Thomson effect, explanation of term  $(\delta U/\delta V)_T$ , Isothermal and adiabatic processes.

**[3 Lectures]**

Thermochemistry: Standard states, heats of reaction, thermochemical equation, standard enthalpy changes (enthalpies of physical changes and enthalpies of chemical changes), Hess's law, standard enthalpy of formation, Kirchhoff's equations and effect of pressure on enthalpy of reactions, bond energy, bond dissociation energy and resonance energy from thermochemical data.

**[3 Lectures]**

Second law of thermodynamics: Reservoirs and heat engines, Carnot cycle, physical concept of Entropy, Carnot engine and refrigerator, Kelvin – Planck and Clausius statements and equivalence of the two statements with entropic formulation, Carnot's theorem, Clausius inequality, entropy change of systems and surroundings for various processes and transformations, Entropy and unavailable work, state functions (Helmholtz energy (A) and Gibb's energy(G)) and their variation with T, P and V, criteria for spontaneity and equilibrium, Thermodynamic relations: Gibbs- Helmholtz equation, Maxwell's relations; pressure dependence of Gibb's energy, chemical potential of pure substances. **[8 Lectures]**

Third law of Thermodynamics: Nernst heat theorem, Third law entropies. **[1 Lecture]**

## **Unit 2**

Properties of States of matter: Properties of gases: Perfect Gas: Properties of gases, concept of pressure and temperature, mixture of gases, concept of partial pressure, Dalton's law, equations of state, Boyle's law, Charle's Law, Avogadro's Law, Ideal gas equation. **[2 Lectures]**

Kinetic theory of gases: Kinetic model of gases, relationship between pressure and molecular speeds, Maxwell-Boltzmann distribution of speeds, mean velocity, root mean square velocity, most probable velocity, relative velocity, collision frequency (similar and different molecules), mean free path, viscosity of gases, effusion, Principle of equipartition of energy and its application to calculate the classical limit of molar heat capacity of gases. **[3 lectures]**

Real Gases: Deviations from perfect behaviour, compressibility factor, Boyle temperature, van der Waals equation and its features, existence of critical state, critical constants in terms of van der Waals constants, virial equation of state, van der Waals equation expressed in virial form and significance of second virial coefficient; principles of corresponding states, intermolecular forces (Debye, Keesom and London interactions; Mie potential, Lennard-Jones potential - elementary idea). **[3 Lectures]**

**[3 Lectures]**

Properties of Liquids: Qualitative description of the structure of liquids, molecular interactions in liquids, the radial distribution function, boiling point, vapour pressure, viscosity, liquid vapour interface, surface tension, curved surfaces, Laplace equation, vapour pressure over curved surface, Kelvin equation, capillary action measurement of surface tension, surface pressure. **[5 Lectures]**

Properties of Solids: General properties of solids, forms of solids, crystal systems, unit cells, Bravais lattice types, symmetry elements, Miller indices of different planes and interplanar distance, Bragg's law, structures of ionic solids (qualitative treatment only); defects in crystals. **[5 Lectures]**

#### **Text Book(s)**

1. Atkins, P. and Paula, J. de. *Atkins' Physical Chemistry*, 10<sup>th</sup> Edn., (Oxford University Press, 2014).
2. Silbey, R. J., Alberty, R. A. and Bawendi, M. J. *Physical Chemistry*, 4<sup>th</sup> Edn., (Wiley, 2004).
3. Levine, I. N., *Physical Chemistry*, 6<sup>th</sup> Edn., (McGraw Higher Ed, 2008).

#### **Reference Book(s)**

1. Laidler, K. J., Meiser, J. H. and Sanctuary, B. C., *Physical Chemistry*, 4<sup>th</sup> Edn., (Brooks Cole, 2002).
2. McQuarrie, D. A. and Simon, J. D., *Physical Chemistry: A Molecular Approach*, (University Science Books, 1997).
3. Mortimer, R. G. *Physical Chemistry*, 3<sup>rd</sup> Edn., (Elsevier, 2008).
4. Adamson, A. A., *A Textbook of Physical Chemistry*, 2<sup>nd</sup> Edn., (Elsevier, 1973).

**Course outcomes:**

On completion of this course, the students will be able to understand:

CO1: Concepts of aliphatic nucleophilic substitution reactions

CO2: Fundamentals of elimination reactions

CO3: Aromatic electrophilic substitution reactions

CO4: Aromatic nucleophilic substitution reactions

CO5: Preparation of alcohols and phenols with their reactivity

**Course Content:****Unit 1****[ 8 Lectures]**

Nucleophilic substitution at  $sp^3$  carbon: Mechanism:  $S_N1$ ,  $S_N2$ ,  $S_Ni$  mechanisms, effect of solvent, substrate structure, leaving group, nucleophiles including ambident nucleophiles, substitution involving NGP; relative rate & stereochemical features.

**Unit 2****[6 Lectures]**

Elimination reaction: E1, E2 and E1cB; reactivity, orientation (Saytzeff / Hofmann) and stereoselectivity; substitution vs elimination.

**Unit 3****[7 Lectures]**

Electrophilic aromatic substitution: Mechanisms:  $\pi$ - and  $\sigma$ -complex, ipso substitution, activating and deactivating groups, orienting influence.

Reactions: Friedel-Crafts alkylation/acylation, nitration, sulfonation, halogenation, formylation.

**Unit 4****[5 Lectures]**

Nucleophilic aromatic substitution: Mechanisms, orientation and reactivity.

**Unit 5****[10 Lectures]**

Alcohols: Classification of alcohols and their synthesis and reactions; Synthesis of phenols: From sodium arylsulphonates, diazonium salts,  $S_NAr$ , Grignard reagents,

cumene-phenol process, boronic acids, Dakin reaction; Reaction of phenols: Reimer-Tiemann reaction, Kolbe's reaction, Lederer-Manasse reaction, Fries rearrangement, Claisen rearrangement, nitration, sulphonation, halogenation, oxidation, coupling with diazonium salt, oxidation of phenols by hypervalent iodine(iii) reagents and other oxidizing agents to quinones; Reactions of quinones: Reactions with HCl, amines, alcohols, Thiele acetylation and dienone phenol rearrangement.

### **Text Book(s)**

1. Clayden, J., Greeves, N., Warren, S., Wothers, P. *Organic Chemistry*, 2<sup>nd</sup> Edn., (Oxford University Press, 2012).
2. Sykes, P. *A Guide book to Mechanism in Organic Chemistry*, 6<sup>th</sup> Edn., (Orient Longman Ltd., New Delhi, 1997).
3. Finar, I. L. *Organic Chemistry* (Volume 1), 6<sup>th</sup> Edn., (Pearson Education, 2002).

### **Reference Book(s)**

1. Zweifel, G. S., Nantz, M. H., Somfai, P. *Modern Organic Synthesis: An Introduction*, 2<sup>nd</sup> Edn., (Wiley, New York, 2017).
2. Norman, R. O. C., Coxon, J. M. *Principles in Organic Synthesis*, 3<sup>rd</sup> Edn., (Blackie Academic & Professional, 1993).
3. Carey, F. A., Sundberg, R. J. *Advanced Organic Chemistry, Part B: Reactions and Synthesis*, 5<sup>th</sup> Edn., (Springer, New York, 2007).
4. March, J., Smith, M. B. *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, 6<sup>th</sup> Edn., (Wiley, 2007).

**CI 207**

**Inorganic Chemistry-I**

**L 3 T 0 P 0 CR 3**

### **Course outcomes:**

On completion of this course the students will be able to understand:

CO1: Concept of acids and bases as well as the hard-soft acid base principle

CO2: History of co-ordination chemistry, nature of ligands, the nomenclature, and the isomerism in coordination complexes

CO3: Concept of oxidation and reduction, redox reactions, electrochemical potentials, and related equations with their implications

CO4: Statistical methods to find error and accuracy in data analysis and their real applications

CO5: Concept of molecular orbital theory (MOT) or band theory classifying the metals, conductors, semiconductors, and insulators

### **Course Content:**

#### **Unit 1** **[8-Lectures]**

Acid -Base concept: Arrhenius concept, Brønsted-Lowery acids and bases, Lewis acids and bases, Hard soft acids - bases and HSAB principle, Acid and base strength.

#### **Unit 2** **[6-Lectures]**

Coordination chemistry: Werner's theory, classification of ligands, coordination number, nomenclature of coordination compounds, isomerism.

#### **Unit 3** **[10 Lectures]**

Oxidation and Reduction: Oxidation numbers, redox potential, half-cell reaction, Nernst equation, electrochemical series, Latimer and Frost diagrams, Pourbaix diagrams.

#### **Unit 4** **[6 Lectures]**

Statistical methods of analysis: Types of errors, accuracy, precision, significant figures, standard and mean deviations, f-test and t-test.

#### **Unit 5** **[6 Lectures]**

Metallic bonding, band theory, semiconductor, bonding in alloys, intermetallic compounds, hydrogen bonding, clathrates.

### **Text Book(s)**

1. Huheey, J. E., Keiter, E. A., Keiter, R. L. and Medhi, O. K. *Inorganic Chemistry: Principles of Structure and Reactivity*, 4<sup>th</sup> Edn., (Pearson Education, 2006).



2. Mendham, J., Denney, R. C., Barnes, J. D., Thomas, M. and Sivasankar, B. *Vogel's Quantitative Chemical Analysis*, 6<sup>th</sup> Edn., (Pearson Education, 2009).

### Reference Book(s)

1. Overton, T., Armstrong, F., Rourke, J. and Weller, M. *Inorganic Chemistry*, 6<sup>th</sup> Edn., (Oxford University Press, 2015).
2. Wulfsberg, G. *Inorganic Chemistry*, 2<sup>nd</sup> Edn., (Viva, 2005).

**CI 209                      Chemistry Laboratory-III**

**L O T O P 3 CR 3**

### Course Content:

#### Unit 1

Inorganic: Qualitative Analysis of Inorganic Mixtures (including interfering radical)

#### Unit 2

Physical:

1. Thermochemistry experiment (determination of heat of hydration)
2. Electrochemistry (determination of redox potential)
3. Chemical kinetics (determination of rate constant of hydrolysis of methyl acetate catalysed by an acid)
4. Conductometric/potentiometric (determination of equivalence conductance of an electrolyte at infinite dilution)
5. UV-VIS spectrophotometric (determination of dissociation constant of ferrithiocyanate complex).

### Text Book(s)

1. Svehla, G. *Vogel's Qualitative Inorganic Analysis*, 7<sup>th</sup> Edn., (Prentice Hall, 1996).
2. Yadav, J. B. *Advance Practical Physical Chemistry*, (Goel Publishing House- Meerut, 2008).

### Reference Book(s)

1. Viswanathan, B., Raghavan, P. S. *Practical Physical Chemistry* (Viva Books Private Limited, 2008).
2. Gurdeep, R. *Advanced Practical Inorganic Chemistry*, (Krishna Prakashan, 2013).

## SEMESTER IV

CI 204

Physical Chemistry-II

L 3 T 0 P 0 CR 3

### Course outcomes:

The courses would fortify the students with in-depth subject knowledge of reaction kinetics. After completion of the course, the learner shall be able to understand:

CO1: Chemical kinetics of simple and complex reactions, Deduction of rate law from the mechanism, Factors affecting the rate of reactions

CO2: Kinetics theories like Hard sphere collision theory, activated complex theory

CO3: Kinetics of reactions in solution phase

CO4: Basics of photo-physical and photo-chemical processes

CO5: Adsorption, adsorption isotherms and their significances and applications

### Course Content:

#### Unit 1

[2 Lectures]

Reaction rate and rate laws: Reaction mechanism, elementary or simple reactions, complex reactions, definition of rate, monitoring the progress of reaction, rate laws and rate constants, order of reactions, reactions having no order, molecularity, Integrated rate law (zeroth, first and second order reactions), half-life, determination of the rate law.

#### Unit 2

[4 Lectures]

Factors affecting the rate of a reaction: Temperature dependence of reaction rate, Arrhenius equation, Arrhenius plot, Activation energy, relationship between activation energy and enthalpy, Pre-exponential factor, Hard-sphere collision theory, the steric requirement, Activated complex theory, Eyring equation, kinetic isotope effect.

#### Unit 3

[6 Lectures]

Kinetics of complex reaction: Complex reactions, evidence of complex reactions, types of complex reactions, steady state approximation, rate limiting step, opposing 1<sup>st</sup> order, consecutive, parallel, chain, and photochemical reactions, Explosion (thermal and chain

branching explosion), kinetic and thermodynamic control of reaction, Law of microscopic reversibility, Lindemann theory of unimolecular reaction.

#### **Unit 4**

**[6 Lectures]**

Catalysis: Classification, characteristic of catalytic reaction, homogeneous and heterogeneous catalysis, turn over number, acid base catalysis, Brönsted relations, autocatalysis, oscillatory reactions, enzyme catalysis, Enzyme Inhibition, Michaelis-Menten equation, Lineweaver-Burk plot, kinetic salt effect (Primary and Secondary salt effect, salting in and salting out), Heterogeneous catalysis, Langmuir- Hinshelwood mechanism, Eley-Rideal mechanism.

#### **Unit 5**

**[6 Lectures]**

Photochemistry: Laws of photochemistry: Grotthus-Draper law, Stark-Einstein law of photochemical equivalence and Lambert-Beer's law; quantum yield and its measurement for a photochemical process, Jablonski Diagram, Fluorescence, Phosphorescence, Chemiluminescence, Quenching, Stern-Volmer equation, Fluorescence lifetime, Photosensitized reactions, Kinetics of HI decomposition, hydrogen-halogen reactions, dimerisation of anthracene.

#### **Unit 6**

**[6 Lectures]**

Reactions in solution: Reactions in solution, cage effect, diffusion-controlled reaction, activation controlled reaction, the material balance equation, Influence of solvent dielectric constant, Influence of ionic strength, influence of hydrostatic pressure, Hammett relationship.

#### **Unit 7**

**[6 Lectures]**

Adsorption: Difference between absorption and adsorption, physical and chemical adsorption, factors influencing adsorption, adsorption isotherms (Langmuir, Freundlich and BET), application of adsorption isotherms for surface area measurement, application of adsorption, Gibbs adsorption isotherm and surface excess. Heterogeneous catalysis (single reactant).

### **Text Book(s)**

1. Atkins, P. and Paula, J. de. *Atkins' Physical Chemistry*, 10<sup>th</sup> Edn., (Oxford University Press, 2014).
2. Levine, I. N., *Physical Chemistry*, 6<sup>th</sup> Edn., (McGraw Higher Ed, 2008).
3. Laidler, K. J., *Chemical Kinetics*, 3<sup>rd</sup> Edn., (Pearson Education India, 2003).

### **Reference Book(s)**

1. Laidler, K. J., Meiser, J. H. and Sanctuary, B. C., *Physical Chemistry*, 4<sup>th</sup> Edn., (Brooks Cole, 2002).
2. Silbey, R. J., Alberty, R. A. and Bawendi, M. J. *Physical Chemistry*, 4<sup>th</sup> Edn., (Wiley, 2004).
3. McQuarrie, D. A. and Simon, J. D., *Physical Chemistry: A Molecular Approach*, (University Science Books,).
4. Connors, K. A. *Chemical Kinetics: A Study of Reaction Rates in Solution*, (Wiley VCH, 1990).
5. Barrow, G. M. *Physical Chemistry*, 5<sup>th</sup> Edn., (Tata McGraw Hill Education, 2006).

**CI 206**

**Organic Chemistry-II**

**L 3 T 0 P 0 CR 3**

### **Course outcomes:**

On completion of the course, the learner shall be able to know:

CO1: Synthesis, properties, and reactions of ethers

CO2: Organonitrogen compound

CO3: Chemistry of aldehydes and ketones

CO4: Carboxylic acids and derivatives

CO5: Understanding of carbohydrate chemistry

### **Course Content:**

#### **Unit 1**

**[ 6 Lectures]**

Ethers: Classification: Dialkyl, aryl alkyl and diaryl ethers; cyclic ethers: epoxides, oxetanes, THF, THP.

Synthesis: Williamson ether synthesis, dehydration of alcohols, alkoxymercuration-demercuration, diaryl- and aryl alkyl ethers by  $S_NAr$ , cycloetherification.

Reactions:  $S_N1/S_N2$  cleavage of ethers by HI, HBr,  $BBr_3$ , TMSI, NaSR.

Synthesis and cleavage of well-known classes of ethers: OMe, OMOM, OTHP, OBn, OPMB

Synthesis and cleavage of well-known silyl ethers: OTMS, OTBS and TBDPS.

## **Unit 2**

**[ 2 Lectures]**

Organonitrogen compounds: Synthesis and reactions of  $RNO_2/ArNO_2$ ,  $RCN/ArCN$ ,  $RNC/ArNC$ ,  $RNH_2/ArNH_2$ , diazonium salts.

## **Unit 3**

**[6 Lectures]**

Aldehydes and ketones: Reactions: Hydrates, cyanohydrin, bisulfite adduct, hemiacetal/acetal/thioacetal, imines, hydrazones, oximes,  $\alpha$ -halogenation, reaction with nitrous acid, Cannizzaro reaction, Tischenko reaction, reactions with Grignard reagents and organolithium compounds, Reformatsky reaction, reaction with diazomethane and related compounds.

## **Unit 4**

**[8 Lectures]**

Carboxylic acids and their derivatives: Synthesis: General synthetic methods of carboxylic acids, esters, acid chlorides, anhydrides and amides.

Reactions: Decarboxylation, esterification, ester hydrolysis, HVZ reaction, nucleophilic substitution at acyl carbon, reactions with Grignard reagents, organolithium and other organometallic compounds, reaction with diazomethane and related compounds.

## **Unit 5**

**[8 Lectures]**

Rearrangements: (i) Rearrangement to electron-deficient carbon:

Wagner-Meerwein rearrangement, pinacol-pinacolone and related rearrangements, dienone-phenol, benzil-benzilic acid rearrangement.

(ii) Rearrangement to electron-deficient oxygen:

Baeyer-Villiger oxidation, hydroperoxide rearrangement cumene hydroperoxide-phenol rearrangement, Dakin reaction.

(iii) Rearrangement to electron-deficient nitrogen (Beckmann rearrangement, Schmidt rearrangement, Hofmann rearrangement, Lossen rearrangement, Curtius rearrangement).

(iv) Aromatic rearrangements:

Migration from oxygen to ring carbon (Fries rearrangement, Claisen rearrangement), migration from nitrogen to ring carbon (Hofmann-Martius rearrangement, Fischer-Hepp rearrangement, N-azo to C-azo rearrangement, Bamberger rearrangement, Orton rearrangement, Benzidine rearrangement).

## Unit 6

[6 Lectures]

Carbohydrates: Monosaccharides, Aldoses up to 6 carbons, structure of D-glucose & D-fructose (configuration & conformation), anomeric effect, mutarotation, Important reactions and conversions including protection/deprotection protocol, Disaccharides and polysaccharide: nature of glycosidic linkages.

### Text Book(s)

1. Clayden, J., Greeves, N., Warren, S., Wothers, P. *Organic Chemistry*, 2<sup>nd</sup> Edn., (Oxford University Press, 2012).
2. Sykes, P. *A Guide book to Mechanism in Organic Chemistry*, 6<sup>th</sup> Edn., (Orient Longman Ltd., New Delhi, 1997).
3. Finar, I. L. *Organic Chemistry* (Volume 1), 6<sup>th</sup> Edn., (Pearson Education, 2002).

### Reference Book(s)

1. Zweifel, G. S., Nantz, M. H., Somfai, P. *Modern Organic Synthesis: An Introduction*, 2<sup>nd</sup> Edn., (Wiley, New York, 2017).
2. Norman, R. O. C., Coxon, J. M. *Principles in Organic Synthesis*, 3<sup>rd</sup> Edn. (Blackie Academic & Professional, 1993).
3. Carey, F. A., Sundberg, R. J. *Advanced Organic Chemistry, Part B: Reactions and Synthesis*, 5<sup>th</sup> Edn., (Springer, New York, 2007).
4. March, J., Smith, M. B. *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, 6<sup>th</sup> Edn., (Wiley, 2007).

**Course outcomes:**

On completion of this course the students will be able to understand:

CO1: Chemistry of boron compounds including their preparation, properties and bonding nature

CO2: Wade's rule for predicting the structure of boron compounds

CO3: Chemistry of inorganic carbon compounds, the allotropy of carbons and their compounds with nitrogen and sulphur

CO4: Chemistry of silanes, silicones, silicon polymers

CO5: Nitrogen and phosphorous chemistry, properties of various compounds of nitrogen and phosphorous such oxides, halides etc.

**Course Content:****Unit 1****[12 Lectures]**

Chemistry of Group 13 Elements: The elements and their properties; Chemistry of Boron; Borides; Boron hydrides (Preparation, structure, bonding, reactions and properties); Wade's rule, Boron halides, Boron-Nitrogen chemistry; Boron-Oxygen chemistry, borane, carborane, metalloborane and metallocarboranes.

**Unit 2****[12 Lectures]**

Chemistry of Group 14 Elements: The elements and their properties; Allotropy of Carbon: Diamond, Graphite, and Fullerenes; Intercalation); Carbides; Carbon halides and oxides; Compounds with C-N and C-S bonds; Silane reagents, Synthesis, properties and modifications on polysilanes. Condensation vs catenation, Silicides, Silicone Polymers; Oxygen compounds of silicon.

### Unit 3

[12 Lectures]

Chemistry of Group 15 Elements: The elements and their properties; Nitrides; Hydrides of Nitrogen; Oxides of Nitrogen; Oxo acids and anions of Nitrogen; Activation of Nitrogen; Reaction of coordinated NO; Phosphides; Phosphorous halides and oxides; Oxoacids of phosphorous and their salts, phosphonitrilic compounds.

#### Text Book(s)

1. Greenwood, N. N., Earnshaw, A. *Chemistry of the Elements*, 2<sup>nd</sup> Edn., (Pergamon Press, 1997).
2. Cotton, F. A., Wilkinson, G., Murillo, C. A. and Bochmann, M. *Advanced Inorganic Chemistry*, 6<sup>th</sup> Edn., (John Wiley, 2007).

#### Reference Book(s)

1. Overton, T., Armstrong, F., Rourke, J. and Weller, M. *Inorganic Chemistry*, 6<sup>th</sup> Edn., (Oxford University Press, 2015).
2. Wulfsberg, G. *Inorganic Chemistry*, 2<sup>nd</sup> Edn., (Viva, 2005).

CI 212

Chemistry Laboratory-IV

L O T O P 3 CR 3

#### Unit 1

Volumetric estimation of iron and copper, determination of water of crystallization in a molecule of Hydrated Mohr's salt, estimation of total Hardness of water.

#### Unit 2

Detection of N, S, and halogens in organic compounds, preparation of suitable derivatives of functional groups and determination of mp/bp

#### Unit 3

One step organic preparation using common organic reactions such as nitration, acetylation, benzylation, diazo-coupling etc.

#### Text Book(s)

1. Mendham, J., Denney, R. C., Barnes, J. D., Thomas, M. and Sivasankar, B. *Vogel's Quantitative Chemical Analysis*, 6<sup>th</sup> Edn., (Pearson Education, 2009).



2. Furniss, B. S., Ford, A. J. H., Smith, P. W. H. and Tatchell, A., R. *Vogel's Textbook of Practical Organic Chemistry*, 5<sup>th</sup> Edn., (John Wiley, 1989).

### Reference Book(s)

1. Vishnoi, R. *Advanced Practical Organic Chemistry*, 2<sup>nd</sup> Revised Edn., (Vikas Publisher, 2007).
2. Gurdeep, R. *Advanced Practical Inorganic Chemistry*, (Krishna Prakashan, 2013).

CI 214

IT Skills for Chemists

L 3 T 0 P 0 CR 3

### Course outcomes:

After completion of the course, the learner shall be able to understand:

CO1: Important mathematical concept widely applied in chemistry

CO2: numerical methods for differentiation and integration

CO3: Computer Programming

CO4: Curve fitting methods

CO5: Different software used in data handling and analysis

### Course Content:

#### Unit 1

[12 Lectures]

Mathematics:

Fundamentals, mathematical functions, polynomial expressions, logarithms, the exponential function, units of a measurement, interconversion of units, constants and variables, equation of a straight line, plotting graphs.

Uncertainty in experimental techniques: Displaying uncertainties, measurements in chemistry, decimal places, significant figures, combining quantities.

Uncertainty in measurement: types of uncertainties, combining uncertainties, statistical treatment, mean, standard deviation, relative error, data reduction and the propagation

of errors, graphical and numerical data reduction, numerical curve fitting: the method of least squares (regression).

Algebraic operations on real scalar variables (e.g. manipulation of van der Waals equation in different forms), roots of quadratic equations analytically and iteratively (e.g. pH of a weak acid), numerical methods of finding roots (Newton-Raphson, binary – bisection, e.g. pH of a weak acid not ignoring the ionization of water, volume of a van der Waals gas, equilibrium constant expressions).

Differential calculus: The tangent line and the derivative of a function, numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations).

Numerical integration (Trapezoidal and Simpson's rule, e.g. entropy/enthalpy change from heat capacity data).

## **Unit 2**

Computer programming:

**[8 Lectures]**

Constants, variables, bits, bytes, binary and ASCII formats, arithmetic expressions, hierarchy of operations, inbuilt functions, elements of the BASIC language, BASIC keywords and commands, Logical and relative operators, strings and graphics, compiled versus interpreted languages, Debugging, simple programs using these concepts, matrix addition and multiplication, statistical analysis.

BASIC programs for curve fitting, numerical differentiation and integration (Trapezoidal rule, Simpson's rule), finding roots (quadratic formula, iterative, Newton-Raphson method).

## **Unit 3**

**[4 Lectures]**

HANDS ON:

Introductory writing activities: introduction to word processor and structure drawing (ChemSketch) software, incorporating chemical structures, chemical equations, and expressions from chemistry (e.g. Maxwell-Boltzmann distribution law, Bragg's law, van der Waals equation, etc.) into word processing documents.

#### **Unit 4**

HANDS ON:

**[4 Lectures]**

Handling numeric data:

Spreadsheet software (Excel), creating a spreadsheet, entering and formatting information, basic functions and formulae, creating charts, tables and graphs, incorporating tables and graphs into word processing documents, simple calculations, plotting graphs using a spreadsheet (Planck's distribution law, radial distribution curves for hydrogenic orbitals, gas kinetic theory- Maxwell-Boltzmann distribution curves as function of temperature and molecular weight), spectral data, pressure-volume curves of van der Waals gas (van der Waals isotherms), data from phase equilibria studies, graphical solution of equations.

#### **Unit 5**

**[4 Lectures]**

HANDS ON:

Numeric modelling:

Simulation of pH metric titration curves, Excel functions LINEST and Least Squares, Numerical curve fitting, linear regression (rate constants from concentration time data, molar extinction coefficients from absorbance data), numerical differentiation (e.g. handling data from potentiometric and pH metric titrations, pKa of weak acid), integration (e.g. entropy/enthalpy change from heat capacity data).

#### **Unit 6**

**[4 Lectures]**

Statistical analysis:

Gaussian distribution and errors in measurements and their effect on data sets. Descriptive statistics using Excel. Statistical significance testing: The  $t$  test, the  $F$  test.

#### **Text Book(s)**

1. McQuarrie, D. A. *Mathematics for Physical Chemistry*, (University Science Books, 2008).
2. Harris, D. C. *Quantitative Chemical Analysis*. 7<sup>th</sup> Edn., (Freeman, 2010).

3. Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis*, (Cambridge University Press, 2001).
4. Venit, S.M. *Programming in BASIC: Problem solving with structure and style*, 2<sup>nd</sup> Edn. (Jaico Publishing House, 2001).

### Reference Book(s)

1. Mortimer, R. *Mathematics for Physical Chemistry*, 4<sup>th</sup> Edn., (Elsevier, 2013).
2. Steiner, E. *The Chemical Maths Book* (Oxford University Press, 2008).
3. Yates, P. *Chemical calculations*, 2<sup>nd</sup> Edn., (CRC Press, 2007).

**CI 216**

**Basic Analytical Chemistry**

**L 3 T 0 P 0 CR 3**

### Learning outcomes:

After completion of the course, the learner shall be able to learn:

CO1: The method of sampling and the presentation of experimental data

CO2: Calculation of characteristic parameters of samples like soil, water, food, cosmetics etc.

CO3: Use of techniques like chromatography, UV-Vis spectroscopy, flamephotometry in sample analysis

### Course Content:

#### Unit 1

**[6 Lectures]**

Introduction to Analytical Chemistry and its interdisciplinary nature, concept of sampling, importance of accuracy, precision and sources of error in analytical measurements, presentation of experimental data and results, from the point of view of significant figures.

#### Unit 2

**[5 Lectures]**

Analysis of soil: composition of soil, concept of pH and pH measurement, complexometric titrations, chelation, chelating agents, use of indicators, determination of pH of soil samples, estimation of Calcium and Magnesium ions as Calcium carbonate by complexometric titration, analysis of Na/K/N contents, clay, porosity and soil density.

**Unit 3****[5 Lectures]**

Analysis of water: Definition of pure water, sources responsible for contaminating water, water sampling methods, water purification methods, determination of pH, acidity and alkalinity of a water sample, determination of dissolved oxygen (DO) of a water sample, analysis of total hardness, analysis of total suspended solid, analysis of total dissolved solid, analysis of oil & grease in water.

**Unit 4****[4 Lectures]**

Analysis of food products: nutritional value of foods, idea about food processing and food preservations and adulteration, identification of adulterants in some common food items like coffee powder, asafoetida, chilli powder, turmeric powder, coriander powder and pulses, etc.; analysis of preservatives and colouring matter.

**Unit 5****[4 Lectures]**

Chromatography: Definition, general introduction on principles of chromatography, paper chromatography, TLC etc.; paper chromatographic separation of mixture of metal ion ( $\text{Fe}^{3+}$  and  $\text{Al}^{3+}$ ), comparison of paint samples by TLC method; column, ion-exchange chromatography etc., determination of ion exchange capacity of anion / cation exchange resin (using batch procedure if use of column is not feasible).

**Unit 6****[4 Lectures]**

Analysis of cosmetics: Major and minor constituents and their function; analysis of deodorants and antiperspirants, Al, Zn, boric acid, chloride, sulphate; determination of constituents of talcum powder: Magnesium oxide, Calcium oxide, Zinc oxide and Calcium carbonate by complexometric titration.

**Unit 7****[2 Lectures]**

Applications: to study the use of phenolphthalein in trap case, to analyze arson accelerants; to carry out analysis of gasoline.

## Unit 8

[6 Lectures]

Instrumental demonstrations: Estimation of macro nutrients: Potassium, Calcium, Magnesium in soil samples by flame photometry, Spectrophotometric determination of Iron in Vitamin / Dietary Tablets, Spectrophotometric Identification and Determination of Caffeine and Benzoic Acid in Soft Drink.

### Text Book(s)

1. Day, R. A. and Underwood, A. L. *Quantitative Analysis*, 6<sup>th</sup> Edn., (Prentice Hall of India, 1991).
2. Skoog, D. A., Holler F. J. and Nieman, T. A. *Principles of Instrumental Analysis*, 6<sup>th</sup> Edn., (Cengage Learning India Ed, 2014).
3. Skoog, D. A.; West, D. M. and Holler, F. J. *Fundamentals of Analytical Chemistry*, 9<sup>th</sup> Edn., (Saunders College Publishing, Fort Worth, 2013).
4. Svehla, G. and Sivasankar, B. *Vogel's Qualitative Inorganic Analysis*, 7<sup>th</sup> Edn., (Pearson Education, 2012).
5. Mendham, J., Denney, R. C., Barnes, J. D., Thomas, M. and Sivasankar, B. *Vogel's Quantitative Chemical Analysis*, 6<sup>th</sup> Edn., (Pearson Education, 2009).

### Reference Book(s)

1. Robinson, J.W. *Undergraduate Instrumental Analysis* 7<sup>th</sup> Edn., (Marcel Dekker, Inc., New York 2014).
2. Dean, J. A. *Analytical Chemistry Notebook*, 2<sup>nd</sup> Edn., (McGraw Hill, 2004).
3. Swaddle, T. W., *Applied Inorganic Chemistry*, (University of Calgary Press, 1990).

## SEMESTER V

CI 301

Physical Chemistry-III

L 3 T 0 P 0 CR 3

### Course outcomes:

After completion of the course, the learner shall be able to understand:

CO1: Fundamentals of equilibrium and equation of states

CO2: Thermodynamic descriptions of pure condensed phase and their mixtures

CO3: Different colligative properties

CO4: Phases, components, Gibbs phase rule, Phase diagrams and applications

### **Course Content:**

#### **Unit 1**

Thermodynamics and Equilibrium: **[15 Lectures]**

Open system, chemical potential and activity, partial molar quantities, chemical potential in terms of Gibb's free energy and other thermodynamic state functions and its variation with temperature and pressure, variation of thermodynamic functions for systems with variable composition (Equations of states for these systems), Gibbs-Duhem equation, variation of thermodynamic functions for systems with variable composition, equations of states for these systems.

Fugacity of gases and fugacity coefficient, standard states of real gases, relation between fugacity and pressure.

Thermodynamic conditions for equilibrium, van't Hoff's reaction isotherm (deduction from chemical potential), equilibrium constant and standard Gibbs free energy change, definitions of  $K_p$ ,  $K_c$  and  $K_x$ ; shifting of equilibrium due to change in external parameters e.g. temperature and pressure, Le Chatelier's principle.

Nernst's distribution law, finding out  $K_{eq}$  using Nernst distribution law for different reactions ( $KI + I_2 = KI_3$  and dimerization of benzene).

Pure ideal gas-its chemical potential and other thermodynamic functions and their changes during a change, Thermodynamic parameters of mixing, chemical potential of an ideal gas in an ideal gas mixture, concept of standard states and choice of standard states of ideal gases.

**Unit 2** **[6 Lectures]**

Condensed Phase: Chemical potential of pure solid and pure liquids, Ideal solution, Ideally dilute solution, Definition, Raoult's law, Henry's law, Mixing properties of ideal solutions, chemical potential of a component in an ideal solution, Choice of standard states of solids and liquids.

Activity, the solvent activity, the solute activity (ideal-dilute solution and real solutes), Activities in terms of molalities, activity coefficients of electrolyte/ion in solution,

Solubility equilibrium and influence of common ions and indifferent ions thereon, pH, buffer solution, buffer capacity, salt hydrolysis (detailed treatment).

### **Unit 3**

**[5 Lectures]**

Colligative Properties: relative lowering of vapour pressure, elevation of boiling point, depression of freezing point, osmotic pressure and their thermodynamic interpretation, applications in calculating molar masses of normal, dissociated and associated solutes in solution.

### **Unit 4**

**[10 Lectures]**

Phase Equilibrium: Definitions of phase, component and degrees of freedom, Phase rule and its derivations, Definition of phase diagram, Phase diagram of component system ( $H_2O$ , S and  $CO_2$ ), two component system, first order phase transition and Clapeyron equation, Clausius-Clapeyron equation -derivation and use, liquid vapour equilibrium for two component systems (phenol-water system), three component systems (water-chloroform-acetic acid system), triangular plots, principle of fractional distillation, Azeotropic solution, Liquid-liquid phase diagram (phenol- water system), Solid-liquid phase diagram, Eutectic mixture, congruent and incongruent melting.

### **Text Book(s)**

1. Atkins, P. and Paula, J. de. *Atkins' Physical Chemistry*, 10<sup>th</sup> Edn., (Oxford University Press, New Delhi, 2014).
2. Silbey, R. J., Alberty, R. A. and Bawendi, M. J. *Physical Chemistry*, 4<sup>th</sup> Edn., (Wiley, 2004).
3. Barrow, G. M. *Physical Chemistry*, 5<sup>th</sup> Edn., (Tata McGraw Hill Education, 2006 ).
4. Levine, I. N., *Physical Chemistry*, 6<sup>th</sup> Edn., (McGraw Higher Ed, 2008).

### **Reference Book(s)**

1. Laidler, K. J., Meiser, J. H. and Sanctuary, B. C., *Physical Chemistry*, 4<sup>th</sup> Edn., (Brooks Cole, 2002).
2. McQuarrie, D. A. and Simon, J. D., *Physical Chemistry: A Molecular Approach*, (University Science Books, 1997).
3. Mortimer, R. G. *Physical Chemistry*, 3<sup>rd</sup> Edn., (Elsevier, 2008).



**Course outcomes:**

After completion of the course, the learner shall be able to understand:

C01: Conformational analysis of acyclic systems and concept of prostereoisomerism

C02: Conformation of cycloalkanes and reactivity of cyclohexane derivatives

C03: Basic concepts of amino acids, proteins and heterocycles

C04: Organic photochemistry and pericyclic reactions

**Course Content:****Unit 1****[4 Lectures]**

Stereochemistry-2: Conformation of acyclic systems, free and restricted rotation, Rotamers, their stability and nomenclature, concept of topicity and prostereoisomerism, Diastereomerism.

**Unit 2****[8 Lectures]**

Stereochemistry-3: Cycloalkanes and Conformational Analysis: Types of cycloalkanes and their relative stability, Baeyer strain theory, cyclohexane, mono and disubstituted cyclohexanes: chair, boat and twist boat forms; relative stability with energy diagrams, symmetry properties and optical activity, conformation & reactivity in cyclohexane system: elimination ( $E_2$ ), rearrangement, nucleophilic substitution ( $S_N1$ ,  $S_N2$ , NGP), oxidation of cyclohexanol, esterification, saponification, lactonisation.

**Unit 3****[6 Lectures]**

Amino acids and proteins: Amino acids: Synthesis: (Strecker, Gabriel, acetamido malonic ester, azlactone), isoelectric point, ninhydrin reaction, Peptides: peptide linkage, synthesis of peptides using N-protection & C-protection, solid phase synthesis, peptide sequence: C-terminal and N-terminal amino acid determination.

Proteins: Amino acids-properties, reactions; peptides, importance of proteins, primary, secondary and tertiary structure of proteins, denaturation, isoelectric point.

**Unit 4****[6 Lectures]**

Heterocycles (monocyclic and bicyclic) with one heteroatom: Heterocyclic compounds: furan, pyrrole, thiophene, pyridine, indole, quinoline and isoquinoline synthesis, structure and bonding, properties.

**Unit 5****[6 Lectures]**

Organic photochemistry: Theory of photochemistry, Jablonski diagram, Frank-Condon principle, Photosensitisers, Einstein's law of photochemical equivalence, typical photoreactions such as photoreaction of benzophenone, photolytic reactions of ketones.

**Unit 6****[6 Lectures]**

Pericyclic reactions: Basic concepts of pericyclic reaction and examples of electrocyclic, cycloaddition and sigmatropic rearrangements reactions, FMO analysis and Woodward Hoffmann selection rules for [2+2] cycloaddition reaction.

**Text Book(s)**

1. Sengupta, S. *Basic Stereochemistry of Organic Molecules*, 1<sup>st</sup> Edn., (Oxford University Press, 2014).
2. Finar, I. L. *Organic Chemistry* (Volumes 1 and 2), 6<sup>th</sup> Edn., (Pearson Education, 2002).
3. Clayden, J., Greeves, N., Warren, S. and Wothers, P. *Organic Chemistry*, 2<sup>nd</sup> Edn., (Oxford University Press, 2012).
4. Sankararaman, S. *Pericyclic reactions—a textbook: reactions, applications and theory*, 1<sup>st</sup> Edn., (Wiley VCH, 2005).
5. Rohatgi-Mukherjee, K. K. *Fundamentals of Photochemistry*, 2<sup>nd</sup> Revised Edn., (New Age international Publishers, 2006).

**Reference Book(s)**

1. Eliel, E. L., Wilen, S. H. and Doyle, M. P. *Basic Organic Stereochemistry*, 1<sup>st</sup> Edn., (Wiley-Interscience, 2001).

2. Kalsi, P. S. *Stereochemistry, Conformation and Mechanism* (New Age international Publishers, 2009).
3. Fleming, I. *Molecular Orbitals and Organic Chemical Reactions*, (Oxford University Press, 2010).
4. Turro, N J., Ramamurthy, V. and Scaiano, J. C. *Modern Molecular Photochemistry of Organic Molecules*, (University Science Books, CA, 2010).

**CI 305**

**Inorganic Chemistry-III**

**L 3 T 0 P 0 CR 3**

**Course outcomes:**

On completion of this course the students will be able to understand:

CO1: The synthesis, structure and bonding analysis of interhalogen, pseudohalogens, xenon and other noble gas compounds

CO2: General properties of 3d transition elements and their comparison with 4d and 5d elements

CO3: Crystal Field Theory (CFT) and crystal field stabilization energy (CFSE)

CO4: Jahn Teller Effects, Term symbol and Orgel diagram

CO5: Basic concept of magnetism viz magnetic dipole, magnetic moment, magnetic susceptibility, magnetic flux and intensity, Bohrs magneton

**Course Content:**

**Unit 1**

**[8 Lectures]**

The chemistry of the halogens and the noble gases: Halogen family: Electronic structure and valences, preparation, interhalogen compounds, polyhalides, pseudohalogens, charge transfer complexes of halogens, oxides and oxoacids of halogens.

**Unit 2**

**[6 Lectures]**

Noble gas family: Atomic and physical properties of the elements, compounds of xenon, bonding in noble gas compounds, compounds of other noble gases.

**Unit 3**

**[14 Lectures]**

Aspects of d- block elements: Elements of first transition series and their comparison with the second and third series, general periodic trends, chemistry of various oxidation

states of first row transition metals and their comparison based on electronic configuration. Crystal Field Theory (CFT): Crystal field splitting of d-orbitals in octahedral, square planar and tetrahedral complexes. CFSE, factors affecting the magnitude of  $\Delta$ , strong and weak field ligands and spectrochemical series, distortion of octahedral complexes and Jahn-Teller Effect, Term symbols and Orgel diagram.

#### Unit 4

[8 Lectures]

Magnetic properties of transition metal complexes: Dia-, para-, ferro- and antiferromagnetic behaviour of compounds, Curie-Weiss law, Curie temperature, Neel temperature.

#### Text Book(s)

1. Huheey, J. E., Keiter, E. A., Keiter, R. L. and Medhi, O. K. *Inorganic Chemistry: Principles of Structure and Reactivity*, 4<sup>th</sup> Edn., (Pearson Education, 2006).
2. Overton, T., Armstrong, F., Rourke, J. and Weller, M. *Inorganic Chemistry*, 6<sup>th</sup> Edn., (Oxford University Press, 2015).

#### Reference Book(s)

1. Greenwood, N. N. and Earnshaw, A. *Chemistry of the Elements*, 2<sup>nd</sup> Edn., (Pergamon Press, 1997).
2. Cotton, F. A., Wilkinson, G., Murillo, C. A. and Bochmann, M. *Advanced Inorganic Chemistry*, 6<sup>th</sup> Edn., (John Wiley, 2007).

CI 307

Quantum Chemistry

L 3 T 0 P 0 CR 3

#### Course outcomes:

After completion of the course, the learner shall be able to understand:

CO1: Drawbacks of classical mechanics and the origin of quantum theory

CO2: Postulates of quantum mechanics. concept of wave functions, operators and eigen value equation

CO3: Wave mechanics of different model system in describing the real system

CO4: Valence bond and molecular orbital theory

C05: Approximation methods for the solution of the Schrodinger equation for many body system.

**Course Content:**

**Unit 1** **[4 Lectures]**

Origin of the quantum theory of matter: Franck- Hertz experiment, Photoelectric effect, Compton Effect, Black body radiation, Planck's law, Wein's law, Bohr's theory and atomic spectra.

**Unit 2** **[2 Lectures]**

Matter wave: Wave-particle duality, uncertainty principle.

**Unit 3** **[8 Lectures]**

Operators and wave functions in quantum mechanics: Operator principles, Hamiltonian and Hermitian operators, postulates of quantum mechanics, Schrödinger equation, free particle, particle in a box (one and three dimensional).

**Unit 4** **[8 Lectures]**

Wave mechanics of simple systems: One dimensional harmonic oscillator, rigid rotator, the hydrogen atom, angular momentum, electron spin, spin-orbit coupling.

**Unit 5** **[6 Lectures]**

Molecular orbital theory: Born-Oppenheimer approximation, LCAO approximation, LCAO MO of  $H_2$  and  $H_2^+$ , VB Theory, comparison of VB and MO.

**Unit 6** **[4 Lectures]**

Approximate methods: Basic idea of variation and perturbation theory.

**Unit 7** **[4 Lectures]**

Many electron wave function: Basic idea of Hartree Fock wave function and SCF MO.

**Text Book(s)**

1. Levine, I. N. *Quantum Chemistry*, 7<sup>th</sup> Edn., (Pearson, 2013).
2. Chandra, A. K. *Introductory Quantum Mechanics*, 3<sup>rd</sup> Edn., (Tata McGraw Hill Publishing Company, New Delhi, 2002).

**Reference Book(s)**

1. Kauzmann, W. *Quantum Chemistry: An Introduction* (Academic Press, 2013).
2. Prasad, R. K. *Quantum Chemistry* (New Age, 2010).
3. Atkins, P. W. and Friedman, R. S. *Molecular Quantum Mechanics* (Oxford University Press, 2010).

**CI 309****Chemistry laboratory-V****L O T O P 4 C R 8****Course Content:****Unit 1**

Inorganic: Inorganic preparations, Gravimetric estimation of copper and Nickel, Paper chromatographic separation of Ag(I), Hg(II) and Pb(II) ions.

**Unit 2**

Organic: Qualitative Analysis of solid and liquid organic compounds containing one or more functional groups.

**Unit 3**

Two step organic preparation using common reagents such as Benzil-Benzilic acid rearrangement, Beckman rearrangement etc.

**Unit 4**

Physical: Rate constant at elevated temperatures, energy of activation, Polarimetry, Partition function, Critical solution temperature etc.

### **Text Book(s)**

1. Mendham, J., Danney, R. C., Barnes, J. D. and Thomas, M. *Vogel's Textbook of Quantitative Chemical Analysis* (Peterson Education, 2004).
2. Viswanathan, B. and Raghavan, P. S. *Practical Physical Chemistry* (Viva Books Pvt. Ltd., 2005).

### **Reference Book(s)**

1. Furniss, B. S., Ford, A. J. H., Smith, P. W. H. and Tatchell, A., R. *Vogel's Textbook of Practical Organic Chemistry*, 5<sup>th</sup> Edn., (John Wiley, 1989).
2. Gurdeep, R. *Advanced Practical Inorganic Chemistry*, (Krishna Prakashan, 2013).

**CI 311                      Green Methods in Chemistry**

**L 3 T 0 P 0 CR 3**

### **Course outcomes:**

After completion of the course, the learner shall be able to know:

CO1. The basic idea of green chemistry

CO2. Twelve principles of green chemistry with special emphasis on the design of green synthesis

CO3. Some typical examples of green synthetic techniques

### **Course Content:**

#### **Unit 1**

**[4 Lectures]**

Introduction: Definitions of Green Chemistry, need for Green Chemistry, goals of Green Chemistry, limitations/ obstacles in the pursuit of the goals of Green Chemistry

#### **Unit 2**

**[20 Lectures]**

Principles of Green chemistry and designing a chemical synthesis: Twelve principles of Green Chemistry with their explanations, designing a green synthesis using these principles, Prevention of Waste/ byproducts, maximum incorporation of the materials used in the process into the final products, Atom Economy, calculation of atom economy of the rearrangement, addition, substitution and elimination reactions.

Prevention/ minimization of hazardous/ toxic products reducing toxicity.

Green solvents– supercritical fluids, water as a solvent for organic reactions, ionic liquids, fluoruous biphasic solvent, PEG, solventless processes, immobilized solvents and how to compare greenness of solvents.

Energy requirements for reactions – alternative sources of energy: use of microwaves and ultrasonic energy.

Selection of starting materials, avoidance of unnecessary derivatization – careful use of blocking/protecting groups.

Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents, catalysis and green chemistry, comparison of heterogeneous and homogeneous catalysis, biocatalysis, asymmetric catalysis and photocatalysis.

Prevention of chemical accidents designing greener processes, inherent safer design, principle of ISD “What you don’t have cannot harm you”, greener alternative to Bhopal Gas Tragedy (safer route to carcarbaryl) and Flixiborough accident (safer route to cyclohexanol) subdivision of ISD, minimization, simplification, substitution, moderation and limitation.

Strengthening/ development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

### **Unit 3**

**[12 Lectures]**

Examples of Green Synthesis/Reactions and some real world cases: Surfactants for carbon dioxide-Replacing smog producing and ozone depleting solvents with CO<sub>2</sub> for precision cleaning and dry cleaning of garments.

Designing of environmentally safe marine antifoulant.

Rightfit pigment: Synthetic azo pigments to replace toxic organic and inorganic pigments.

An efficient, green synthesis of a compostable and widely applicable plastic (polylactic acid) made from corn.

### **Text Book(s)**

1. Ahluwalia, V. K. and M. R. Kidwai, *New Trends in Green Chemistry*, (Anamalaya Publishers, 2012).



- Anastas, P. T. and Warner, J. K. *Green Chemistry - Theory and Practical*, (Oxford University Press, 2005).
- Cann, M.C. and Connely, M. E. *Real-World cases in Green Chemistry*, (American Chemical Society, Washington, 2000).

### Reference Book(s)

- Matlack, A. S. *Introduction to Green Chemistry*, 2<sup>nd</sup> Edn., (Marcel Dekker, 2010).
- Ryan, M. A. and Tinnesand, M. *Introduction to Green Chemistry*, (American Chemical Society, Washington, 2002).
- Lancaster, M. *Green Chemistry: An Introductory Text*, 2<sup>nd</sup> Edn., (RSC Publishing, 2010).

**CI 313**

**Industrial Chemistry**

**L 3 T 0 P 0 CR 3**

### Course outcomes:

After completion of the course, the learner shall be able to learn:

CO1: The basics of unit operations involved in different industrial processing.

CO2: Processes involved in different industries like oil, petrochemical, coal, agrochemical, cement, tea industries.

### Course Content:

#### Unit 1

**[6 Lectures]**

Unit operations - distillation, extraction, leaching and drying, unit process in organic synthesis - sulfonation, chlorination, nitration, oxidation, hydrogenation and hydrolysis.

#### Unit 2

**[2 Lectures]**

Process water, DM water, steam, industrial gases.

#### Unit 3

**[4 Lectures]**

Petroleum: Origin and history of petroleum, exploration, reservoir conditions, core, formation water, production, produced water, secondary enhanced oil recovery, drilling fluid, oil-field chemicals, tertiary enhanced oil recovery, transportation of petroleum.

**Unit 4** **[4 Lectures]**

Petrochemicals: refining, composition of petroleum, hydrotreating, cracking of oil, reforming, isomerization, unleaded oil, cracking of natural gas, petrochemicals.

**Unit 5** **[4 Lectures]**

Coal: origin and classification of coal, desulphurization, production of coal chemicals.

**Unit 6** **[4 Lectures]**

Agrochemicals: production of ethanol and methanol, cellulosic products - pulp & paper.

**Unit 7** **[4 Lectures]**

Tea industry - processing of tea, natural fiber- eri and muga production and processing.

**Unit 8** **[4 Lectures]**

Polymers: raw materials, polymer processing, paints, rubber.

**Unit 9** **[4 Lectures]**

Cement – production, various grades of cement, analysis and testing of cement Fertilizer - raw materials and process, sulfuric acid, iron and steel – various grades of products, glass and ceramics, dyes – raw materials and process, dyeing, detergents – raw materials, production, specification and detergency, chlor-alkali industry, electrochemical industry, pharmaceutical industry, fats and oils, fat hardening. Statistical methods for analysis of quality of product, hazards and risk analysis of industry, pollution of air, water and soil, remediation.

**Text Book(s)**

1. Heaton, A. *The Chemical Industry*, 2<sup>nd</sup> Edn., (Blackie Academic, 1996).
2. Thompson, R. *Industrial Inorganic Chemicals: Production and Uses* (Royal Soc. of Chem., 1995).

**Reference Book(s)**

1. Kent, J. A. *Kent and Riegel's Handbook of Industrial Chemistry and Biotechnology*, (Springer, 2010).
2. Speight, J. G. *The Chemistry and Technology of Petroleum*, 5<sup>th</sup> Edn., (Dekker, 2014).
3. Dawe, R. A. *Modern Petroleum Technology*, **Vol. 1** (Upstream), 6<sup>th</sup> Edn., (John Wiley., 2002).
4. Lucas, A. G. *Modern Petroleum Technology*, **Vol. 2** (Downstream), 6<sup>th</sup> Edn., (John Wiley., 2002).

**CI 302**

**Physical Chemistry-IV**

**L 3 T 0 P 0 CR 3**

**Course outcomes:**

After completion of the course, the learner shall be able to understand:

CO1: Transport processes in liquid phase and factors affecting the transport processes

CO2: Basic principle of laws of electrochemistry.

CO3: Understanding about electro chemical cells and cell reactions, electrode potential , potentiometric titration

CO4: Basics of colloidal dispersion

**Course Content:**

**Unit 1**

**[8 Lectures]**

Transport processes: Diffusion processes: Flux, force, Fick's laws, phenomenological coefficients & their inter-relationship (general form), different examples of transport properties.

General features of fluid flow (streamline flow and turbulent flow), Reynold number, nature of viscous drag for streamline motion, Newton's law of viscosity, viscosity coefficient, Poiseuille's equation (with derivation), temperature dependence of viscosity, principle of determination of viscosity coefficient of liquids by falling sphere method.

**Unit 2**

**[20 Lectures]**

Electrochemistry:

Ionics: Ion conductance, Conductance and measurement of conductance, cell constant, specific conductance and molar conductance, Variation of specific and equivalent

conductance with dilution for strong and weak electrolytes, Kohlrausch's law of independent migration of ions, Equivalent and molar conductance at infinite dilution and their determination for strong and weak electrolytes, Ostwald's dilution law, Ionic mobility, Debye-Huckel theory of Ion atmosphere (qualitative)-asymmetric effect, Transport number, Principles of Hittorf's and Moving-boundary method, relaxation effect and electrophoretic effect, Wien effect, Debye-Falkenhagen effect, Walden's rule Application of conductance measurement (determination of solubility product and ionic product of water), Conductometric titrations.

Electrodics: Types of electrochemical cells and examples, cell reactions, emf and change in free energy,  $\Delta H$  and  $\Delta S$  of cell reactions from emf measurements, Thermodynamic derivation of Nernst equation, Standard cells, Half-cells / electrodes, different types of electrodes (with examples), Standard electrode potential (IUPAC convention) and principles of its determination, types of concentration cells, Liquid junction potential and its minimisation.

Glass electrode and determination of pH of a solution, Ion-selective electrodes, Potentiometric titrations (acid-base and redox).

Electrical double layer, polarization and overvoltage.

Batteries, fuel cell, corrosion and its prevention.

### **Unit 3**

**[8 Lectures]**

Definition of colloids and crystalloids, classification of colloids, preparation and purification techniques of colloidal dispersion, Tyndall effect, Brownian movement, electrophoresis, electro-osmosis, protective colloids, gold number, zeta potential, lyophobic and lyophilic sols, origin of charge and stability of lyophobic colloids, coagulation and Schultz-Hardy rule, Zeta potential, DLVO theory, electrokinetic phenomenon (qualitative idea only), amphiphiles, surfactants, micelles, critical micelles concentration, emulsions, microemulsions, gels.

### **Text Book(s)**

1. Atkins, P. and Paula, J. de. *Atkins' Physical Chemistry*, 10<sup>th</sup> Edn., (Oxford University Press, New Delhi, 2014).

2. Levine, I. N., *Physical Chemistry*, 6<sup>th</sup> Edn., (McGraw Higher Ed, 2008).
3. Laidler, K. J., Meiser, J. H. and Sanctuary, B. C. *Physical Chemistry*, 4<sup>th</sup> Edn., (Brooks Cole, 2002).
4. Silbey, R. J., Alberty, R. A. and Bawendi, M. J. *Physical Chemistry*, 4<sup>th</sup> Edn., (Wiley 2004).

#### Reference Book(s)

1. Adamson, A. A. *A Textbook of Physical Chemistry*, 2<sup>nd</sup> Edn., (Elsevier, 1973).
2. Glasstone, S. *An introduction to Electrochemistry*, (Maurice Press, 2008).
3. Bockris, J. O. M. and Reddy, A. K. N. *Modern Electrochemistry*, Vol. 1 & 2 (Plenum Press, 2001).

**CI 304                      Organic Chemistry-IV**

**L 3 T 0 P 0 CR 3**

#### Course outcomes:

After completion of the course, the learner shall be able to understand:

CO1: Oxidations of alcohol, alkene and alkynes

CO2: Reduction involving hydrogenation, dissolving metal reducing agents and complex metal hydrides

CO3: Selected organic name reactions

CO4: Concept of retrosynthetic analysis

#### Course Content:

##### Unit 1

**[ 10 Lectures]**

Oxidation:

(A) Oxidation of alcohols to aldehydes/ketones/carboxylic acids:

Transition metal-based oxidants: Jones reagent, Collins Reagent, PCC, PDC,  $\text{KMnO}_4$ ,  $\text{MnO}_2$ ,  $\text{Mn}(\text{OAc})_3$ ,  $\text{RuCl}_3/\text{NaIO}_4$  ( $\text{RuO}_4$ ).

Dimethyl sulfoxide-based oxidation: Moffatt-Pfitzner Oxidation, Parikh-Doering Oxidation, Corey-Kim Oxidation, Swern Oxidation.

Other oxidants: Dess-Martin reagent, TEMPO, TPAP.

(B) Oxidation of alkenes/alkynes:

Ozonolysis,  $\text{KMnO}_4$ , Prévost dihydroxylation, Woodward dihydroxylation, Upjohn dihydroxylation, epoxidation by peroxy acids and related reagents

(C) Other oxidation processes: Allylic oxidation by  $\text{SeO}_2$ , Oxidation of aldehydes/ketones by  $\text{SeO}_2$ , Cleavage of 1,2-diols, Hunsdiecker reaction.

## Unit 2

[ 8 Lectures]

Reduction:

(A) Hydrogenation:  $\text{H}_2/\text{Pd-C}$ ,  $\text{H}_2/\text{Lindlar Catalyst}$ ,  $\text{H}_2/\text{Wilkinson's Catalyst}$ , transfer hydrogenation, diimide reduction.

(B) Dissolving Metal Reductions for: alkynes, aldehydes/ketones, esters,  $\alpha,\beta$ -unsaturated ketones, aromatic compounds (Birch reduction), Clemmensen Reduction.

(C) Aluminium-based reagents: lithium aluminum hydride (LAH), lithium trimethoxyaluminum hydride (LTBA), lithium tri-(*tert*-butoxy)aluminum hydride (LTBA), Sodium *bis*(2-methoxyethoxy)aluminum hydride (Red-Al), selectrides, diisobutylaluminum hydride, alane.

Boron-based reagents: Sodium borohydride, zinc Borohydride, lithium borohydride, sodium cyanoborohydride, sodium triacetoxyborohydride, borane.

(D) Other reduction processes: Wolff-Kishner reduction, Clemmensen Reduction, MPV reduction.

## Unit 3

[6 Lectures]

Selected important reactions: Aldol addition and condensation, directed aldol addition, Mukaiyama aldol addition, Robinson Annulation, Knoevenagel condensation, Perkin condensation, Stobbe condensation, Michael addition, Claisen condensation, Dieckmann condensation, acyloin condensation, Stork enamine reaction, Pinacol Coupling Reaction, McMurry Reaction, benzoin condensation, Stetter reaction, Wittig and related reactions, Nef carbonyl synthesis.

**Unit 4****[2 Lectures]**

Active methylene compounds: Preparation and synthetic applications of diethyl malonate and ethyl acetoacetate.

**Unit 5****[4 Lectures]**

Reactions involving free radical intermediates: Addition reaction (Peroxide effect), substitution reaction (allylic and benzylic halogenation), cyclization of free radical intermediates, Baldwin rules, fragmentation and rearrangement reactions by radical pathways.

**Unit 6****[ 6 Lectures]**

Retrosynthetic analysis: Basic concepts of retrosynthetic analysis, Analysis of one group disconnection approach for alcohol and keto compound, synthons, donor and acceptor synthons, functional group interconversion, C-C disconnections and synthesis, reconnection (1,6-di carbonyl), natural reactivity and umpolung, protection-deprotection strategy.

**Text Book(s)**

1. Clayden, J., Greeves, N., Warren, S. and Wothers, P. *Organic Chemistry*, 2<sup>nd</sup> Edn., (Oxford University Press, 2012).
2. Carey, F. A. and Sundberg, R. J. *Advanced Organic Chemistry, Part B: Reactions and Synthesis*, 5<sup>th</sup> Edn., (Springer, New York, 2007).
3. March, J. and Smith, M. B. *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, 6<sup>th</sup> Edn., (Wiley, 2007).

**Reference Book(s)**

1. Zweifel, G. S., Nantz, M. H. and Somfai, P. *Modern Organic Synthesis: An Introduction*, 2<sup>nd</sup> Edn. (Wiley, New York, 2017).
2. Norman, R. O. C. and Coxon, J. M. *Principles in Organic Synthesis*, 3<sup>rd</sup> Edn. (Blackie Academic & Professional, 1993).

**Course outcomes:**

On completion of this course the students will be able to understand:

CO1: Definition of organometallic chemistry, EAN and 18-electron rule

CO2: Preparation and bonding analysis of metal carbonyls, allyl, enals, carbenes, metallocene

CO3: Kinetic and thermodynamic stability of metal complexes, stability constants

CO4: Importance of metals in biological systems and heme-proteins

CO5: Nuclear stability, isotopes and laws of radioactivity, carbon dating

**Course Content:****Unit 1****[12 Lectures]**

Introduction to Organometallic Chemistry: Classification of ligands, EAN rule, preparation, properties and bonding of metal carbonyls and olefin complexes.  $\pi$ -allyl and enyl systems; Transition metal-carbon  $\sigma$ -bond: metal-alkyls, metal-carbenes, metal-carbynes, Metallocene.

**Unit 2****[10 Lectures]**

Metal-ligand equilibria in solution: Stepwise and overall formation constants. Factors affecting the stability of metal complexes, chelate effect, determination of binary formation constants, inert and labile complexes.

**Unit 3****[8 Lectures]**

Bioinorganic chemistry: Essential and trace elements in biological systems, heme-proteins- haemoglobin, myoglobin, dioxygen binding, co-operativity, Bohr effect, Picket-fence model.

**Unit 4****[6 Lectures]**



Nuclear chemistry: Nuclear stability, isotopes, isobars and isotones, laws of radioactivity, artificial radioactivity, nuclear fission and fusion, radiocarbon dating.

### **Text Book(s)**

1. Huheey, J. E., Keiter, E. A., Keiter, R. L. and Medhi, O. K. *Inorganic Chemistry: Principles of Structure and Reactivity*, 4<sup>th</sup> Edn., (Pearson Education, 2006).
2. Cotton, F. A., Wilkinson, G., Murillo, C. A. and Bochmann, M. *Advanced Inorganic Chemistry*, 6<sup>th</sup> Edn., (John Wiley, 2007).

### **Reference Book(s)**

1. Overton, T., Armstrong, F., Rourke, J. and Weller, M. *Inorganic Chemistry*, 6<sup>th</sup> Edn., (Oxford University Press, 2015).
2. Bertini, I., Gray, H. B., Lippard, S. J. and Valentine, J. S. *Bioinorganic Chemistry*, (Viva Books Pvt. Ltd., 2004).

## **CI 308 Principles of Spectroscopy**

**L 3 T 0 P 0 CR 3**

### **Course outcomes:**

After completion of the course, the learner shall be able to understand:

CO1: The basic principles involved in the interaction of electromagnetic radiation with matter.

CO2: Different types of spectra

CO3: Spectroscopic techniques like IR, UV-Vis, NMR and the theory involved.

CO4: Use of the spectroscopy in deducing the chemical structure.

### **Course Content:**

#### **Unit 1**

**[4 Lectures]**

Basic principle of spectroscopy: Interaction of matter and electromagnetic radiation, Factors affecting widths and intensity of spectral lines.

#### **Unit 2**

**[10 Lectures]**

IR spectroscopy: Principle, instrumentation, and applications of IR spectroscopy.

**Unit 3****[10 Lectures]**

Electronic spectroscopy: Basic principle, Lambert-Beer law, types of electronic transitions in organic molecules, applications in functional group detection.

**Unit 4****[12 Lectures]**

NMR spectroscopy: Origin of chemical shifts, factors affecting the chemical shifts and their Interpretation, spin-spin coupling, relaxation process.

**Text Book(s)**

1. Banwell, C. N. and McCash, E. M. *Fundamentals of Molecular Spectroscopy* (Tata McGraw Hill, 1994).
2. Kemp, W. *Organic Spectroscopy*, 3<sup>rd</sup> Edn., (McMillan Press, 1991).

**Reference Book(s)**

1. Silverstein, *Spectrometric Identification of Organic Compounds*, 7<sup>th</sup> Edn., (John Wiley & Sons, 2005).
2. Chandra, S. *Molecular Spectroscopy* (Narosa, 2009).

**CI 310****Chemistry Laboratory-VI****L O T O P 4 CR 4****Course Content:****Unit 1**

Computational practical

1. DOS, WINDOWS and UNIX operating systems

**Unit 2**

1. Programming with FORTRAN77

### Unit 3

1. Numerical methods in chemistry (using MS EXCEL)
2. Generation of an EXCEL chart to display the variation of the  $H_{1s}$  radial function with radial distance from the nucleus
3. Generation of an EXCEL chart to display the variation of the  $H_{2s}$  radial function with radial distance from the nucleus
4. Generation of an EXCEL chart to display the variation of the  $H_{2p}$  radial function with radial distance from the nucleus
5. EXCEL charts for the hydrogenic radial distribution functions

### Unit 4

1. Generation of the numerical radial wave function for the helium atom "1s" atomic orbital.
2. Generation of the numerical radial wave functions  $Li_{1s}$  and  $Li_{2s}$  orbitals etc.

### Unit 5

Quantum Chemical Calculations with GAUSSIAN and GAMESS

### Text Book(s)

1. Balagurusamy, E. *Numerical Methods*, (Tata McGraw-Hill Publishing Company Limited, 2002).
2. Billo, E. J. *Excel for Chemists: A Comprehensive Guide*, (Wiley-VCH, 2001).

### Reference Book(s)

1. Quinn, C. M. *Computational Quantum Chemistry: An Interactive Guide to Basis Set Theory*, (Academic Press, 2002).

CI 312 Introduction to Polymer Chemistry

L 3 T 0 P 0 CR 3

### Course outcomes:

After completion of the course, the learner shall be able to understand:

CO1: Basic concepts of polymers

CO2: Polymerization techniques and characterization of polymers

C03: Molecular weight and structure property relationship

C04: Properties of some important polymers

**Course Content:**

**Unit 1**

**[6 Lectures]**

Introduction: Historical background, basic nature and classification, importance of polymers as a class of material, polymer raw materials.

**Unit 2**

**[12 Lectures]**

Polymerization techniques: Special features of polymerization, step polymerization, radical chain polymerization, living and non-living chain polymerization, co-ordination polymerization, co-polymerization, ionic polymerization, ring opening polymerization, characterization of polymers, GPC, Spectroscopy of polymer, rheology.

**Unit 3**

**[8 Lectures]**

Structure-property relationship: Stereochemistry of polymers, modification of polymers, cross-linking, polymer architecture, polymer processing and fabrication, polymer composites.

**Unit 4**

**[8 Lectures]**

Natural and synthetic polymers: rubber, natural fibers, silk fibers, PS, Nylon, etc.

Applications of polymers: Applications and future prospects.

**Text Book(s)**

1. Gowarikar, V.R; Viswanathan, N.V. and Sreedhar, J. *Polymer Science* (Wiley-Eastern Limited, 1986).
2. Misra, G. S. *Introductory Polymer Chemistry* (Wiley Eastern Limited, 1993).

**Reference Book(s)**

1. Sperling, L.H. *Introduction to Physical Polymer Science* (Wiley-Interscience, 1986).
2. Odian, G. *Principles of Polymerization* (Wiley, 2004.)
3. Sun, S. F. *Physical Chemistry of Macromolecules*, 2<sup>nd</sup> Edn., (Wiley, 2004).

CI 314

Seminar

L 1 T 0 P 0 CR 1

Presentation by students on chosen topics in the consultation with the course instructor.

**SEMESTER-VII**

CI 401 Principles of Inorganic Chemistry

L 3 T 0 P 0 CR 3

**Course outcomes:**

On completion of this course the students will be able to understand:

CO1: Periodic properties of elements including lanthanides

CO2: Valence bond, molecular orbital theory and VSEPR model of inorganic systems

CO3: Fundamentals of group theory, Application of group theory in predicting the IR and Raman active vibrational modes, orbital symmetry and chemical reactions

CO4: Trace and essential metals in biological systems

CO5: Sodium potassium pump, heme and non-heme proteins and their biological importance

**Course Content:**

**Unit 1**

**[10 Lectures]**

Brief review of the following: Periodic properties, lanthanide contraction, ionic bonding, valence bond theory and LCAO-MO theory, orbital symmetry and overlap, bond energy and covalent radii, VSEPR model and Walsh diagram, Introduction to non-covalent interaction.

**Unit 2**

**[16 Lectures]**

Group theory: Symmetry elements and symmetry operations, symmetry groups, molecular dissymmetry and optical activity, symmetry point groups for compounds having co-ordination number 2 to 9, Historical development of Evariste Galois theory of

groups, matrix representation of groups, reducible and irreducible representation, the great orthogonality theorem, Direct product representation. Projection operator, symmetry adapted linear combination, vibrational modes as bases for group representation, symmetry selection rules for IR and Raman spectra, orbital Symmetry and Chemical reactions –Woodward and Hoffman rules for electrocyclic and cycloaddition reactions.

### Unit 3

[10 Lectures]

Bioinorganic chemistry: scope, inorganic elements in biological systems, basic bioenergetics, active transport of cations across membranes, Na<sup>+</sup>/K<sup>+</sup> pump, heme-proteins–haemoglobin and myoglobin: structure, thermodynamics and kinetics of oxygenation, Cytochrome P<sub>450</sub>, Hemerythrin, Ferritin and Transferrin.

### Text Book(s)

1. Cotton, F. A., Wilkinson, G., Murillo, C. A. and Bochmann, M. *Advanced Inorganic Chemistry*, 6<sup>th</sup> Edn., (John Wiley, 2007).
2. Huheey, J. E., Keiter, E. A., Keiter, R. L. and Medhi, O. K. *Inorganic Chemistry: Principles of Structure and Reactivity*, 4<sup>th</sup> Edn., (Pearson Education, 2006).

### Reference Book(s)

1. Cotton, F. A., *Chemical Application of Group Theory*, 3<sup>rd</sup> Edn., (John Wiley & Sons, 2008).
2. Bertini, I., Gray, H. B., Lippard, S. J. and Valentine, J. S. *Bioinorganic Chemistry*, (Viva Books Pvt. Ltd., 2004).

### CI 403 Chemical and Statistical Thermodynamics

L 3 T 0 P 0 CR 3

#### Course outcomes:

After completion of the course, the learner shall be able to understand:

CO1: Fundamentals of equilibrium thermodynamics

CO 2: Thermodynamics of phase transition and phase diagrams

CO3: Basics of statistical thermodynamics

CO4: Basics of non-equilibrium thermodynamics

## **Course Content:**

### **Unit 1**

**[12 Lectures]**

Brief review of thermodynamic functions and laws of thermodynamics: Temperature dependence of thermodynamic functions, Experimental determination of thermodynamic functions, Thermodynamic description of mixtures, Gibbs-Duhem equation, Chemical equilibrium, Thermodynamic description of phase transitions, Clapeyron-Claussius equation, Phase diagrams, Thermodynamics of nonideal systems – fugacity and activity concepts, excess properties.

### **Unit 2**

**[12 Lectures]**

Concepts of statistical thermodynamics, entropy and probability, ensembles, distribution laws of MB, FD and BE, partition functions and statistical formulation of macroscopic variables. Use of statistical thermodynamics including calculation of electrical and magnetic properties, and heat capacity of solids, application of BE statistics to helium.

### **Unit 3**

**[12 Lectures]**

Non-equilibrium thermodynamics, thermodynamic criteria for non-equilibrium states, Assumptions of non-equilibrium thermodynamics, uncompensated heat, entropy production and entropy flow, entropy balance, Onsager formalism, relation between forces and fluxes, transformations of generalized fluxes and forces, microscopic reversibility and Onsager's reciprocity relations.

Electrokinetic phenomena, diffusion, electric conduction, irreversible thermodynamics for biological systems, coupled reactions.

### **Text Book(s)**

1. Engel, T. and Reid, P. *Thermodynamics, Statistical Thermodynamics and Kinetics*, 2<sup>nd</sup> Edn., (Pearson, New Delhi, 2011).
2. Kalidas, C. and Sangaranarayanan, M. V. *Non-equilibrium Thermodynamics, Principles and applications*, (McMillan, New Delhi, 2002).

## Reference Book(s)

1. Atkins, P. and Paula, J. de. *Atkins' Physical Chemistry*, 10<sup>th</sup> Edn., (Oxford University Press, New Delhi, 2014).
2. Berry, R. Rice S. A. and Ross, J. *Physical Chemistry*, 2<sup>nd</sup> Edn., (Oxford, London, 2010).

**CI 407 Principles of Organic Chemistry**

**L 3 T 0 P 0 CR 3**

### Course outcomes:

After completion of the course, the learner shall be able to understand:

CO1: Understanding of structure-activity relationship of organic molecules.

CO2: Stereochemistry of organic molecules, prostereogenic elements and asymmetric synthesis.

CO3: Basic concepts of nucleophilic substitution, elimination, addition and neighbouring group participation reactions with stereochemical outcomes of products.

CO4: Chemistry of five, six and fused heterocyclic compounds

### Course content:

#### Unit 1

**[4 Lectures]**

Structure and Bonding: Reactivity of organic molecules, aromaticity, n-annulenes and hetero-annulenes, fullerenes (C<sub>60</sub>), Graphene, Cryptans, bonds weaker than covalent: addition compounds, inclusion compounds and rotaxenes.

#### Unit 2

**[3 Lectures]**

Thermodynamics and Kinetics: Acids and bases, concept of hard and soft acids and bases, symbiosis, labeling and kinetic isotope effects, Hammett equation,  $\sigma$ - $\rho$  relationship, non-classical carbenuim ion (or carbocation), kinetic and thermodynamic control, Hammand principle, Curtin-Hammett principle, transition state and intermediates.



**Unit 3****[10 Lectures]**

Stereochemistry: Chirality and isomerism in organic system, conformational analysis of simple cyclic and acyclic systems, conformation of saturated heterocycles, interconversion of Fischer, Newman and Sawhorse formula, *E-Z* isomerism, *R-S* nomenclature, diastereomerism in acyclic and cyclic systems, newer methods of asymmetric synthesis (including enzymatic and catalytic nexus), enantio-, and diastereoselective synthesis, determination of enantiomeric and diastereomeric excess, stereospecific synthesis, effect of conformation on reactivity, methods of resolution, optical purity, optical activity in absence of chiral atom, neighbouring group participation reactions and examples involving non-classical carbocation.

**Unit 4****[8 Lectures]**

General reaction mechanism, aliphatic substitution reaction,  $S_N1$ ,  $S_N2$ , mixed  $S_N1$  and  $S_N2$  and  $S_Ni$  reaction, SET reaction, classical and nonclassical carbocations, electrophilic substitution reaction,  $S_E1$ ,  $S_E2$ ,  $S_Ei$  mechanism, electrophilic and nucleophilic aromatic substitution reaction,  $S_NAr$ , Benzyne,  $SRN^1$  mechanism, reactivity, effect of substrate, leaving group and attacking nucleophile, elimination reaction,  $E^1$   $E^2$  and  $E^1Cb$ , protection-deprotection chemistry of selected functional groups such as aldehydes, ketone and  $-OH$ ,  $NH_2$ .

**Unit 5****[ 6 Lectures]**

Addition Reaction: Mechanism and stereochemical aspects of addition reaction in carbon-carbon multiple bonds, region and chemoselectivity, orientation and reactivity, mechanism of condensation reactions involving enolates- Aldol, cross Aldol, Knoevenagel, Claisen, Perkin and Stobbe reactions.

**Unit 6****[5 Lectures]**

Heterocyclic Chemistry:  $\pi$ -excessive and  $\pi$ -deficient heterocycles, synthesis, reactions and reactivity of heterocycles, e.g. furan, thiophene, pyrrole, pyridine, pyrazoles,

pyridazines, pyrimidines, isoxazoles, tetrazoles, quinoline, isoquinoline and indole, Skraup synthesis, Fischer-Indole synthesis, Vilsmeier-Heck formylation reaction.

### **Text Book(s)**

1. Carey, F. A. and Sundberg, R. J. *Advanced Organic Chemistry, Part A: Structure and Mechanisms*, 5<sup>th</sup> Edn., (Springer, New York, 2007).
2. Clayden, J., Greeves, N., Warren, S. and Wothers, P. *Organic Chemistry*, 2<sup>nd</sup> Edn., (Oxford University Press, 2012).
3. March, J. and Smith, M. B. *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, 6<sup>th</sup> Edn., (Wiley, 2007).
4. Sengupta, S. *Basic Stereochemistry of Organic Molecules*, 1<sup>st</sup> Edn., (Oxford University Press, 2014).
5. Kalsi, P. S. *Stereochemistry, Conformation and Mechanism*, (New Age international Publishers, 2009).
6. Finar, I. L. *Organic Chemistry (Volume 1)*, 6<sup>th</sup> Edn., (Pearson Education, 2002).

### **Reference Book(s)**

1. Sykes, P. *A Guide Book to Mechanism in Organic Chemistry*, 6<sup>th</sup> Edn., (Longman, 1986).
2. Carey, F. A. and Sundberg, R. J. *Advanced Organic Chemistry, Part B: Reactions and Synthesis*, 5<sup>th</sup> Edn., (Springer, New York, 2007).
3. Eliel, E. L., Wilen, S. H. and Doyle, M. P. *Basic Organic Stereochemistry*, 1<sup>st</sup> Edn., (Wiley-Interscience, 2001).
4. Zweifel, G. S., Nantz, M. H. and Somfai, P. *Modern Organic Synthesis: An Introduction*, 2<sup>nd</sup> Edn., (Wiley, New York, 2017).

**CI 409 Quantum Chemistry and Chemical Bonding-I**

**L 3 T 3 P 0 CR 3**

### **Course outcomes:**

After completion of the course, the learner shall be able to learn:

CO 1: Basic mathematics involved in quantum chemistry

CO2: Origin of quantum chemistry

CO3: The solution of the Schrodinger equation for different model systems and their correlation with real systems

CO4: Approximate methods used in the solution of Schrodinger equations

### **Course Content:**

#### **Unit 1**

**[10 Lectures]**

Mathematical Review: Basic vector algebra, matrix, determinant, eigen value equations, quantum mechanical operators, orthogonal functions, Schmidt's orthogonalization technique.

#### **Unit 2**

**[14 Lectures]**

Planck's quantum theory, wave-particle duality, uncertainty principle, postulates of quantum mechanics, Schrödinger equation, free particle, particle in a box, degeneracy, harmonic oscillator, rigid rotator, the hydrogen atom, angular momentum, electron spin, spin-orbit coupling.

#### **Unit 3**

**[12 Lectures]**

Approximate methods in quantum mechanics: The variation theorem, linear variation principle and perturbation theory (first order and non-degenerate), application of variation method and perturbation theory to the Helium atom, antisymmetry, Slater determinant, term symbols and spectroscopic states.

### **Text Book(s)**

1. Atkins, P. W. and Friedman, R. S., *Molecular Quantum Mechanics*, (Oxford University Press, 1997).
2. Levine, I. N *Quantum Chemistry*, (Pearson Education Inc., 2004).

## Reference Book(s)

1. McQuarrie, D. A. *Quantum Chemistry* 2<sup>nd</sup> Edn., (University Science Books, 2007).
2. Prasad, R. K. *Quantum Chemistry* (New Age, 2010).

## CI 411 Principles and Applications of Spectroscopy

L 3 T 3 P 0 CR 3

### Course outcomes:

On completion of this course the students will be able to understand:

CO 1: Basic principles of spectroscopy, interaction of electromagnetic radiation with matter, atomic and molecular spectroscopy

CO 2: Selection rules and allowed transitions, factors effecting the molecular and electronic transitions

CO 3: Different laws and principles like Beer-Lamberts Law, Frank-Condon principle, Woodward-Fieser rules, Raman Effect, Mössbauer effect, Mc-Lafferty rule etc.

CO 4: Different spectroscopic parameters like absorption wavelength, peak intensity, peak half width, chemical shift value, g-value, isomer shift value

CO 5: Basic principles and instrumentation of various spectroscopic techniques viz FTIR, Raman, UV-vis, NMR including 2D, ESR, Mössbauer spectroscopy and Mass spectrometry

### Course Content:

#### Unit 1

[8 Lectures]

Rotational and Vibrational spectra: Basic principles, selection rule, fundamental vibrations, Raman effect, identification of some representative organic and inorganic compounds.

#### Unit 2

[5 Lectures]

Electronic spectra: Frank-Condon principle, Fluorescence, Phosphorescence, electronic spectra of diatomic molecules, chromophores, auxochromes, absorption and intensity shifts, solvent effects, Woodward Fieser rules.

**Unit 3****[10 Lectures]**

Nuclear Magnetic Resonance Spectroscopy: Basic principles, origin of chemical shifts, factors affecting the chemical shifts and their interpretation, spin-spin coupling, relaxation processes, coupling constants, Nuclear Overhauser effect (NOE) 2D-NMR, DEPT, HMQC, HMBC,  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{31}\text{P}$ ,  $^{15}\text{N}$  and  $^{19}\text{F}$  NMR spectra of selected compounds, Shift reagents, spin tickling.

**Unit 4****[3 Lectures]**

Mass spectrometry: Basic principles and instrumentation, mass spectral fragmentation of organic compounds, applications to organometallic compounds.

**Unit 5****[5 Lectures]**

EPR spectroscopy: Basic principles, origin of g-shifts, hyperfine and super hyperfine coupling, spin orbit coupling, line shape, zero field splitting, Kramer degeneracy, ESR analysis of organic compounds, transition metal complexes of vanadium, copper, cobalt and iron.

**Unit 6****[5 Lectures]**

Mössbauer spectroscopy: Nuclear resonance absorption, recoil energy, Doppler effect, Mössbauer effect, Isomer shift, quadruple interactions, effect of magnetic field, determination of oxidation states of iron (including bioinorganic systems, ferredoxins) tin and cobalt compounds.

**Text Book(s)**

1. Banwell, C. N. and McCash, E. M. *Fundamentals of Molecular Spectroscopy*, (Tata McGraw Hill, 1994).
2. Pavia, D. L., Lampman, G. M., Kriz, G. S. and Vyvyan, J. R. *Introduction to Spectroscopy*, (Cengage India, 2015).

**Reference Book(s)**

1. Drago, R. S. *Physical Methods for Chemistry*, (Saunders Company, 1992).
2. Nakamoto, K. *Infrared and Raman Spectra: Inorganic and Coordination Compounds*, 6<sup>th</sup> Edn., (John Wiley, 2009).
3. Dutta, R.L. and Syamal, A. *Elements of Magnetochemistry*, 2<sup>nd</sup> Edn., (East West Press, 1993).

## **CI 405 Laboratory Course in Organic Chemistry**

**L O T O P 6 CR 6**

### **Unit 1**

Separation techniques of organic compounds and their spectroscopic identification.

Experiments involving the separation and purification of organic compounds from a mixture, using chromatographic techniques, steam distillation, fractional crystallization and sublimation.

### **Unit 2**

Synthesis of organic compounds using common reagents: At least eight preparation (involving two or more than two steps) involving the following representative reactions: (a) Oxidation of alcohol, (b) Reduction of carbonyl group, (c) Nucleophilic substitution, (d) Cycloaddition reaction, (e) Condensation reaction, (f) Aromatic electrophilic substitution, (g) Preparation of dyes, (h) Heterocyclic synthesis, (i) Solid phase synthesis etc.

### **Unit 3**

Natural product extraction: Caffeine, Nicotine, Carotenoides etc.

### **Unit 4**

Estimation of glucose, acetic acid in vinegar, -OH groups etc.

### **Unit 5**

Determination of acid value and saponification value of fat/ oil.

## Unit 6

Green experiments

### Text Book(s)

1. Pasto, D., Johnson and Miller, M. *Experiments and Techniques in Organic Chemistry*, (Prentice Hall, 1992).
2. Williamson, K. L. *Macroscale and Microscale Organic Experiments*, (D. C. Heath & Company, 1999).

### Reference Book(s)

1. Furniss, B. S., Ford, A. J. H., Smith, P. W. H. and Tatchell, A. R. *Vogel's Textbook of Practical Organic Chemistry*, 5<sup>th</sup> Edn., (Wiley, 1989).

## SEMESTER-VIII

**CI 408                      Chemistry of Transition Elements**

**L 3 T 0 P 0 CR3**

### Course outcomes:

On completion of this course the students will be able to understand:

CO1: Crystal Field and Ligand Field theory of transition metal complexes

CO2: Charge transfer transition, and optical properties of metal complexes

CO3: Kinetic and thermodynamic stability of metal complexes, stability constants

CO4: Reaction mechanism of square and octahedral complexes, trans effect, outer and inner sphere mechanism in metal complexes

CO5: Magnetism, Magnetic Properties of transition metal complexes and lanthanides

### Course Content:

#### Unit 1

**[12 Lectures]**

Electronic structure and spectra of transition metal complexes: Spectroscopic states, Crystal Field Theory, Orgel and Tanabe-Sugano diagrams, selection rules, band intensities and band width, Adjusted Crystal Field Theory, Spectrochemical and Nephelauxetic series, molecular orbital theory of complexes (including complexes with

and without  $\pi$  bonding), MO diagrams for octahedral and tetrahedral complexes, Jahn-Teller effect, Charge-transfer spectra, optical properties of lanthanides and actinides.

## **Unit 2**

**[10 Lectures]**

Magnetic properties of transition metal complexes: Types of magnetic behaviour: dia-, para-, ferro- and anti-ferromagnetic compounds, spin-orbit coupling, temperature independent paramagnetism, application of Crystal Field Theory to explain magnetic properties, spin-crossover. Thermodynamic effects-hydration, ligation, lattice energy, magnetic properties of lanthanides and actinides.

## **Unit 3**

**[14 Lectures]**

Reaction Mechanism of inorganic complexes: Stepwise and overall formation constants. Factors affecting the stability of metal complexes, chelate effect, determination of binary formation constants, Energy profile of a reaction, inert and labile complexes, kinetics of substitution in octahedral complexes, acid hydrolysis and base hydrolysis. Dissociative, associative and interchange mechanism, trans-effect, isomerisation and racemisation in tris-chelate complexes, electron-transfer reactions, stereo-chemical non-rigidity and fluxional molecules.

## **Text Book(s)**

1. Huheey, J. E., Keiter, E. A., Keiter, R. L. and Medhi, O. K. *Inorganic Chemistry: Principles of Structure and Reactivity*, 4<sup>th</sup> Edn., (Pearson Education, 2006).
2. Cotton, F. A., Wilkinson, G., Murillo, C. A. and Bochmann, M. *Advanced Inorganic Chemistry*, 6<sup>th</sup> Edn., (John Wiley, 2007).

## **Reference Book(s)**

1. Greenwood, N. N. and Earnshaw, A. *Chemistry of the Elements*, 2<sup>nd</sup> Edn., (Pergamon Press, 1997).
2. Carlin, R. L. *Magnetochemistry*, (Springer Verlag, 1986).



**Course outcomes:**

After completion of the course, the learner shall be able to understand:

C01: Chemical kinetics of simple and complex reactions

C02: Analysis techniques for fast reactions

C03: Kinetics of reactions in solution phase

C04: Chemistry of ions in solution

C05: Electrode-electrolyte interface and different electrochemical processes.

**Course Content:****Unit 1****[15 Lectures]**

Brief review of chemical kinetics: Determinations of reaction rates; Kinetics and mechanism; Steady state kinetics, Kinetic and thermodynamic control of reactions, Composite reactions, chain reactions, Oscillatory reactions.

Photophysical and photochemical processes; Fast reactions; study of fast reactions by flow method, relaxation method, flash photolysis, T and P jump and nuclear magnetic resonance method, Femto-chemistry.

Reactions in solutions, Ionic reactions, kinetic salt effect, Electron transfer and proton transfer reactions, Kinetics of enzyme catalysis and micellar catalysis, Phase transfer catalysis, Kinetics and techniques of polymerization, Polymer molecular weight control.

**Unit 2****[5 Lectures]**

Theories of reaction rates: Arrhenius theory, Collision theory, Activated complex theory, Treatment of unimolecular reactions, Lindemann-Hinshelwood, RRK, Marcus and RRKM theory.

### Unit 3

[8 Lectures]

Equilibrium electrochemistry of ions, hydration number, activity coefficient, Debye-Hückel theory, Debye-Hückel-Onsager treatment and its extension, ion-solvent interactions, Debye-Hückel-Jerum model, electro-capillarity, ion transport, ion channels, Diffusion of ions and molecules in solutions.

### Unit 4

[ 8 Lectures]

Electrodes and electrochemical cells, hydrogen electrode, cell reactions, Nernst equation, electrode kinetics, electrode/electrolyte interface, electrical double layer, various models, Exchange current density, Butler-Volmer equation, over potential, Tafel plot, voltammetry, polarography, half-wave potential, Electrocatalysis – influence of various parameters, batteries, solid state battery, fuel cells, electrochemistry of corrosion, anodic/cathodic corrosion and its prevention.

### Text Book(s)

1. Atkins, P. and Paula, J. de. *Atkins' Physical Chemistry*, 10<sup>th</sup> Edn., (Oxford University Press, New Delhi, 2014).
2. Engel, T. and Reid, P. *Thermodynamics, Statistical Thermodynamics and Kinetics*, 2<sup>nd</sup> Edn., (Pearson, New Delhi, 2011).

### Reference book(s)

1. Laidler, K. J. *Chemical Kinetics*, 4<sup>th</sup> Edn., (McGraw Hill, New Delhi, 2007).
2. Bokris, J. O. M. and Reddy, A. K. N. *Modern Electrochemistry, Vol. I & II*, (Plenum, 2001).
3. Bard, A. J. and Faulkner, L. R. *Electrochemical Methods: Fundamentals and applications*, 2<sup>nd</sup> Edn., (Wiley, 2000).

**Course outcomes:**

After completion of the course, the learner shall be able to learn:

CO1: Born Oppenheimer approximation

CO2: Hartree-Fock method for the solution of Schrodinger equation for many particle system

CO3: Models of chemical bonding-Molecular orbital (MO) and Valence bond (VB) theory

CO4: Hückel  $\pi$ -electron theory and Walsh diagram

**Course Content:****Unit 1****[16 Lectures]**

Born-Oppenheimer approximation, Hartree-Fock method, Brillouin theorem, Koopman's theorem, Roothan's equations, models of chemical bonding - Molecular orbital (MO) and Valence bond (VB) theories, application to diatomic molecules such as,  $H_2$ ,  $H_2^+$ ,  $N_2$ ,  $O_2$ , and CO. Hybridisation and MOs of  $H_2O$ ,  $NH_3$  and  $CH_4$ , Introduction to the SCF method.

**Unit 2****[20 Lectures]**

Quantitative MO theory - Huckel  $\pi$ -electron theory and its application to ethylene, butadiene and benzene, energy levels of di- and tri- atomic molecules, Walsh diagrams and molecular geometry, Extended Hückel MO theory and calculation on some simple molecules.

**Text Book(s)**

1. Atkins, P. W. and Friedman, R. S., *Molecular Quantum Mechanics*, (Oxford University Press, 1997).
2. Levine, I. N *Quantum Chemistry*, (Pearson Education, Inc. 2004).

**Reference Book(s)**

1. McQuarrie, D. A. *Quantum Chemistry* (Viva Books Private Limited, 2003).
2. Prasad, R. K. *Quantum Chemistry* (New Age, 2010).

**Course Outcomes:**

On completion of the course, the the learner shall be able to understand:

CO1: Uses of various types of oxidants, reducing agents, selective organometallic reagents in organic synthesis.

CO2: Generation of reaction intermediates and their reaction pathways.

CO3: Important name reactions and molecular rearrangement reactions.

CO4: Pericyclic reactions, photochemical reactions and concept of retrosynthetic analysis.

**Course Content:****Unit 1****[5 Lectures]**

Reduction: Catalytic hydrogenation and dehydrogenation, dissolving metal reduction, hydride reduction of functional groups, Meerwein-Ponndorf-Verley reduction, hydroboration and related reaction, reaction of alkyl borane and tributyltin hydride, Wolff-Kishner reduction, non-metallic reducing agents such as diimide.

**Unit 2****[ 6 Lectures]**

Oxidation: Oxidation by Cr and Mn compounds; oxidation of alcohol, aldehyde, C=C, C-H bonds, PCC, oxidation with per acids and peroxides: C=C, Sharpless epoxidation, Baeyer-Villiger oxidation. Other types: Prevost and Woodward hydroxylation, cis- and trans-hydroxylation, glycol cleavage reagents;  $\text{KMnO}_4$ ,  $\text{OsO}_4$ ,  $\text{HIO}_4$ ,  $\text{Pb}(\text{OAc})_4$ , mercuric acetate,  $\text{SeO}_2$  oxidation of allylic C-H bond.

**Unit 3****[5 Lectures]**

Rearrangement reactions: Formation and stability of carbenium ions, carbanions, carbenes, nitrenes, radicals, ylides and arynes. Rearrangement reactions involving carbocation (Wagner-Meerwein, Pinacol-Pinacolone rearrangement), carbenes (Wolff &

Arndt- Eistert synthesis), nitrenes (Hoffman, Curtius, Schmidt, Lossen, Beckman), acylation, PPA cyclization and Fries rearrangement.

#### **Unit 4**

**[4 Lectures]**

Photochemistry: Cis-trans isomerisation, Paterno-Buchi reaction, Norrish type I & II reaction, photoreduction of Ketones, dipimethane rearrangement, photochemistry of arenes, Barton reaction.

#### **Unit 5**

**[6 Lectures]**

Pericyclic reactions: Orbital symmetry, selection rules and stereochemistry of electrocyclic reaction, cycloaddition and sigmatropic shift, Cheletropic reactions, Diels-Alder reaction-endo/exo-regioselectivity, effect of Lewis acid on Diels-Alder reaction, Claisen, Cope, Sommelet-Hauser rearrangement, Group transfer reactions-ene reaction; and 1,3-dipolar cycloaddition including ozonolysis and reaction of ketene with alkenes.

#### **Unit 6**

**[3 Lectures]**

Free radical reactions: Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, reactivity of the attacking radicals, the effect of solvents on reactivity, allylic halogenation by NBS, oxidation of aldehydes to carboxylic acids, auto-oxidation.

#### **Unit 7**

**[4 Lectures]**

Selected organic reaction and reagents: Favörski, Hofmann-Löffler-Freytag, ene, Stork-enamine, Michael addition, Robinson annulation, Mannich, Shapiro, Chichibabin and Wittig reaction, Gilman's reagent, DCC, LDA, 1,3-dithiane, Baker's Yeast, Phase-transfer catalysts. Boron: organoboron reagents and reactions; Silicon: Organosilicon compounds and their reactions, organotin compounds and their applications.

#### **Unit 8**

**[3 Lectures]**

Retrosynthetic analysis: Synthesis backwards, disconnections, synthons (donor and acceptor), choosing disconnections, functional group interconversion, disconnection

approach of alcoholic and keto compound, C-C disconnections, natural reactivity and umpolung.

### **Text Book(s)**

1. Clayden, J., Greeves, N., Warren, S. and Wothers, P. *Organic Chemistry*, 2<sup>nd</sup> Edn., (Oxford University Press, 2012).
2. March, J. and Smith, M. B. *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, 6<sup>th</sup> Edn., (Wiley, 2007).
3. Carey, F. A. and Sundberg, R. J. *Advanced Organic Chemistry, Part B: Reactions and Synthesis*, 5<sup>th</sup> Edn., (Springer, New York, 2007).
4. Caruthers, W. and Coldham, I. *Modern Methods of Organic synthesis*, 4<sup>th</sup> Edn., (Cambridge University Press, 2004).
5. Norman, R. O. C. and Coxon, J. M. *Principles of Organic Synthesis*, (Blackie Academic and Professional, 1993).

### **Reference Book(s)**

1. Zweifel, G. S., Nantz, M. H. and Somfai, P. *Modern Organic Synthesis: An Introduction*, 2<sup>nd</sup> Edn., (Wiley, New York, 2017).

## **CI 412 Laboratory Course in Inorganic Chemistry**

**L 0 T 3 P 6 CR 6**

### **Unit 1**

Quantitative estimation involving volumetric (redox and complexometry), gravimetric and spectrophotometric methods of analysis of constituents in three component mixtures, alloys and minerals.

### **Unit 2**

Synthesis and characterization of inorganic compounds, including those involving green synthetic methodology: Characterization includes elemental analysis, studies by IR, electronic spectra, magnetic susceptibility, conductance measurements, cyclic voltammetry. TG, DSC.

### **Text Book(s)**

1. Mendham, J., Denney, R. C., Barnes, J. D., Thomas, M. and Sivasankar, B. *Vogel's Quantitative Chemical Analysis*, 6<sup>th</sup> Edn., (Pearson Education, 2009).
2. Marr, G. and Rockett, B. W. *Practical Inorganic Chemistry*, (Van Nostrand, 1972).

### **Reference Book(s)**

1. Wollins, J. D. *Inorganic Experiments*, 3<sup>rd</sup> Edn., (VCH, 1994).
2. Parshall, G. W. (Ed. in Chief). *Inorganic Synthesis, Vol. 15*, (McGraw Hill, 1974).

**CI 416**

**History of Chemistry**

**L 0 T 3 P 6 CR 6**

### **Course outcome:**

On completion of this course, the students will be able to learn:

CO1: Develop understanding of various branches of science during different eras in different parts of the world

CO2: Analyze the role played by the science in different eras in the evolution of modern day science

CO3: Ethics in science

### **Course content:**

#### **Unit 1**

**[10 Lectures]**

Old traditions of Chemical sciences in various countries

Ancient Technology

Medicine in the ancient times

Ayurvedic Chemistry

Alchemy

India, Islamic & Chinese Alchemy

Metal extraction in the ancient times

Fiber, cloth and dyeing chemistry in the ancient times

Paper and ink in ancient times

## **Unit 2**

**[8 Lectures]**

Construction materials in the ancient times

The iron pillar of Delhi

Science & Technology in the West

Medieval and Renaissance Medicine

## **Unit 3**

**[8 Lectures]**

Modern traditions and methods

The Chemical Revolution: From Boyle to Dalton

Priestley's discovery of dephlogisticated air

Lavoisier and oxygen

## **Unit 4**

**[10 Lectures]**

Discoveries and Inventions in the context of state of art and impact

Development of chemistry during the industrial revolution

Development of chemistry during World War

Ethics in science

### **Text Book(s)**

1. Brock, W. H. *The Chemical Tree: A History of Chemistry*, (W. W. Norton & Co.: New York, 2000).
2. Bell, M. S. *Lavoisier in the Year One*, (W. W. Norton & Co.: New York, 2005).
3. Tripathi, V. Ed. *Archaeometallurgy in India*, (Cambridge University Press, 1998).

### **Reference Book(s)**

1. Singh, M. V. and Shrivastava, B. B. *Science and Technology in ancient India*, (Centrum Press, New Delhi, 2011).
2. Needham J. *Science and Civilization in China: Chemistry and Chemical Technology*, Volume V (Cambridge University Press, 1956).
3. Chattopadhyay, D. P. *History of Science and Technology in Ancient India*, (Firma KLM Kolkata, 1986).
4. Ray, P. C. *History of Chemistry in ancient and medieval India*, (Indian Chemical Society, Kolkata, 1956).



## **SEMESTER-IX**

**CI 501**

**Bio-Organic Chemistry**

**L 3 T 0 P 0 CR 3**

### **Course outcomes:**

On completion of this course, the students will be able to learn:

C01: Structure, Synthesis, Physical and Chemical properties of amino acids

C02: Structure and therapeutic applications of proteins, Structure of enzyme, Mechanism of enzyme action

C03: Details about nucleosides, nucleotides, RNA, and DNA including mutagenesis, codon, anticodon, genetic code, transcription and translation.

C04: Basics, classification, properties, synthesis and biosynthesis of Terpenoids, Alkaloids and Prostaglandins

C05: Biosynthesis of Shikimic acid, polyketide, derived natural products

### **Course Content:**

#### **Unit 1**

**[6 Lectures]**

Bio-organic chemistry: Structure of amino acids and physical and chemical properties, method of synthesis (including Merrifield synthesis) of peptides and polypeptides, naming of polypeptides chain, amino acid sequence determination (N-terminal and C-terminal), structure of protein (Helical and pleated structure), denaturation of protein, biosynthesis of proteins, therapeutic and diagnostic applications.

#### **Unit 2**

**[6 Lectures]**

Structure of purines and pyrimidine bases and their biosynthesis, nucleosides and nucleotides and their nomenclature, structure of RNA and DNA, replication of DNA and mutagenesis, codon, anticodon, t-RNA, structure and genetic code, transcription and translation.

#### **Unit 3**

**[6 Lectures]**

Enzymes: Mechanism of enzyme action and models, kinds of reactions catalyzed by enzymes, nomenclature, stereochemical aspects, cofactors, co-enzyme chemistry, structure and function of NADH, FAD, ADP and ATP.

**Unit 4** **[5 Lectures]**

Terpenoids: Classification, structure, chemistry and biosynthesis of some important mono, sesqui, di and tri-terpenes. e.g. limonene, carvone or carveol etc..

**Unit 5** **[5 Lectures]**

Alkaloids: Characteristic reaction, general methods of degradation, structure and chemistry of some well-known alkaloids, e.g. quinine, cocaine, morphine, heroin.

**Unit 6** **[4 Lectures]**

Biosynthetic pathway for Shikimic acid, polyketide derived natural products.

**Unit 7** **[4 Lectures]**

Prostaglandins: General structure, classification, biosynthetic pathway, stereoselective synthesis of Prostaglandins E<sub>2</sub> and F<sub>2</sub>.

**Text Book(s)**

1. Finar, I. L. *Organic Chemistry* (Volume 2), 6<sup>th</sup> Edn. (Pearson Education, 2002).
2. Lehninger, A. L. *Principles of Biochemistry*, (Worth Publishers, 1993).
3. Blackburn, G. M., Gait, M. J., Loakes, D. and Williams, D. M. ed., *Nucleic Acids in Chemistry and Biology*, 3<sup>rd</sup> Edn., (RSC publishing, 2006).

**Reference Book(s)**

1. Salerini, O. L. *Natural and synthetic organic medicinal compounds*, (C. V. Mosby Co. 1976).
2. Mann, J.; Davidson, R. S.; Hobbs, J. B.; Banthrope, D. V. and Harborne, J. B. *Natural Products, their chemistry and biological significance*, (Longmann, Essex., 1994).
3. Norman, R. and Coxon, J. M. *Principles of Organic Synthesis*, (Blackie, Academic and Professional, 1997).

**CI 525 Organometallic Chemistry**

**L 3 T 0 P 0 CR 3**

**Course outcomes:**

On completion of this course the students will be able to understand:

C01: Organometallic compounds with different type of ligands like  $\pi$ -acids, carbenes, alkyls, allyls etc.

C02: Structure and bonding analysis of organometallic compounds using the MO theory

CO3: Organometallic compounds of main group elements and their structure and bonding analysis

CO4: Application of organometallic compounds as homogeneous and heterogeneous catalysts and their role in industrial revolution

**Course Content:**

**Unit 1** **[8 Lectures]**

$\pi$ - Acid complexes: MO treatment, Preparation, properties, structures and bonding of metal complexes with CO, N<sub>2</sub>, NO, PR<sub>3</sub>, AsR<sub>3</sub> as ligands, metal carbonyl hydrides and metal carbonyl clusters. LNCC and HNCC, Compounds with metal-metal multiple bonds.

**Unit 2** **[8 Lectures]**

Organometallics: Structure, bonding, synthesis and reactions of metal complexes with alkyls, aryls, alkenes, alkynes and allyls, double and multidecker sandwich complexes.

**Unit 3** **[8 Lectures]**

Main Group Organometallics: Structure and bonding involving main group (Li, Be, Zn, Hg, Tl, Si, Sn and related systems) and transition elements (Cu, Ag, Au), metal organyls, isolobal analogy.

**Unit 4** **[12 Lectures]**

Homogeneous and heterogeneous catalysis: Oxidative addition and reductive elimination reactions, insertion and extrusion reactions, reactions involving coordinated ligands, cyclometallation reactions. Catalytic reactions of alkenes— isomerisation, hydrogenation, carbonylation, hydroformylation and polymerization, Fischer-Tropsch process, hydroboration, hydrosilation, hydrocyanation, hydroamination.

**Text Book(s)**

1. Elschenbroich, C. and Salzer, A. *Organometallics – A Concise Introduction*, 2<sup>nd</sup> Edn., (VCH Publication, 1992).

**Reference Book(s)**

1. Crabtree, R. H. *The Organometallic Chemistry of the Transition Metals*, 6<sup>th</sup> Edn., (John Wiley, 2014).
2. Powell, P. *Principles of Organometallic Chemistry*, 2<sup>nd</sup> Edn., (Chapman, London, 1988).

**Unit 1**

Purification of chemicals and calibration of analytical instruments; Error analysis- primary and secondary data, accuracy and precision, averaging of data, types of experimental error, significant figures, estimation and representation of error, and minimization of errors; Handling of basic instruments, e.g., potentiometer, conductivity meter, spectrophotometer, etc., through three basic experiments.

**Unit 2**

Four minor experiments chosen from: Kinetics by spectrophotometry, polarimetry and conductometry, Relative strength of two acids by conductance, Interfacial tension between two liquids by Tensiometer, Determination of a weak acid and a strong acid in mixture by potentiometry, Study of liquid-liquid phase diagram, Determination of fluoride by ion selective electrode, nitrate spectrophotometry, Determination of average molecular weight of a polymer by viscometry, etc.

**Unit 3**

Four major experiments chosen from: Study of non-Newtonian polymer solutions by Brookfield viscometer, Study of excess adiabatic compressibility of binary system by ultrasonic interferometry, Simultaneous determination of CMC and partition equilibrium constant by spectroscopic method, Kinetics of the catalytic decomposition of  $\text{H}_2\text{O}_2$  by manganese (IV) oxide, Determination of CMC by Du Nouy Tensiometry, Micellar catalysis by spectroscopy, Determination of  $pK_a$  by spectroscopy, Determination of stoichiometry and the stability constant of the complex formation, Study of pseudo-ternary phase diagram of oil-water-(surfactant-cosurfactant) system, Determination of activation energy of reaction by polarometry, Preparation and characterization of nanoparticles, etc.

**Text Book(s)**

1. Viswanathan, B. and Raghavan, P. S. *Practical Physical Chemistry*, (Viva Books Pvt. Ltd., 2005).
2. James, A. M. and Prichard, F. E. *Practical Physical Chemistry*, 3<sup>rd</sup> Edn., (Longman, 1974).

## Reference Book(s)

1. Jadaav, J. B. *Advanced Practical Physical Chemistry*, (Krishna Prakashan, 2015).
2. Garland, G. W., Nibler, J. W. and Shoemaker, D. P. *Experiments in Physical Chemistry*, 7<sup>th</sup> Edn., (McGraw- Hill, 2008).

## CI 519 Physical Chemistry of Surface and Condensed Systems L3 T0 P0 CR 3

### Course outcomes:

On completion of this course, the students will be able to understand:

C01: Basic understanding of surface phenomena like curve surface, capillary action, adsorption

C02: Structure and properties of different colloidal dispersion

C03: Polymer thermodynamics

C04: Structure and properties (optical electronic etc.) of solids

C05: Phenomena occurred on solid surfaces

### Course Content:

#### Unit 1

[8 Lectures]

Thermodynamic description of surface and interphase, Surface tension, capillary action, pressure across curved surface, vapor pressure of droplet, Gibbs adsorption isotherm, BET equation, estimation of surface area, Surface film of liquids. Various adsorption isotherms: Freundlich isotherm, Langmuir isotherm, Dubinin-Radushkevich isotherm, Temkin isotherm.

#### Unit 2

[8 Lectures]

Colloids; Surfactants, micelle, thermodynamics of micellization, microemulsion, micellar catalysis. Host-guest chemistry. Lipids and biological membranes, functions of cell membrane, ion transport through cell membrane, nerve conduction, biological cell and its constituents, biomolecules, bioenergetics.

### Unit 3

[6 Lectures]

Polymer molecular weight determination of polymers and biopolymers, Thermodynamics of polymerization, Thermodynamics of polymer and biopolymer solution, phase separation of polymer solutions, Polymer solution properties, Stereochemistry of polymer.

### Unit 4

[10 Lectures]

Structures of solids and liquids, liquid crystals, Nanoparticles and nanotechnology, Defects in solids, thermodynamics of Schottky and Frenkel defect formation, Thin films, Langmuir-Blodgett film. Electrical properties of solids, intrinsic and extrinsic semiconductors, doping of semiconductors, p-n junction, super conductors, conducting polymers, organic conductors, molecular electronic devices, nonlinear optical materials, optical reflectance, photoconduction, ionic conductors.

### Unit 5

[4 Lectures]

Reactions on solid surfaces, Diffusion in solids, Solid state reactions, Solid state batteries. Zeolites: Synthesis, structure, surface area and catalytic properties; glasses, ceramics and composites.

### Text Book(s)

1. Atkins, P. and Paula, J. de. *Atkins' Physical Chemistry*, 10<sup>th</sup> Edn., (Oxford University Press, New Delhi, 2014).
2. Chakrabarty, D. K. *Solid State Chemistry*, 1<sup>st</sup> Edn., (New Age Publishers, 2005).
3. Anslyn, E. V. and Dougherty, D. A. *Modern Physical Organic Chemistry*, (University Science Books, 2005).

### Reference Book(s)

1. West, A. R. *Solid State Chemistry and its Applications*, 2<sup>nd</sup> Edn., (Wiley, 2014).
2. Billmeyer, F.W. *Textbook of Polymer Science*, 2<sup>nd</sup> Edn., (Wiley, 2007).

**Course outcomes:**

On completion of this course the students will be able to understand:

CO1: Instrumentation technique of various analytical tools like XRD, AAS, cyclic voltammetry, chromatography, optical and electronic microscopy

CO2: Basic principles of those instrumentation techniques

CO3: Application of analytical tools (XRD, SEM, TEM, TGA, AAS, ICP-OES) in characterization and elemental detection of chemical compounds: solids (crystalline, amorphous, nanomaterials), liquids and gases.

CO4: Application of radiochemical techniques in chemical reactions

CO5: Electrochemical techniques for understanding electron transfer reaction mechanism, fuel cell application, Li-ion battery

**Course Content:**

**Unit 1**

**[4 Lectures]**

X-ray methods: X-ray diffraction, X-ray fluorescence and X-ray absorption and X-ray emission spectroscopy.

**Unit 2**

**[4 Lectures]**

Thermoanalytical methods: Thermo gravimetric analysis, differential thermal analysis and differential scanning calorimetry.

**Unit 3**

**[6 Lectures]**

Electrochemical methods: Coulometry, Polarography, anode-stripping voltammetry, pulse techniques, cyclic voltammetry, electrogravimetry, spectroelectrochemistry.

**Unit 4**

**[5 Lectures]**

Chromatographic methods: Adsorption, liquid-liquid partition, ion-exchange, paper and thin-layer chromatography, HPLC, gel permeation chromatography and gas chromatography, HPTLC, Flash chromatography.

**Unit 5****[4 Lectures]**

Radiochemical methods: Tracers in chemical analysis, isotopic exchange, isotopic dilution technique, labeling experiments in studying reaction mechanism.

**Unit 6****[8 Lectures]**

Optical microscopy: Optical Rotatory Dispersion and Circular Dichroism: Definition, Deduction of absolute configuration, octane rule for ketones.

Transmission electron microscopy (TEM) and Scanning electron microscopy (SEM).

**Unit 7****[5 Lectures]**

Atomic absorption spectroscopy: Inductively coupled Plasma- mass spectroscopy (ICP-MS), ICP-AES (Atomic Emission Spectroscopy).

**Text Book(s)**

1. Drago, R. S. *Physical Methods in Chemistry*, (Saunders College Publishing, 1992).
2. Hollas, J. M. *Modern Spectroscopy*, (John Wiley, 1996).

**Reference Book(s)**

1. Willard, H. H. *Instrumental Methods of Analysis*, (East West Press, 1998).
2. Bard, A. J. and Faulkner, L. R. *Electrochemical Methods, Fundamentals and Applications*, (John Wiley, 2000).

**CI 523 Chemical Technology and Society****L 3 T 0 P 0 CR 3****Course outcomes:**

On completion of this course, the students will be able to understand:

C01: Basic principles of the techniques generally involved in chemical processing in Industry

C02: Types of equipment needed in chemical industry

C03: Exploration of societal and technological issues from a chemical perspective

**Course Content:****Unit 1****[20 Lectures]**

Chemical Technology: Basic principles of distillation, solvent extraction, solid-liquid leaching and liquid-liquid extraction, separation by absorption and adsorption. An introduction into the scope of different types of equipment needed in chemical



technology, including reactors, distillation columns, extruders, pumps, mills, emulgators. Scaling up operations in chemical industry. Introduction to clean technology.

## **Unit 2**

**[16 Lectures]**

Exploration of societal and technological issues from a chemical perspective. Chemical and scientific literacy as a means to better understand topics like air and water (and the trace materials found in them that are referred to as pollutants), energy from natural sources (i.e. solar and renewable forms), from fossil fuels and from nuclear fission, materials like plastics and polymers and their natural analogues, proteins and nucleic acids, and molecular reactivity and interconversions from simple examples like combustion to complex instances like genetic engineering and the manufacture of drugs. Adverse effects of pesticides, chemical fertiliser, growth hormones and use of aromatic solvents.

### **Text Book(s)**

1. Hill, J. W., McCreary T. W. and Kolb, D. K. *Chemistry for changing times*, 13<sup>th</sup> Edn., (Prentice Hall, 2012)

## **SEMESTER-X**

### **Elective I**

**CI 506**

**Catalysis (Physical)**

**L 3 T 0 P 0 CR 3**

#### **Course outcomes:**

On completion of this course the students will be able to understand:

CO1: Various aspects of homogeneous and heterogeneous catalysis

CO2: Catalysts for industrially important reactions like alkene polymerization

CO3: Different spectroscopic and physicochemical techniques for catalyst characterization

CO4: Microporous and Mesoporous materials, their catalytic activity and industrial importance (e.g. in petrochemical industries)

CO5: Reactor design and industrial plant for large scale productions, Future catalysts for environment, biofuels, and energy production

## **Course Content:**

### **Unit 1**

**[10 Lectures]**

Introduction: Definition, role of catalysts, classification of catalysts. Homogeneous catalysts: Mechanism of homogeneous catalysis, acid-base catalysis, enzyme catalysis, micellar catalysis, phase transfer catalysts, homogeneous catalysis in industry, Ziegler-Natta catalysts, olefin and acetylene polymerization, isomerization, hydrogenation and HY addition, carbonylation reactions, hydroformylation, oxidation of olefins, metallocene catalysts.

### **Unit 2**

**[6 Lectures]**

Theory and mechanism of heterogeneous catalysts: Adsorption and catalysis, mechanism of heterogeneous catalysis, kinetics of heterogeneous catalytic reactions, volcano principle, shape and size selectivity of catalysts.

### **Unit 3**

**[4 Lectures]**

Characterization of catalysts and their surfaces: Methods of surface analysis, surface area, pore size, void fraction, particle size, mechanical strength, surface chemical composition, surface acidity and reactivity.

### **Unit 4**

**[8 Lectures]**

Examples of heterogeneous catalysts: Clays, zeolites, bimetallic, semiconductor and oxide catalysts, supported catalysts, polymer catalysts. Production and design of industrial catalysts: Materials and methods, precipitated catalysts, impregnated catalysts, skeletal catalysts, fused and molten catalysts, calcination, reduction, shape formation of catalyst particles, optimal shape and size of catalysts particle.

### **Unit 5**

**[2 Lectures]**

Reactors: Definition, classification, reactor design, choosing reactors in laboratory and plant.

### **Unit 6**

**[3 Lectures]**

Catalyst promotion and deactivation: Promotion and promoters, causes and mechanism of deactivation, poisoning, sintering, prevention of catalyst decay, regeneration of catalysts.

## Unit 7

[3 Lectures]

Examples of heterogeneous catalytic reactions: Catalytic processes in petroleum industry- reforming, cracking and hydrotreating, hydrogenation, hydrodesulphurization, Fischer-Tropsch process, etc.

Future Trends: Environmental aspect.

### Text Book(s)

1. Bartholomew, C. H. and Furrauto, R. J. *Fundamentals of Industrial Catalytic Processes*, 2<sup>nd</sup> Edn., (Wiley Interscience, 2006).
2. Chakrabarty, D. K. and Viswanathan, B. *Heterogeneous Catalysis* (New Age Int., 2008).

### Reference Book(s)

1. Gates, B. C. *Catalytic Chemistry*, (John Wiley & Sons, 1992).
2. Wijngaarden, R. J. *Industrial Catalysis*, (Wiley-VCH, 1998).
3. Augustine, R. L. *Heterogeneous Catalysts for Synthetic Chemists*, (Marcel- Dekker, 1996).

## CI 508      Methods in Organic Synthesis

L3 T0 P0 CR 3

### Course outcomes:

On completion of this course, the students will be able to understand:

CO1: Enolate chemistry and organometallic reagents

CO2: Important nucleophilic addition reactions, olefination reactions and other name reactions

CO3: Use of umpolung reagents in organic synthesis

CO4: Protection-deprotection chemistry

CO5: Heteroatoms in organic synthesis and retrosynthetic analysis

### Course Content:

## Unit 1

[8 Lectures]

Alkylation of carbon via enolates and specific enolate equivalents: Generation of carbon nucleophiles by proton abstraction, kinetic vs thermodynamic control in formation of

enolates, alkylation of enolates, generation and alkylation of dianions, solvent effect in enolate alkylations, oxygen vs carbon as the site of alkylation, alkylation of aldehydes, esters, lactones and nitro compounds, use of enol derivatives (enamines, vinyl acetates, vinyl-silyl-ethers, C- or O-Sn- derivatives, boron aluminium enolates). Michael addition: 1,2- vs 1,4-addition, conjugate addition followed by alkylation, conjugate substitution reactions (Baylis-Hillmann reaction, nucleophilic epoxidation), conjugate addition of organometallic reagents such as Cu-derivatives (Gilman reagents), Grignard reagents, improvements of the Robinson annulation –with alpha –silyl methylvinyl ketone use of vinyl pyridine, Michael addition of vinyl-silyl-ethers and allylsilanes.

## **Unit 2**

**[6 Lectures]**

Reaction of nucleophilic carbon species with carbonyl groups: Aldol and related condensation reaction, diastereoselective aldol reaction and Michael addition, Mukaiyama aldol reaction, Darzen reaction, Mannich reaction, acylation of nucleophilic carbon, carbonyl olefination (Wittig types reaction and methylenation, recent improvements of the use of phosphorous compounds, ylides, Stereoselective synthesis of alkenes: Julia olefination, Peterson elimination, Wittig reaction, HWE reaction, Still-Gennari modification, Shapiro reaction, McMurry reaction. Metal-mediated alkene synthesis [Tebbe olefination, Petasis reaction, Heck reaction, Suzuki reaction, metathesis (cross metathesis, enyne metathesis, RCM)], stereoselective addition to alkynes (Birch reduction and Lindlar's O<sub>2</sub> reduction).

## **Unit 3**

**[2 lectures]**

Umpolung of reactivity in carbonyl chemistry: Addition of electrophiles to carbonyl carbons, enolate cations (use of ketene thioacetates etc.), homoenolate anions (metalated allyl ethers amines, thio-ethers, silanes), bis-homoenolate cations. Addition reactions of C-C multiple bonds (oxymercuration, hydroboration etc.) and organoboranes.

## **Unit 4**

**[ 8 Lectures]**

Organometallic compounds in organic synthesis, protective groups (hydroxyl, amine, carbonyl and carboxylic and C-C double bond protecting groups) in organic synthesis. New greener techniques to carry out organic reactions with examples (crown ethers and cryptates, phase transfer catalyzed reaction, micellar catalysis, solid phase synthesis,

solvent-free reaction involving mechanical, thermal and microwave energies, use of greener solvents, enzyme catalyzed reaction).

### **Unit 5**

**[ 6 Lectures]**

Heteroatoms in organic synthesis: Sulfur: Sulfur stabilized anions, sulfonium salts, sulfonium ylides, sulfur stabilized cations, sulfoxides, oxidations using selenium. Important catalyzed reactions such as palladium catalyzed reactions including Heck, Stille, Sonogashira, Kumada, Suzuki & Negishi, alkene metathesis, enyne metathesis, reactions of organoboranes; reactions of organosilicon compounds, reactions of organotin compounds.

### **Unit 6**

**[6 Lectures]**

Retrosynthetic analysis of multistep synthesis, Synthesis: Illustrative synthesis of complex natural products with relevant examples.

### **Text Book(s)**

1. Clayden, J., Greeves, N., Warren, S. and Wothers, P. *Organic Chemistry*, 2<sup>nd</sup> Edn., (Oxford University Press, 2012).
2. March, J. and Smith, M. B. *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, 6<sup>th</sup> Edn., (Wiley, 2007).
3. Carey, F. A. and Sundberg, R. J. *Advanced Organic Chemistry, Part B: Reactions and Synthesis*, 5<sup>th</sup> Edn., (Springer, New York, 2007).
4. Caruthers, W. and Coldham, I. *Modern Methods of Organic synthesis*, 4<sup>th</sup> Edn., (Cambridge University Press, 2004).
5. Norman, R. O. C. and Coxon, J. M. *Principles of Organic Synthesis*, (Blackie Academic and Professional, 1993).

### **Reference Book(s)**

1. Zweifel, G. S., Nantz, M. H. and Somfai, P. *Modern Organic Synthesis: An Introduction*, 2<sup>nd</sup> Edn., (Wiley, New York, 2017).
2. Mundy, B. P. and Eller, M. G. *Name reaction and reagent in organic synthesis*, (John Wiley and Sons. 1998).
3. Smith, M. B. *Organic Synthesis*, 2<sup>nd</sup> Edn., (McGraw Hill, 2002).

**Course outcomes:**

On completion of this course the students will be able to understand:

CO1: Non-covalent force of interactions and supramolecular systems

CO2: MOF, COF and Inorganic host like zeolites for host-guest compounds

CO3: Photochemical reactions involving inorganic complexes and redox active centres

CO4: Photocatalyst for water splitting reactions, semiconductors, Ru-complexes, role of co-catalyst, quencher, quantum yield

CO5: Structure, electronic and bonding properties of unusual organometallic compounds, Computational study of organometallic compounds

**Course Content:****Unit 1****[8 Lectures]**

Introduction to Supramolecular Chemistry, nature of supramolecular interactions, host design, nanochemistry, host-guest chemistry, supramolecular synthesis of metal-organic and inorganic compounds.

**Unit 2****[12 Lectures]**

Inorganic Photochemistry: Excited states, ligand field states, charge-transfer states and Triplet states; Phosphorescence and fluorescence; Photochemical reactions: substitution and redox reactions of Cr (III), Ru(II) and Ru(III) complexes, photosystem-I and II, artificial photosynthesis, photocatalytic water splitting, dye sensitized solar cell.

**Unit 3****[6 Lectures]**

Pi-pi bonding in heavier main group chemistry, concept of Frustrated Lewis Pair (FLP) and their applications, Chemistry of N-heterocyclic carbnes, silylenes and germylenes, Aurophilic interactions.

**Unit 4****[10 Lectures]**

Theoretical study of the electronic structure of some organometallic compounds.

### **Text Book(s)**

1. Elschenbroich, C. and Salzer, A. *Organometallics – A Concise Introduction*, 2<sup>nd</sup> Edn., (VCH Publication, 1992).
2. Cotton, F. A., Wilkinson, G., Murillo, C. A. and Bochmann, M. *Advanced Inorganic Chemistry*, 6<sup>th</sup> Edn., (John Wiley, 2007).
3. Ramamurthy, V. and Schanze, K. S. *Multimetallic and Macromolecular Inorganic Photochemistry molecular and Supramolecular Photochemistry*, 4<sup>th</sup> Edn., (Marcel Dekker, 1999).
4. Steed, J. W. and Atwood, J. L. *Supramolecular Chemistry-2<sup>nd</sup> Edn.*, (John Wiley Publication, 2009).

### **Reference Book(s)**

1. Crabtree, R. H. *The Organometallic Chemistry of the Transition Metals*, 6<sup>th</sup> Edn., (John Wiley, 2014).
2. Hammer, F. *Inorganic Photochemistry*, (Sarup Book Publishers, 2009).

## **CI 532: Chemistry of Paints and Surface Coating Technology L 3 T 0 P 0 CR 3**

### **Course outcomes:**

On completion of this course, the students will be able to understand:

CO1.The chemistry behind paints, pigments and surface coating technology

CO2.Industrial processes of making paints

CO3.Chemical modification of vegetable oils

CO4.Basic ideas of polymer blends

### **Course Content:**

#### **Unit I**

**[ 6 Lectures]**

Introduction of paints and surface adhesion, classification- paints, varnishes and lacquers, their components and functions, binders, pigments, extenders, and additives, global picture of paint industry.

**Unit II****[ 8 Lectures]**

Chemical modifications of vegetable oils- monoglyceride preparation, thermal polymerization, dehydration of the oil, oxidation, auto oxidations, iodination, hydrolysis, alcoholysis, acidolysis, saponification, sulfonation, epoxidations. Preparation of alkyd resins, acrylic polymers, phenolics, amino resins, epoxy resins, polyurethane resins and polysiloxanes. Curing parameters for all the resins and properties of all the resins.

**Unit III****[ 7 Lectures]**

Pigments: classifications (organic, inorganic pigments), purification and surface modification of pigments, properties of pigments; extenders, fillers and nano fillers; solvents, thinners and diluents, paint additives, physical chemistry of paint formations: wetting, dispersion, stabilization, adsorption, flocculation, rheology; particle size analysis.

**Unit IV****[8 Lectures]**

Industrial process for making paints-three roll mill process; ball and pebble mills; sand, bead and short mills, high speed disc dispenser, testing and analysis of paints, general industrial paints, problems of paints and coatings.

Coating Driers: composition, mechanism of drier action; manufacture of driers; evaluation of driers; combination of driers; drier dosage; drier related paint film defects; driers for water based coatings.

**Unit V****[7 Lectures]**

Definition and basic concepts of polymer blends, alloys and composites; matrix resins, importance of polymer blends and alloys, principle of polymer miscibility and compatibility, inter-chain forces, interpenetrating network, thermodynamics of polymer miscibility, morphology and phase separation in polymer blends.



**Text Books:**

1. Swaraj Paul, Surface Coatings: Science and Technology, 2<sup>nd</sup> Edition, CBS publishers, New Delhi, 2014.
2. Dright G. Welden, Failure Analysis of Paints and Coatings, Wiley, 2009.
3. I.E Nielsen, Mechanical Properties of Polymers and Composites, Vols. 1 & 2, Dekker, New York, 1995

**Reference Book:**

1. Oil and Colour Chemists' Association, Surface Coating (2 Vols), Tafe Educational Books, Randwick, 1987.

**Elective II****CI 514****Biomolecular Chemistry****L3 T0 P0 CR 3****Course outcomes:**

On completion of this course, the students will be able to understand:

CO1: Understanding of interface of Chemistry and Biology

CO2: Molecular design of life, biochemical reactions, Chemical and physical foundations of biomolecules

CO3: Detection and isolation of natural biomolecules

CO4: Synthetic and semi synthetic path of biomolecules

**Course Content:****Unit 1****[4 Lectures]**

Interface of Chemistry and Biology, interaction between drug molecule and receptor sites.

**Unit 2****[ 14 Lectures]**

The molecular design of life, biochemical reactions, Chemical and physical foundations of biomolecules : water, acid, base and buffers; the biosynthesis, structure and functions

of key biomolecules (nucleic acids, amino acids, peptides and proteins, lipids and carbohydrate); synthesis and oxidations of fatty acids; biological membranes; membrane structure and transport mechanisms, membrane channels and pumps, molecular motors, cell signalling and signal transduction pathways, Principle of thermodynamics; bioenergetics and energy metabolism in cells, carbohydrate and glycobiology, glycolysis and gluconeogenesis, citric acid cycle, oxidative phosphorylation; light reaction of photosynthesis, Calvin cycle.

### **Unit 3**

**[14 Lectures]**

Detection and isolation of natural biomolecules, synthetic and semi-synthetic ways to different biomolecules, stereochemical consequences, protein and DNA X-ray crystallography, biomolecular spectroscopy (absorption and emission spectroscopy, polarization in light scattering, NMR, fluorescence spectroscopy, mass spectrometry for protein identification, vibrational spectroscopy).

### **Unit 4**

**[4 Lectures]**

Biodiversity of natural products

### **Text Book(s)**

1. Blackburn, G. M., Gait, M. J., Loakes, D. and Williams, D. M. *Nucleic Acids in Chemistry and Biology*, 3<sup>rd</sup> Edn., (RSC publishing, 2006).
2. Lehninger, A. L. *Principles of Biochemistry*, (Worth Publishers, 1993).

### **Reference Book(s)**

1. Nogradi, M. *Stereoselective synthesis, A Practical approach*, 2<sup>nd</sup> Edn., (VCH, Weinheim, 1995).
2. Thomas, G. *Medicinal Chemistry, An Introduction*, (Wiley, 2000, Single Edition).
3. Patrick, G. L. *An Introduction to Medicinal Chemistry*, 2<sup>nd</sup> Edn., (Oxford University Press, 2001).

**Course outcomes:**

On completion of this course, the students will be able to understand:

CO1: The numerical methods of integration and differentiations

CO2: Molecular mechanics calculation of complex system

CO3: Quantum mechanical calculation of complex systems

**Course Content:****Unit 1****[8 Lectures]**

Data analysis, mean and standard deviation, absolute and relative errors, linear regression, covariance and correlation coefficient. Curve fitting, solution of polynomial equation, numerical integration (Trapezoidal Rule, Simpson's Rule, Gaussian Quadrature), solution of ordinary differential equations (Euler's Method, Runge-Kutta methods, predictor-corrector method), matrix multiplication, inversion and diagonalization.

**Unit 2****[6 Lectures]**

Molecular Mechanics: Basic geometrical description of molecules; force-field development, intermolecular interactions, origin and modelling of dispersion forces & hydrogen bonds, strengths, weaknesses and applicability of currently available force-fields.

**Unit 3****[8 Lectures]**

Static properties of complex systems: Introduction to Monte Carlo as a way of averaging. Metropolis Monte Carlo algorithm: introduction and applications.

Dynamical properties of complex systems: Molecular Dynamics as a way of averaging. Integration of the Newton's equations: initial conditions, numerical algorithms (Verlet and leap-frog), and thermostats.

**Unit 4****[6 Lectures]**

Quantum Chemistry: Many electron systems, Hartree-Fock method, basis sets, electron correlation and its treatment, basics of density functional theory, DFT based reactivity descriptors. Introduction to popular softwares (like Gaussian, DMol, GAMESS). Applications to simple molecular systems.

**Unit 5****[8 Lectures]**

Combined QM/MM methods: Implications of the choice of QM and MM methods; Application of QM/MM methods in organic, inorganic and organometallic systems including bio-organic and bio-inorganic molecules.

Quantitative structure activity relation (QSAR): Early approaches, topological indices, fragmental models; quantum mechanical descriptors.

**Text Book(s)**

1. Lewars, E. *Computational Chemistry*, (Springer, 2003).
2. Balagurusamy, E. *Numerical Methods*, (Tata McGraw-Hill Publishing Company Limited, 2002).

**Reference Book(s)**

1. Leach, A. R. *Molecular Modeling: Principles and Applications*, 2<sup>nd</sup> Edn., (Pearson Prentice Hall, 2001).
2. Cramer, C. J. *Essentials of Computational Chemistry* (Wiley 2002).
3. Jensen, F. *Introduction to Computational Chemistry* (Wiley 1999).

**CI 518      Organic Solid States Chemistry****L3 T0 P0 CR 3****Course outcomes:**

On completion of this course, the students will be able to learn:

CO 1: Types of intermolecular interactions

CO 2: Crystal design and crystal design strategies

CO 3: Crystallization techniques of organic solids

CO 4: Concept of polymorphism

CO 5: Understanding of multi-component crystal and coordination polymer

## **Course Content:**

### **Unit 1**

**[2 Lectures]**

Intermolecular Interactions: General Properties, van der Waals Interactions, Hydrogen Bonds, Halogen Bonds, Other Interactions.

### **Unit 2**

**[ 5 Lectures]**

Crystal Engineering: Organic Solid States, Properties, Structure activity Relationship, X-ray Crystallography, Pharmaceutical Developments.

### **Unit 3**

**[5 Lectures]**

Crystal Design Strategies: Synthesis in Chemistry, Supramolecular Chemistry, Synthons in Crystal Engineering.

### **Unit 4**

**[6 Lectures]**

Crystallization of Organic Solids, nucleation, thermodynamics and kinetics of crystallization, crystal growth mechanism, crystal morphology and habit, crystal morphology engineering.

### **Unit 5**

**[ 6 Lectures]**

Polymorphism: Definition and occurrence, thermodynamic and kinetic relationships of the formation of polymorphs, Methods of polymorph characterization, properties of polymorphs, case studies from the pharmaceutical industry, polymorphism today.

### **Unit 6**

**[ 6 Lectures]**

Multi-component crystals: classification, definition and nomenclature, solid solutions, Host-Guest compounds, solvates and hydrates, Donor-Acceptor complexes, co-crystals of pharmaceutical importance.

### **Unit 7**

**[6 Lectures]**

Coordination Polymers: Definition, classification and design strategies, network topologies, supramolecular isomerism, interpenetration, porous coordination polymers, properties and applications.

## **Text Book(s)**

1. Desiraju, G. R.; Vittal, J. J. and Ramanan, A. *Crystal Engineering: A Textbook*, (World Scientific Publishing Company, 2011).

2. Bernstein, J. *Polymorphism in Molecular Crystals, Monographs on Crystallography*, No. 14, (Clarendon Press/International Union of Crystallography, 2002).

### Reference Book(s)

1. Desiraju, G. R. *Crystal Design: Structure and Function*, (John Wiley & Sons, 2003).
2. Steed, J. W. and Atwood, J. L. *Supramolecular Chemistry*, (John Wiley & Sons, 2009).

**CI 520 Environmental and Green Chemistry**

**L3 T0 P0 CR 3**

### Course outcomes:

On completion of this course, the students will be able to learn:

CO1: Environmental impact and quality parameters of air, water and soil

CO2: Analysis and purification of water, wastewater, solid-wastes and air pollution.

CO3: Environmental protection and pollution prevention

CO4: Green chemistry principles and Design of green synthesis

### Course Content:

#### Unit 1

**[6 Lectures]**

Environment and chemistry; Matter and cycles of matter; The atmosphere and atmospheric chemistry: The geosphere and geochemistry; Aquatic chemistry, CO<sub>2</sub> distribution, acid-base and redox equilibrium in water, pE-pH curves, water quality parameters.

#### Unit 2

**[6 Lectures]**

Chemistry and environmental pollution: Chemical hazards, chemical disasters, Water pollution, air pollution and soil pollution; Industrial pollution, vehicular pollutions, agricultural pollution, pollution by plastics; environmental biochemistry, toxicological chemistry.

#### Unit 3

**[6 Lectures]**

Environmental analysis: Analysis of water and wastewater, solid-wastes and air pollution.

**Unit 4****[6 Lectures]**

Environmental protection: pollution prevention, green chemistry, biodegradation, water and wastewater purification – removal of arsenic, iron, fluoride, etc.; air purification, waste minimization, industrial and municipal waste treatment and soil remediation.

**Unit 5****[6 Lectures]**

Green chemistry principles: Principles of green chemistry, atom economy, less hazardous chemical syntheses, designing safer chemicals, safer solvents and auxiliaries, design for energy efficiency, renewable feedstock, catalysis, design for degradation, real time analysis for pollution prevention, and inherently safer chemistry for accident prevention.

**Unit 6****[6 Lectures]**

Design of green synthesis: Ideal synthesis, clean routes, supercritical solvents, ionic liquids, green catalyst, auto-exhaust catalyst and clean technology  
Real world examples.

**Text Book(s)**

1. Manahan, S. E. *Environmental Chemistry*, 9<sup>th</sup> Edn. (CRC Press, Boca Raton, 2010).
2. Anastas, P. T. and Warner, J. C. *Green Chemistry: Theory and Practice*, (Oxford University Press, 1998).

**Reference Book(s)**

1. Hutzinger, O. *Handbook of Environmental Chemistry*, (Springer-Verlag, 1991).
2. Cann M. C. and Connelly, M. E., *Real World Cases in Green Chemistry*, (ACS, 2000).

**CI 534 Industrial Polymers****L3 T0 P0 CR 3****Course outcomes:**

On completion of this course, the students will be able to learn:

CO 1: Fundamentals of industrial polymers

CO 2: Synthesis, processing and properties of some industrially important polymers

CO 3: Discussion of the applications of the polymeric products

## **Course Content:**

### **Unit I**

**[4 Lectures]**

Fundamentals of industrial polymers including monomer, initiator, catalyst; manufacturing techniques, structure and property, modification, applications, etc.

### **Unit II**

**[ 8 Lectures]**

Industrial commodity thermoplastics like polyethylene, polypropylene, polystyrene, poly(vinyl chloride), high impact polystyrene, etc.; their preparative methods, microstructures, physical, mechanical, thermal, chemical and aging properties; various commodity to advanced applications.

### **Unit III**

**[ 8 Lectures]**

Industrial engineering thermoplastics like poly(acrylonitrile), nylon 6, nylon 6,6, polyesters, polycarbonates, polyurethanes, poly(tetrafluoroethylene), etc. their preparative methods, microstructures, physical, mechanical, thermal, chemical and aging properties; various commodities to advanced applications.

### **Unit IV**

**[ 8 Lectures]**

Industrial thermosetting resins like phenolic resins, amino-resins, alkyds, unsaturated polyesters, polyurethanes, epoxy resins, etc.; their preparative methods, microstructures, physical, mechanical, thermal, chemical and aging properties; various commodity to advanced applications.

### **Unit V**

**[8 Lectures]**

Industrial elastomers like natural rubber, styrene-butadiene rubber, acrylonitrile-butadiene rubber, synthetic isoprene rubber, isobutylene-isoprene rubber, chloroprene rubber, ethylene-propylene diene rubber, chlorosulphonated polyethylene rubber, silicone rubber, fluororubbers, etc. their preparative methods, microstructures, physical, mechanical, thermal, chemical and aging properties; various commodity to advanced applications.



### **Text Books**

1. P. Ghosh, Polymer Science and Technology: Plastics, Rubbers, Blends and Composites, Third Edition, McGraw Hill Education Private Limited (India), 2011
2. J. A. Brydson, Plastics Materials, 4<sup>th</sup> edn., Butterworths, London, 1982
3. J. A. Brydson, Rubbery materials and their compounds, Elsevier Applied Science, London, 1988

### **Reference Book**

1. M. Chanda, S. K. Roy, Industrial Polymers, Specialty Polymers, and Their Applications, 1st Edition, CRC Press, 2019.
2. E. Alfredo Campo, Industrial Polymers, Carl Hanser Verlag GmbH & Co. KG, Berlin, 2007

### ***Elective III***

**CI 522 Polymer Chemistry (Physical/ Polymer)**

**L3 T0 P0 CR 3**

### **Course outcomes:**

On completion of this course, the students will be able to understand:

CO 1: Historical background and basics of polymer chemistry

CO 2: Kinetics of polymerization reaction

CO 3: Basic characterization of polymers

CO 4: Thermodynamics of polymer solutions

CO 5: Structure-property relationship of polymers

### **Course Content:**

#### **Unit 1**

**[3 Lectures]**

Introduction: Historical background, basic nature, classification, raw materials for polymers, gas cracker, naphtha cracker.

**Unit 2****[5 Lectures]**

Kinetics and mechanism of polymerization: Degree of polymerization and molecular weight of polymer, kinetics of various types of polymerization, co-polymerization, reactivity ratio, molecular weight distribution, control of molecular weight.

**Unit 3****[3 Lectures]**

Polymerization techniques: Special features of polymerization, various polymerization techniques, polymerization reactors.

**Unit 4****[7 Lectures]**

Polymer characterization: Determination of molecular weight and molecular weight distribution, GPC, light scattering, end group analysis method, Zimm plot, viscosity of polymer solutions, thermal, mechanical, rheological and electrical properties of polymers, polyelectrolytes, ion-exchange resins.

**Unit 5****[7 Lectures]**

Thermodynamics of polymer solutions: Chain conformation, molecular dimensions in solution, solubility of polymers, solubility parameters, lattice theory,  $\Delta H$ ,  $\Delta S$  and  $\Delta G$  of mixing in polymer solution, dilute polymer solutions,  $\chi_1$  and  $\theta$ -temperature, phase separation, fractionation.

**Unit 6****[3 Lectures]**

Structure-property relationship: Stereochemistry of polymers, cross-linking, polymer architecture, elasticity, viscoelasticity, crystallinity.

**Unit 7****[ 8 Lectures]**

Natural polymers: rubber, natural fibers, silk fibers, Synthetic polymers: HDPE, LDPE, PP, PS, Nylon; synthetic polymeric resins and rubbers, moulding, Applications and Future trends: Applications, degradation and future trends.

### **Text Book(s)**

1. Misra, G. S. *Introductory Polymer Chemistry* (Wiley Eastern Limited, 1993).
2. Billemeier, F. *Textbook of Polymer Science* (Wiley, 1984).

### **Reference Book(s)**

1. Odian, G. *Principles of Polymerization* (Wiley, 2004).
2. Sun, S. F. *Physical Chemistry of Macromolecules*, 2<sup>nd</sup> Edn., (Wiley, 2004).
3. Seymour, R. B. *Polymer Chemistry: An Introduction* (Marcel-Dekker, 1984).

## **CI 524 Heterocyclic Compounds and Medicinal Applications (Organic)**

**L3 T0 P0 CR 3**

### **Course outcomes:**

On completion of this course, the students will be able to understand:

CO1: Modern approaches to drug design and clinical trials

CO2: Importance of heterocyclic compounds in medicinal chemistry and drug design

CO3: Nomenclature, classification, synthesis and reactivity of non-aromatic, aromatic, benzo-fused heterocycles containing one, two or more heteroatom

### **Course Content**

#### **Unit 1**

**[ 6 Lectures]**

History of medicinal chemistry, interaction between drug molecule and receptor sites, drug action mechanism, drug metabolism, approaches to drug design; pharmacokinetics-pharmacodynamics, xenobiotics. Drug development, screening, lead optimisation, phase I, II and III trials.

#### **Unit 2**

**[ 4 Lectures]**

Introduction to heterocyclic compounds: Nomenclature, classification, heterocycles and aromaticity, importance of heterocycles in medicinal chemistry.

**Unit 3** **[ 7 Lectures]**

Non-aromatic heterocycles: Syntheses and reactivities of small ring non-aromatic strained heterocycles like epoxides, aziridines, azetidines, oxetanes, thietanes. Syntheses, conformations and medicinal importance of six-membered non-aromatic heterocycles like piperdines, piperzines, morpholines, tetrahydropyrans.

**Unit 4** **[ 7 Lectures]**

Benzo-fused heterocycles containing one heteroatom: Syntheses and reactions of benzo-fused heterocycles containing one heteroatom *e.g.* benzofurans, 2,3-dihydrobenzofurans, benzothiophenes, benzopyrans, 1,2,3,4-tetrahydroquinolines etc. Examples and selected syntheses of some important drugs containing this class of benzo-fused heterocycles.

**Unit 5** **[ 6 Lectures]**

Aromatic heterocyclic compounds containing one hetero atom: Preparation and properties of furan, thiophene, pyrrole, indole, quinoline and isoquinoline derivatives.

**Unit 6** **[ 6 Lectures]**

Heterocyclic compounds containing two or more hetero atoms: Synthetic methods of preparation, properties and applications in medicinal chemistry—*e.g.*, azoles (pyrazole, imidazole, oxazole and thiazole derivatives), diazines (pyrazine, pyrimidine and pyridazine derivatives), benzo-diazines, heterocyclic compounds containing one nitrogen atom and an oxygen or sulphur atom (oxazine, phenoxazine and thiazine derivatives), triazines and tetrazines.

**Text Book(s)**

1. Abraham, D. J. ed., *Burger's Medicinal Chemistry and Drug Discovery (6 volume set)*, 6<sup>th</sup> Edn., (Wiley Interscience, 2003).
2. Thomas, G. *Medicinal Chemistry, An Introduction*, (Wiley, 2000, Single Edition).
3. Finar, I. L. *Organic Chemistry (Volumes I and II)*, 6<sup>th</sup> Edn., (Pearson Education, 2002).
4. Joule, J. A. and Mills, K. *Heterocyclic Chemistry*, 5<sup>th</sup> Edn., (Wiley, New York, 2010).

## Reference Book(s)

1. Gilchrist, T. L. *Heterocyclic Chemistry*, 3<sup>rd</sup> Edn., (Pearson India, 2008).
2. Patrick, G. L. *An Introduction to Medicinal Chemistry*, 2<sup>nd</sup> Edn., (Oxford University Press, 2001).

## CI 526 Bio-inorganic Chemistry (Inorganic)

L3 T0 P0 CR 3

### Course outcomes:

On completion of this course the students will be able to understand:

CO1: .Biological importance of calcium, Na and K

CO2: Metalloenzymes, non-heme proteins and their biological functions

CO3: Toxicity of metals like mercury, cadmium and lead

CO4: Metal complexes as anticancer drugs

CO5: Application of metals for medical diagnosis

### Course Content:

#### Unit 1

[8 Lectures]

Calcium in biology: Calcium in living cells, transport and regulation, molecular aspects of intramolecular processes, extracellular binding proteins. Role in muscle contraction, blood clotting mechanism and biological calcification. Na-K Pump.

#### Unit 2

[16 Lectures]

Proteins and enzymes of Fe, Co, Cu, Mo and Zn: Hemerythrin, ferritin and transferrins, peroxidase, catalase, cytochrome P-450. Iron-sulphur proteins: rubredoxin and ferredoxins. Cytochrome C oxidase and superoxide dismutase, ceruloplasmin, Vitamin B12, B12 co-enzymes and cobalamines, carbonic anhydrase, carboxy peptidase, metallothionins, interchangeability of Zn and Co in enzymes. Structural and functional models, Biological nitrogen fixation.

#### Unit 3

[12 Lectures]

Metals in medicine: Toxicity of mercury, cadmium, lead, chromium, beryllium, selenium and arsenic, biological defence mechanisms, chelation therapy, metals used for diagnosis

and chemotherapy, platinum complexes as anticancer drugs, complexes of gold, copper, zinc, mercury, arsenic and antimony as drugs.

### **Text Book(s)**

1. Cowan, J. A. *Inorganic Biochemistry- An Introduction*, (Wiley- VCH, 1997).
2. Hanzlik, R. P. *Inorganic Aspects of Biological and Organic Chemistry*, (Academic Press, 1976).

### **Reference Book(s)**

1. Lippard, S. J. and Berg, J. M. *Principles of Bioinorganic Chemistry*, (University Science Book, Mill Valley, 1994).
2. Hay, R. W. *Bioinorganic Chemistry*, (Ellis Hollwood, 1984).

**CI 536                      Chemistry of Materials**

**L3 T0 P0 CR 3**

### **Course outcomes:**

On completion of this course, the students will be able to understand:

C01: Solid state conductors, both electron and ion conductors, and their structure-property correlation and application

C02: Polymeric materials (organic and inorganic) and their properties

C03: Liquid crystals, their characteristic properties and applications

C04: Clay-polymer and carbon composite

### **Course Content:**

#### **Unit 1**

**[ 8 Lectures]**

Solid state ionic conductors: Structure, physico-chemical principles, applications.

Ferrous alloys, Fe-C phase transformations in ferrous alloys; non-ferrous alloys-properties and applications of ferrous and non-ferrous alloys, magnetic alloy. Metallic glass, ceramics, Nano-materials and optical materials.

#### **Unit 2**

**[ 6 Lectures]**

Polymeric materials: Molecular shape, structure and configuration, crystallinity, stress-strain behaviour, thermal behaviour, polymer types and their applications, conducting and ferro-electric properties.

**Unit 3****[7 Lectures]**

Inorganic Polymers: Polysiloxanes, polysilanes, polyphosphazenes, polymeric sulphur – synthesis, structure, properties and applications. co-ordination polymers and organometallic polymers.

**Unit 4****[7 Lectures]**

Liquid crystals: Nematic, smectic, cholesteric – properties and applications. High Tc materials: Defect Perovskites- high Tc superconductivity in cuprates, 1-2-3 and 2-1-4 materials; anisotropy, temperature dependence of electrical resistance, optical phonon modes, superconducting state, heat capacity, coherence length, elastic constants, position lifetimes, micro-wave absorption pairing and multigap structure in high Tc materials, applications of high Tc materials.

**Unit 5****[ 8 Lectures]**

Organic solids: Conducting organics, organic superconductors, Magnetism in organic materials.

Fullerenes: doped fullerenes as superconductors.

Molecular devices: molecular rectifiers and transistors, artificial photosynthetic devices, sensors.

Clay-polymer composite and carbon composites, phosphor and laser materials.

**Text Book(s)**

1. Keer, H. V. *Principles of the Solid State* (Wiley Eastern, 1993).
2. Ashcroft, N. W. and Mermin, N. D. *Solid State Physics* (Saunders College, 1993).

**Reference Book(s)**

1. Callister, W. D. *Material Science and Engineering- An Introduction* (Wiley, New York, 1985).
2. Lever, K. D.; Alexander, J. M. and Rawlings, R. D. *Materials Science* (J.C. Senderson, ELBS).
3. Marck, J. E.; Allcock, H. R. and West, R. *Inorganic Polymers* (Prentice Hall, 1992).

## Annexure

The CBCS structure of the programme involves three different types of courses viz. Core Courses, Elective Courses and Ability Enhancement Courses. The significance of each type of course and the details of credit system is given below:

### **Types of Course:**

**i) Core Course:** A course, which should compulsorily be studied by a candidate as a core requirement is termed as a Core course.

- The Core Course cannot be substituted by any other course.
- It will be offered by the Chemistry department.
- A core course offered in a discipline/subject may be treated as an elective by other discipline/subject/vice versa and such electives may also be referred to as Generic Elective.
- Dissertation/Project: A core course designed to acquire special/advanced knowledge, such as Project work/ Dissertation work is carried out by a candidate on his/her own with an advisory support from the faculty member.

**ii) Elective Course:** Generally a course which can be chosen from a pool of courses and which may be very specific or specialized or advanced or supportive to the discipline/subject of study or which provides an extended scope or which enables an exposure to some other discipline/subject/domain or nurtures the candidate's proficiency/skill is called an Elective Course.

- **Discipline Specific Elective (DSE) Course:** Elective courses may be offered by the main discipline/subject of study is referred to as Discipline Specific Elective. The University/Institute may also offer discipline related Elective courses of interdisciplinary nature (to be offered by main discipline/subject of study).
- **Generic Elective (GE) Course:** An elective course chosen generally from an unrelated discipline/subject, with an intention to seek exposure is called a Generic Elective. A core course offered in a discipline/subject may be treated as



an elective by other discipline/subject/vice versa and such electives may also be referred to as Generic Elective.

iii) **Ability Enhancement Courses (AEC):** The Ability Enhancement (AE) Courses may be of two kinds

- **Ability Enhancement Compulsory Courses (AECC):** AECC" courses are the courses based upon the content that leads to Knowledge enhancement viz. Environmental Science, English Communication/MIL Communication etc. AECC should compulsorily be studied by a candidate to complete the requirement of a degree in a said programme/ discipline of study. AECC cannot be substituted by any other course.
- **Skill Enhancement Courses (SEC):** These courses may be chosen from a pool of courses designed to provide value-based and/or skill-based knowledge.

### **Credit System:**

- Credit defines the quantum of content/syllabus prescribed for the course. It may be a unit prescribed for a course and is determined by the number of hours of instruction required per week. Thus, in each course credits will be assigned on the basis of the number of hours required per week for lectures/tutorials/lab work/field work to complete the course in a single semester.
  - 1 credit = 1 hour of direct teaching per week
  - 1 credit = 2 hours of lab work/field work/project work per week
- A course of study may have only lecture (L) component or only practical/practice (P) component or combination of any two or all the three components. The third being Tutorial (T) component.
- The total credits earned by a student at the end of semester upon successfully completing the course is L+T+P.

### **Credit requirement:**

Minimum Credit requirement: 210

Minimum duration: 05 years (10 semesters)

Maximum duration: 07 years (14 semesters)

<b>Semester</b>	<b>Total Credit</b>	<b>Semester</b>	<b>Total Credit</b>
<b>I</b>	<b>21</b>	<b>VI</b>	<b>20</b>
<b>II</b>	<b>22</b>	<b>VII</b>	<b>21</b>
<b>III</b>	<b>23</b>	<b>VIII</b>	<b>21</b>
<b>IV</b>	<b>22</b>	<b>IX</b>	<b>21</b>
<b>v</b>	<b>22</b>	<b>X</b>	<b>17</b>