

Post Graduate Department of Chemistry

# **FACULTY OF SCIENCES**

# **SYLLABUS FOR**

**Programme Code:** *MCHE* 

**Programme Name: M.Sc. Chemistry** 

Examinations: 2024-2025

Batch 2024: Semester I-II

Batch 2023: Semester III-IV



# Department of Chemistry Khalsa College, Amritsar

Note: (a) Copy rights are reserved. Nobody is allowed to print it in any form.

(b)) Subject to change in the syllabi at any time.

(c) Please visit the College website time to time.

Academic Session: 2024-25



# Post Graduate Department of Chemistry

S.No.	PROGRAMME OBJECTIVES
1.	The course was introduced to cater the needs of Academic Institutes (Universities, College, and Schools), Chemical, Pharmaceutical industry, Textile, Sugar Industry, Research Institutes.
2.	Students will be able to develop the theoretical aspects of all the fields of chemistry Organic, Inorganic, Physical and Analytical Chemistry and some interdisciplinary courses needed for better understanding the subject from technology point of view.
3.	Students will be able to develop the better understanding of the Practical aspect of chemistry through lab work and research project.
4.	Continue to acquire relevant knowledge and skills appropriate to professional activities and demonstrate highest standards of ethical issues in the subject concerned. Develop the ability to identify unethical behavior such as fabrication, falsification or misrepresentation of data and adoptive objectives, unbiased and truthful actions in all aspects.
5.	Create awareness to become an enlightened citizen with commitment to deliver one's responsibilities within the scope of bestowed rights and privileges.
6.	Integrating multicultural awareness such as race, gender, physical ability, age, income and other social variables, and by creating an environment that is, "welcoming for all students".
7.	Ability to think, acquire knowledge and skills through logical reasoning and to inculcate the habit of self-learning throughout life, through self- paced and self- directed learning aimed at personal development, and adapting to changing academic demands of work place through knowledge/ skill.



# Post Graduate Department of Chemistry

S.No.	PROGRAMME SPECIFIC OUTCOMES (PSOS)
PSO-1	Students will develop the advanced theoretical and practical skills in the field of INORGANIC CHEMISTRY in specialized areas of Group Theory, Ligand Field Theory, Reaction Mechanism, Organometallics, Bioinorganic and Metal Clusters, Photoinorganic chemistry, Oxidative addition and Insertion reactions, Structure and bonding of d-Block elements, <i>Techniques for Structure Elucidation of Inorganic Compounds</i> , Practical Techniques of qualitative and quantitative analysis of inorganic compounds.
PSO-2	Students will develop the advanced theoretical and practical skills in the field of ORGANIC CHEMISTRY through some specialized areas like Reaction Mechanism-Substitution reactions, Techniques for Structure Elucidation of Organic Compounds, Reaction Mechanism-Addition, Elimination and Rearrangements, Supramolecular, Reactive Intermediates and Disconnections, Natural Products, Pericyclic & Photochemistry, Asymmetric synthesis, Green Chemistry and Heterocyclic Chemistry, Practical Techniques of qualitative and quantitative analysis of organic.
PSO-3	Students will develop the advanced theoretical and practical skills in the field of PHYSICAL CHEMISTRY through specialized areas of Thermodynamics, Quantum Chemistry, Electrochemistry and Chemical Dynamics, Analytical Techniques, Surface and Polymer Chemistry Practical Techniques of qualitative and quantitative analysis and use of various electrical and non-electrical Instruments for analysis.
PSO-4	Student will develop the understanding regarding the use of mathematical tools, biological processes, use of computer and software's for chemistry purpose.
PSO-5	The students to get knowledge of Research Methodology, Advance Analytical Techniques and learn about various tools of Organic and Inorganic synthesis

**Eligibility:-** The candidate having passed B.Sc. degree (10+2+3 system of education) i.e. B. Sc. (Medical), B. Sc. (Non-Medical), or equivalent with Chemistry as one of the elective subject in all semesters and with at least 50% marks in aggregate from Guru Nanak Dev University or any other UGC recognized University.



# Post Graduate Department of Chemistry

# Batch 2024 Sem. I-II

	COURSE SCHEME										
	SEMESTER - I										
Course	Course Name	Hours	C	redi	its	Total		Max	Mark	S	Page
Code		/Week	L	Т	P	Credits	Th	P	IA	Total	No.
CHE 411 /CHH 411	Inorganic Chemistry-I: (Ligand Field and Group Theory)	4	4	0	0	4	75		25	100	8-9
CHE 412	Organic Synthesis-I (Reaction Mechanism-Substitution reactions)	4	4	0	0	4	75		25	100	10-12
CHE 413 /CHH 413	Physical Chemistry-I: Thermodynamics	4	4	0	0	4	75		25	100	13-14
CHE 414 /CHH 414	Spectroscopy A: Techniques for Structure Elucidation of Organic Compounds	6	6	0	0	6	112		38	150	15-17
CHE 415 /CHH 415	Inorganic Chemistry Lab-I (Quantitative Analysis)	6	0	0	3	3		56	19	75	18-19
CHE 416	Organic Chemistry Lab- I Quantitative analysis and Multistep Synthesis	6	0	0	3	3		56	19	75	20-21
CHE 417/CHH 417	Basics and Application of Chemistry Software's	6	2	0	2	4	37	38	25	100	22-24
	TOTAL	36				28				700	



# Post Graduate Department of Chemistry

	SEMESTER - II										
Course	Course Name	Hours	Credits			Total	Max Marks				Page
Code	Course Name	/Week	L	T	P	Credits	Th	P	IA	Total	No.
	Major Courses										
CHE 421	Inorganic Chemistry-II: (Reaction Mechanism, Organometallics and Catalysis)	4	4	0	0	4	75		25	100	26-28
CHE 422 / CHH 422	Organic Synthesis-II (Reaction Mechanism-Addition, Elimination and Rearrangements)	4	4	0	0	4	75		25	100	29-30
CHE 423/ CHH423	Physical Chemistry-II: Quantum Chemistry	4	4	0	0	4	75		25	100	31-32
CHE 424 / CHH 424	Spectroscopy B: Techniques for Structure Elucidation of Inorganic Compounds	6	6	0	0	6	112		38	150	33-35
CHE 425 / CHH 425	Organic synthesis-III(Supramolecular, Reactive Intermediates and Disconnections)	4	4	0	0	4	75		25	100	36-38
MH CHX 421 Or BT CHX 421	Mathematics for Chemists (Med. Students) Or Biology for Chemists (Non Med. Students)	3	3	0	0	3	56		19	75	39-40 41-42
CHE 426 / CHH 426	Physical Chemistry Lab-I	6	0	0	3	3		56	19	75	43-44
CHE 427 /CHH 427	Inorganic Chemistry Lab- II	6	0	0	3	3		56	19	75	45-47
	TOTAL	37				31				775	

Important Note: M. Sc. (Chemistry) and M. Sc. Chemistry (Under the Honours Scheme) have some common subjects. The subject code of M. Sc. (Chemistry) starts with CHE

The subject codes of M. Sc. Chemistry (Under the Honours Scheme) starts with CHH



# Post Graduate Department of Chemistry

# Batch 2023 Sem. III-IV

	SEMESTER - III										
Course		Hours	(	Credits		Total		Max	Marl	ks	Page
Code	Course Name	/Week	L	T	P	Credits	Th	P	I A	Total	No.
		Major (	Cour	ses							
CHE 531 / CHH 531	Inorganic Chemistry-III: (Bioinorganic and Metal Clusters)	4	3	1	0	4	75		25	100	49-51
CHE 532/ CHH 532	Organic Synthesis-IV (Natural Products)	4	3	1	0	4	75		25	100	52-54
CHE 533	Physical Chemistry-III (Electrochemistry and Chemical Dynamics)	6	5	1	0	6	112		38	150	55-57
CHE 534/ CHH 534	Organic Synthesis-V (Pericyclic & Photochemistry)	4	3	1	0	4	75		25	100	58-60
CHE 535/ CHH 535	Physical Chemistry-IV (Analytical Techniques)	4	3	1	0	4	75		25	100	61-63
CHE 536	Organic Chemistry Lab- II	6	0	0	3	3		56	19	75	64-65
CHE 537	Physical Chemistry Lab-II	6	0	0	3	3		56	19	75	66-67
	Allocation of Project work										
	TOTAL	34				28	·			700	

	SEMESTER - IV										
Course		Hours	(	Cred	its	Total		Max	Marl	ks	Page
Code	Course Name	/Week	L	Т	P	Credits	Th	P	I A	Total	No.
	Major Courses										
CHE 541/ CHH 541	Inorganic Chemistry-IV: (Advanced Inorganic Chemistry)	6	5	1	0	6	112		38	150	69-70
CHE 542/ CHH 542	Organic Synthesis-VI (Asymmetric synthesis, Green Chemistry and Heterocyclic Chemistry)	6	5	1	0	6	112		38	150	71-73
CHE 543/ CHH 543	Physical Chemistry-V (Surface and Polymer Chemistry)	6	5	1	0	6	112		38	150	74-75
	PROJECT WORK (Non-Evaluative)										
	TOTAL									450	

Post Graduate Department of Chemistry

# Semester-I

Academic Session: 2024-25

7



# Post Graduate Department of Chemistry

M.Sc. Chemistry/M. Sc. Chemistry (Under the Honours Scheme) (Semester-I) CHE 411/CHH 411: Inorganic Chemistry-I

Ligand Field and Group Theory

Total Hours: 60 Total Hours/week: 4 Total Credits: 4

Total Credits: 4
L T P
4 0 0

Maximum Marks: 100

Theory: 75
Internal Assessment: 25

### INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi.
- III. Section-I will consist of EIGHT questions and students are required to attempt any SIX short questions carrying 2.5 Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 15 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

### **COURSE OBJECTIVES:**

The main objective of this course is to teach the use of mathematical tool of Group Theory in the field of chemistry for evaluating the properties of the molecules. The Ligand field Theory and its use to predict spectral, magnetic and other physical properties of inorganic compounds will also be the main focus of this course.

### **COURSE CONTENTS:**

#### UNIT-I

# 1. Group theory and its applications-I

15 Hrs

Symmetry, symmetry elements and operations, Determination of point groups (flow chart), Order and class of point group, Reducible and irreducible representations (H<sub>2</sub>O and BF<sub>3</sub>).

Multiplication tables and derivation of character tables for  $C_{2V}$ ,  $C_{3V}$  and cyclic group, Great orthogonality theorem, Mullikens notations.

#### **UNIT-II**

#### 2. Group theory and its applications-II

15 Hrs

Crystallographic Symmetry, Sub groups, determination of symmetry of atomic orbitals under different point groups. Hybridization of atomic orbitals: sp, sp<sup>2</sup>,sp<sup>3</sup>,dsp<sup>2</sup>,sp<sup>3</sup>d and d<sup>2</sup>sp<sup>3</sup> and group theory, Matric representation of symmetry operations, group theory and CFT.

Separation of d-orbitals under the influence of  $T_d$ , square planar,  $O_h$  and trigonal bipyramid symmetry, Vibrational modes in non-linear molecules, representation of vibrational modes in  $H_2O$ ,  $NH_3$  and  $BF_3$ . Group theory and linear molecules.



# Post Graduate Department of Chemistry

#### **UNIT-III**

# 3. Ligand Fields-I

Concept and scope of ligand fields, d and other orbitals, Qualitative determination of ligand field effects, the physical properties affected by LF, Ionic model of coordination compounds, Spin-orbit coupling, free ion in weak CF, Effect of cubic field on S,P,D,F,G,H,I terms.

Heat of ligation and CFSE, Standard electrode potential and CFSE, Cation distribution in lattice, spinels, interionic separation and CFSE and chemical stability.

#### **UNIT-IV**

# 4. Ligand Fields-2

Free ion in medium and strong fields. Transition from weak to strong fields, Correlation and Tanabe Sugano diagrams for d<sup>2</sup> to d<sup>9</sup> (O<sub>h</sub> and T<sub>d</sub>), Elementary MOT, Bonding in octahedral and tetrahedral complexes.

Qualitative calculations of 10 Dq. Electronic spectra of complexes, Selection rules and band widths and factors, Jahn Teller effect. Spectra of  $[M(H_2O)_6]^{+2}$ .

Spectra of spin free and paired complexes, distorted O<sub>h</sub> and T<sub>d</sub> complexes, Spectrochemical and Nephelauxetic series and CT spectra.

### **BOOKS PRESCRIBED:**

- 1) Chemical applications of group theory by F.A. Cotton.
- 2) Introduction to Ligand fields by B.N. Figgis.
- 3) Group theory by Raman.
- 4) Group theory in Chemistry by Gopinathan and Ramakrishnan.

#### **COURSE OUTCOMES:**

S. No.	On completing the course, student will be able to
CO1	Identify elements of symmetry on chemical compounds on the basis of their structure and correlate these elements of symmetry with point groups to which the molecule belongs
CO2	Apply the mathematical concepts of matrices, determinants on various symmetry operations.
CO3	Apply the mathematical tool of 'Group Theory' on various molecules to derive reducible and irreducible representation. This also leads to the use of group theory derive the type of hybridisations and IR active and Raman active modes of vibrations in the molecules
CO4	Develop the understanding of Bonding in coordination compounds in terms of CFT and LFT.
CO5	Construct orgel diagrams, Correlation diagrams and Tunabe-Sugano diagrams along with the study of electronic, magnetic and spectrochemical properties of the coordination compounds.



# Post Graduate Department of Chemistry

# M.Sc. Chemistry (Semester-I) CHE 412: Organic Synthesis-I

Reaction Mechanism-Substitution Reactions

Total Hours: 60 Total Hours/week: 4 Total Credits: 4

Maximum Marks: 100 Theory: 75

L T P Internal Assessment: 25

4 0 0

### INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi.
- III. Section-I will consist of EIGHT questions and students are required to attempt any SIX short questions carrying 2.5 Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 15 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

#### **COURSE OBJECTIVE:**

The course is designed to introduce the quantitative aspects of reactivity, effect of structure and the different reactive intermediate involved in the organic reactions. Further, the course provides an in-depth knowledge of mechanisms of different types of substitution reaction of aliphatic as well as aromatic organic compounds.

#### **COURSE CONTENTS:**

UNIT-I

#### 1. Reaction Mechanism: Structure and Reactivity

15 Hrs

Type of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle, Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects. Hard and soft acids and bases.

Generation, structure, stability and reactivity of carbenes and nitrenes with special emphasis on cycloaddition, rearrangement and Insertion reaction.

Effect of structure on reactivity- resonance and field effects, steric effect, quantitative treatment. The Hammett equation and linear free energy relationship, substituent and reaction constants. Taft equation.

**UNIT-II** 

# 2. Stereochemistry:

8 Hrs

R/S Nomenclature, Calculation of number of stereoisomers for molecule with one or more chiral center, Crams Rule, Sharpless asymmetric epoxidation Elements of symmetry, chirality, molecules with more than one chiral center. Threo and erythro isomers, methods of resolution, optical purity.



# Post Graduate Department of Chemistry

Prochirality – enantiotopic and diastereotopic atoms, groups and faces.

Stereospecific and stereoselective synthesis. Asymmetric synthesis. Optical activity in absence of chiral carbon (Biphenyls, Allenes, Spiranes). Chirality due to helical shape.

### 3. Aliphatic Electrophilic Substitutions

7 Hrs

Bimolecular mechanisms-  $S_E2$  and  $S_Ei$ : The  $S_E1$  mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity, Hell-Volard-Zelinsky reaction.

**UNIT-III** 

# 4. Aliphatic Nucleophilic Substitutions

8 Hrs

The  $S_N2$ ,  $S_N1$ , missed  $S_N1$  and  $S_N2$  and SET mechanisms. The neighboring group mechanism, neighboring group participation by  $\pi$  and  $\sigma$  bonds, anchimeric assistance.

Classical and non-classical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations. The S<sub>N</sub>*i*mechanisum,

Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium,

Phase transfer catalysis and ultrasound, ambident nucleophile, regioselectivity. Gabriel synthesis

### 5. Aromatic Nucleophilic Substitution

7 Hrs

The  $S_NAr$ ,  $S_N1$ , benzyne an  $SR_N1$  mechanisms, Reactivity-effect of substrate structure, leaving group and attacking nucleophile.

The von Richter, Sommelet-Hauser, and Smiles rearrangements.

**UNIT-IV** 

#### 6. Aromatic electrophilic substitution

8 Hrs

The arenium ion mechanism, orientation and reactivity in mono substitution and disubstituted aromatics, energy profile diagram, the *ortho/para* ratio, ipso attack, orientation in other ring systems, quantitative treatment of reactivity in substrates and electrophiles.

Diazo coupling, Vilsmeir reaction, Gatterman-Koch reaction, Bechmann reaction, Hoben-Hoesch reaction.

#### 7. Free Radical Reactions

7 Hrs

Types of free radical reactions, free radical substitution mechanism, and mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in the attacking radicals. The effect of solvents on reactivity.

Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, autooxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.

Academic Session: 2024-25

11



# Post Graduate Department of Chemistry

# **BOOKS PRESCRIBED:**

- 1. Stereochemistry Eliel
- 2. Advanced Organic Chemistry Jerry March.
- 3. Advanced Organic Chemistry, F. A. Carey, R. J. Sundberg, Volume I and II
- 4. Highlights of Organic Chemistry, W.J. L. Nobel; An Advanced Text Book.
- 5. Stereochemistry conformation and Mechanism P. S. Kalsi

# **COURSE OUTCOMES:**

S. No.	On completing the course, student will be able to
CO1	Understand various methods of generation of carbocations, carbanions, free radicals, carbenes, nitrenes and their applications in organic synthesis.
CO2	Study the mechanism of different types of free radical substitution reactions and free radical rearrangements.
CO3	Learn the mechanism of different aliphatic/aromatic nucleophilic and electrophilic substitution reactions
CO4	Able to assign R/S configuration to the molecules with one or more than one chiral centers, allenes, biphenyls, and spiranes and can analyze the effect of structure on reactivity of compound quantitatively.
CO5	Develop interest in writing and finding mechanisms of substitution and rearrangement reactions.

Academic Session: 2024-25

12



# Post Graduate Department of Chemistry

M.Sc. Chemistry/M. Sc. Chemistry (Under the Honours Scheme) (Semester-I)

CHE 413/CHH 413 Physical Chemistry-I Thermodynamics

Total Hours: 60 Total Hours/week: 4

**Total Credits: 4** 

L T P 4 0 0

Maximum Marks: 100

Theory: 75

**Internal Assessment: 25** 

### INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi.
- III. Section-I will consist of EIGHT questions and students are required to attempt any SIX short questions carrying 2.5 Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 15 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

#### **COURSE OBJECTIVE:**

The Course is thoughtfully prepared to give first the overview of the classical laws of thermodynamics and its applications. Further, the course elaborates the concept of statistical thermodynamics to inter-relate the quantum mechanics and thermodynamics. Also, the irreversible thermodynamics based on real life examples has been formulated.

### **COURSE CONTENTS:**

**UNIT-I** 

# 1. Classical Thermodynamics-I

15Hrs

Brief resume of concepts of thermodynamics, Helmholtz and Gibb's free energy, chemical potential and entropy. Partial molar properties, partial molar free energy, partial molar volume and partial molar heat content and their significances. Determination of these quantities. Concept of fugacity and determination of fugacity.

UNIT-II

#### 2. Classical Thermodynamics-II

15 Hrs

Non-ideal systems: Excess functions for non-ideal solutions. Activity, activity coefficients, Debye-Huckel theory for activity coefficient of electrolytic solutions, determination of activity and activity coefficients, ionic strength.

**UNIT-III** 

#### 3. Statistical Thermodynamics:

15Hrs

Thermodynamic probability, Most probable distribution, Stirling approximation, Maxwell-Boltzmann distribution law, Entropy and probability, Ensemble averaging, postulates of



# Post Graduate Department of Chemistry

ensemble averaging. Types of ensemble systems, Lagrange's method of undetermined multipliers. Partition functions: Translational, rotational, vibrational and electronic partition function, calculation of thermodynamic properties in terms of partition functions. Application of partition functions in the determination of equilibrium constants and heat capacity behavior of solids-chemical equilibria. Types of statistics: Fermi-Dirac statistics-distribution laws, Bose-Einstein statistics- distribution law and application to helium.

#### **UNIT-IV**

#### 4. Non Equilibrium Thermodynamics:

15 Hrs

Thermodynamic criteria for non-equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes: heat flow, chemical reactions. transformations of generalized fluxes and forces, non-equilibrium stationary states, phenomenological equations, microscopic reversibility, irreversible thermodynamics for biological systems, coupled reactions.

### **BOOKS PRESCRIBED:**

- 1. S. Glasstone: Thermodynamics for Chemists
- 2. P.W. Atkins: Physical Chemistry
- 3. S.H. Maron& C.F. Prutton: Principles of Physical Chemistry
- 4. Introduction to the Thermodynamics of Biological Processes by D. Jou& J. E. LLebot.
- 5. Pitts: Non equilibrium thermodynamics
- 6. I Prigogine: Introduction to thermodynamics of irreversible processes

#### **COURSE OUTCOMES:**

S. No.	On completing the course, student will be able to
CO1	Students will learn about the classical thermodynamics and revise the basic concepts
CO2	Learn to conceptualise the statistical mechanics derivations
CO3	Understands the link between classical mechanics and quantum mechanics by studying statistical mechanics
CO4	Deriving the thermodynamic parameters from quantum chemistry
CO5	Studying the irreversible thermodynamics and correlating real life problems

Academic Session: 2024-25



# Post Graduate Department of Chemistry

M.Sc. Chemistry/M. Sc. Chemistry (Under the Honours Scheme) (Semester-I)

# CHE 414/CHH 414 Spectroscopy-A

Techniques for Structure Elucidation of Organic Compounds

Total Hours: 90

Total Hours/week: 6 Maximum Marks: 150

Total Credits: 6 Theory: 112
L T P Internal Assessment: 38

6 0 0

#### INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi.
- III. Section-I will consist of EIGHT questions and students are required to attempt any SIX short questions carrying 4 Marks each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 22 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

#### **COURSE OBJECTIVE:**

The course is well designed for the introduction of various concepts in molecular spectroscopy covering UV, IR, 1HNMR, 13C-NMR, 2D NMR and mass spectroscopy. It enables the students for interpretation of spectra and data analysis leading to skill enhancement. This course makes students employable in industries.

#### **COURSE CONTENTS:**

**UNIT-I** 

#### 1. General Features of Spectroscopy:

7 Hrs

The Electromagnetic Spectrum, Characteristics of Electromagnetic Radiations, Units of Frequency, Wavelength, Wave number and their conversion factors, Interaction of radiation with matter, Absorption of Electromagnetic Radiation by Organic Molecules, Absorption and emission spectroscopy, electronic and nuclear energy levels, Transition probability and Selection Rules, Basic features of different spectrometers, Line widths and Broadening.

#### 2. Nuclear Magnetic Resonance Spectroscopy-I

15Hrs

Principal of NMR, Natural abundance of  $^{13}$ C,  $^{19}$ F and  $^{31}$ P nuclei; The spinning nucleus, effect of external magnetic field, precessional motion and frequency, Chemical shift and its measurements. Factors influencing chemical shift, anisotropic effect, vander Waals deshielding, Integrals of protons, proton exchange, spin-spin coupling-splitting theory, one, two and three bond coupling, virtual, long range and allylic coupling, magnitude of coupling constant; factors affecting the coupling constant, Chemical and magnetic equivalence, First and second order spectra,  $A_2$ , AB, AX,  $AB_2$ ,  $AX_2$ ,  $A_2B_2$  and  $A_2X_2$   $AX_3$ ,  $A_2X_3$ , AMX, ABC spin systems.

UNIT-II

Academic Session: 2024-25



# Post Graduate Department of Chemistry

# 3. Nuclear Magnetic Resonance Spectroscopy-2

23 Hrs

Simplification of complex spectra: increased field strength, spin decoupling or double resonance and lanthanide shift reagents, <sup>13</sup>C-NMR: Natural Abundance <sup>13</sup>C, Resolution and multiplicity of <sup>13</sup>C NMR, Proton coupled <sup>13</sup>C spectra, <sup>14</sup>H Decoupled <sup>13</sup>C spectra; off-resonance <sup>13</sup>C spectra. NOE effect, Cross polarization and origin of nuclear overhauser effect. <sup>13</sup>C Solvents, Heteronuclear coupling. NMR spectra of diastereotopic systems.

Structural applications of <sup>13</sup>C-NMR., pulse sequences, pulse widths, spins and magnetization vectors, The DEPT experiment & its use in structural elucidation, INEPT.

Introduction to 2D-NMR, COSY, TOCSY, & HETCOR, HSQC spectra, NOE-based experiments: NOESY.

#### **UNIT-III**

#### 3. Mass Spectra:

11 **Hrs** 

Introduction, methods of ionization EI & CI, Brief description of LD, FAB, SIMS, FD etc., Ion analysis methods (in brief), isotope abundance, Metastable ions, general rules predicting the fragmentation patterns. Nitrogen rule, determination of molecular ion peak, index of H deficiency, fragmentation patterns for aliphatic compounds, amines, aldehydes, Ketons, esters, amides, nitriles, carboxylic acids ethers, aromatic compounds etc.

### 4. UV and Visible Spectroscopy of organic molecules:

12 Hrs

Measurement techniques, Beer – Lambert's Law, molar extinction coefficient, oscillator strength and intensity of the electronic transition, Frank Condon Principle, Ground and first excited electronic states of diatomic molecules, relationship of potential energy curves to electronic spectra, Chromophores, auxochromes, blue shift, red shift, hypo and hyperchromic effect,  $n-\sigma^*,\pi-\pi^*$ ,  $n-\pi^*$  transitions in organic molecules.

Woodward rules for conjugated dienes and  $\alpha,\beta$ -unsaturated carbonyl groups, extended conjugation and aromatic sterically hindered systems.

#### **UNIT-IV**

# 5. Infrared Spectroscopy

11 Hrs

Vibrational Energy Levels, Degree of freedom, Selection Rules, Force Constant, Fundamental Vibrational frequencies, Factors influencing Vibrational Frequencies (Vibrational Coupling, Hydrogen Bonding, electronic effect, Bond Angles, Field Effect). Sampling Techniques, Absorption of Common functional Groups, Interpretation, Finger print Regions.

Applications in Organic Chemistry

- (a) Determining purity
- (b) Studying reaction kinetics.
- (c) Studying hydrogen bonding.
- (d) Studying molecular geometry & conformational analysis.
- (e) Studying reactive species

## 6. Solution of Structural Problems by Combined Use of the following Spectroscopic Techniques

11Hrs

- (a) Electronic spectra
- (b) Vibrational spectroscopy
- (c) NMR (1H and 13C) spectroscopy
- (d) Mass Spectroscopy



# Post Graduate Department of Chemistry

# **BOOKS PRESCRIBED:**

- 1. Pavia, Lampman&Kriz, Introduction to Spectroscopy.
- 2. C.N Banwell "Fundamentals of Molecular Spectroscopy".
- 3. R. M. Silverstein, G.C.Bassler, T.C. Morrill, "Spectrometic Identification of Organic Compounds.
- 4. W. Kemp, "Organic Spectroscopy".
- 5. D.H. Williams, I. Fleming, "Spectroscopic Methods in Organic Chemistry".
- 6. D.H. Williams, I. Fleming, "Spectroscopic Problems in Organic Chemistry", 1967.
- 7. R.C. Banks, E.R. Matjeka, G. Mercer, "Introductory Problems in Spectroscopy", 1980.
- 8. G.M. Barrow "Introduction to Molecular Spectroscopy".

# **COURSE OUTCOMES:**

S. No.	On completing the course, student will be able to							
CO1	Learn the basic principles of interpret uv-visible, vibrational, 1-D and 2-D NMR and Mass spectroscopy for the structure identification of organic compounds							
CO2	Students will gain an understanding of molecular-level critical thinking skills							
CO3	Analyse and interpret uv-visible, vibrational, 1-D and 2-D NMR and Mass spectral data of organic compounds							
CO4	Analyse the mass of organic molecule and fragments present in the molecule from mass spectral studies							
CO5	Evaluate various structural possibilities and arrive at the most logical structure of organic compounds by analysis and interpretation of uv-visible, vibrational, 1-D/2-D NMR and Mass spectral data.							



# Post Graduate Department of Chemistry

M.Sc. Chemistry/M. Sc. Chemistry (Under the Honours Scheme) (Semester-I)

# CHE 415/CHH 415 Inorganic Chemistry Lab-I

Quantitative analysis

Total Hours: 90 Total Hours/week: 6 Total Credits: 3 L T P

Maximum Marks: 75 Theory: 56

**Internal Assessment: 19** 

0 0 3

# **INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES:**

I. The exam will be conducted on two sessions ie Morning and Evening

II. Students will perform two practicals.

III Students will be asked to complete write up of both practical within first 30 minutes on the first sheet provided.

IV. On the second sheet provided after 30 minutes, students will perform and note the record on second sheet during the conduct of practical exam

V. The split of marks will be as under:

(Write-up = 20, Performance = 20, Viva-Voce = 10, Practical notebook = 6)

#### **COURSE OBJECTIVES:**

To analyse quantitative estimation of metal ions and anions using Oxidation-Reduction Titrations, . Precipitation Titrations, Complexometric Titrations and Gravimetric Analysis

#### **COURSE CONTENTS:**

#### I. Oxidation-Reduction Titrations

- 1. Standardization with sodium oxalate of KMnO<sub>4</sub> and determination of Ca<sup>2+</sup>ion.
- 2. Standardization of ceric sulphate with Mohr's salt and determination of Cu<sup>2+</sup>, NO<sub>3</sub>-land C<sub>2</sub>O<sub>4</sub>-lons.
- 3. Standardization of K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub>with Fe<sup>2+</sup>and determination of Fe<sup>3+</sup> (Ferric alum)
- 4. Standardization of hypo solution with potassium iodate / K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> and determination of available Cl<sub>2</sub>in bleaching powder, Sb<sup>3+</sup>and Cu<sup>2+</sup>.
- 5. Determination of hydrazine with KIO<sub>3</sub>titration.

#### **II. Precipitation Titrations**

- 1. AgNO<sub>3</sub>standardization by Mohr's method by using adsorption indicator.
- 2. Volhard's method for Cl-determination.
- 3. Determination of ammonium / potassium thiocyanate.

#### **III. Complexometric Titrations**

- 1. Determination of Cu<sup>2+</sup>and Ni<sup>2+</sup>by using masking reagent by EDTA titration.
- 2. Determination of Ni<sup>2+</sup>(back titration).



# Post Graduate Department of Chemistry

3. Determination of Ca<sup>2+</sup>(by substitution method).

# IV. Gravimetric Analysis

- 1. Determination of Ba<sup>2+</sup>as its chromate.
- 2. Estimation of lead as its lead molybdate.
- 3. Estimation of chromium (III) as its lead chromate.
- 4. Estimation of Cu<sup>2+</sup>using Ammonium/ Sodium thiocyanate.

#### **BOOKS PRESCRIBED:**

Book: Vogel's book on Inorganic Quantitative Analysis.

### **COURSE OUTCOMES:**

S. No.	On completing the course, student will be able to
CO1	Prepare the exact solution and Standardization for quantitative analysis of the solutions.
CO2	Determine of different ions like Ca <sup>2+</sup> , Fe <sup>2+</sup> , Oxalate, nitrate, available chlorine in bleaching powder using oxidation reduction titrations
CO3	Able to perform Precipitation Titrations using Volhard's method and Mohr's methods
CO4	Determine of different ions (Cu <sup>2+</sup> , Ni <sup>2+</sup> and Ca <sup>2+</sup> ) using complexometric Titrations
CO5	Estimate of ions using gravimetric techniques.

Academic Session: 2024-25

19



# Post Graduate Department of Chemistry

M.Sc. Chemistry (Semester-I)
CHE416: Organic Chemistry Lab-I
Quantitative analysis and Multistep Synthesis

Total Hours 90
Total Hours/week: 6
Total Credits: 3
L T P

0 0 3

Maximum Marks: 75

Theory: 56

**Internal Assessment: 19** 

### **INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES:**

- I. The exam will be conducted on two sessions ie Morning and Evening
- II. Students will perform two practicals.

III Students will be asked to complete write up of both practical within first 30 minutes on the first sheet provided.

IV. On the second sheet provided after 30 minutes, students will perform and note the record on second sheet during the conduct of practical exam

V. The split of marks will be as under:

(Write-up = 20, Performance = 20, Viva-Voce = 10, Practical notebook = 6)

#### **COURSE OBJECTIVES:**

This course aims to impart to the student knowledge of: Laboratory set up, safe handling of chemicals, workup procedures and effective disposal of organic waste. The practicals include various methods of preparing organic compounds in a multiple step as well as Quantitative Analysis of Organic Compounds.

#### **COURSE CONTENTS:**

# 1. Quantitative Analysis

- (a) Extraction of Organic Compounds from Natural Sources
- 1. Extraction of Caffeine from tea leaves
- 2. Isolation of casein from milk
- 3. Extraction of natural products using Soxhlet apparatus
- (b) Quantitative Analysis of Organic Compounds:
- 1. Estimation of phenol/aniline using bromate-bromide solution.
- 2. Estimation of reducing sugar by Fehling solution method.
- 3. To determine the saponification value of the given fat or oil sample.
- 4. To determine the iodine number of the given fat or oil sample.

#### 2. Multistep Organic Synthesis

- 1. Synthesis of 2-chloro-4-bromoaniline from aniline (Bromination and chlorination)
- 2. Photochemical synthesis of benzpinacol and its pinacol rearrangement.
- 3. Synthesis of 2,4-dinitrophenyl hydrazine from chloro benzene. (Electrophilic and nucleophilic substitution reactions on aromatic ring).
- 4. Synthesis of 2-phenyllndole-Fischer Indole Synthesis. Synthesis of 3-nitrobenzoic from



# Post Graduate Department of Chemistry

benzoic acid

- 5. Cannizaro's reaction of 4-chlorobenzaldehyde.
- 6. Green synthesis of dihydropyrimidones and their structure confirmation by spectroscopic techniques

### 4. Applications of chromatographic techniques

#### 1. TLC analysis:

TLC Analysis of the the purified samples along with the mixture in same TLC plates (component 1 with mixture and component 2 with mixture on separate TLC plate) and calculation of Rf values-Reporting and recording

### 2. Column Chromatography:

Separation of a mixture by column chromatography of o-nitroaniline and p-nitroaniline.

3. UV, IR, <sup>1</sup>H NMR, <sup>13</sup>C NMR, EI mass spectral identification of drug molecules from a library of compounds

# 3. Microwave Organic Synthesis

MW-assisted synthesis of substituted pyridines under solvent and catalyst free conditions

#### **BOOK PRESCRIBED:**

- 1. Vogel's Textbook of Practical Organic Chemistry
- 2. Advanced Practical Organic Chemistry by N. K. Vishnoi
- 3. Lab Mehods in Organic Chemistry by Solomon Marmor
- 4. Yin G, Liu Q, Maa J, She N. Solvent and catalyst free synthesis of new hydroxylated trisubstituted pyridines under microwave irradiation. Green Chemistry, 2012, 14, 1796-98.

### **COURSE OUTCOMES:**

S. No.	On completing the course, student will be able to
CO1	Predict the results and identify errors associated with a chemical analysis based on the analytical technique and nature of the sample.
CO2	Justify the steps to prepare and standardize different solutions.
CO3	Do hands on expertise to synthesize organic compounds. Able to check Purity of organic compounds & the progress of the reaction by performing TLC Techniques individually
CO4	Characterize the structure of the organic compound by interpreting IR, UV, 1H NMR and Mass spectral data.
CO5	Gain hands-on practice of handling Laboratory Equipment.



# Post Graduate Department of Chemistry

M.Sc. Chemistry/M. Sc. Chemistry (Under the Honours Scheme) (Semester-I)

Basics and Applications of Chemistry Softwares (Theory)

CHE 417/CHH 417

Total Hours: 90 Total Hours/week: 6 Total Credits: 4 L T P

2 0 2

Maximum Marks: 100 Theory + Practical: 37 + 38 Internal Assessment: 25

# **INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES (Theory):**

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi.
- III. Section-I will consist of EIGHT questions and students are required to attempt any SIX short questions carrying 1.5 Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 7 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

#### **COURSE OBJECTIVES:**

- 1. To comprehend how to use MS Excel for data processing to generate various types of graphs, carry out calculation based upon formulae and curve fitting of the data along with systematic presentation of graph.
- 2. To comprehend how to use MS power point for presentation of theoretical articles and research outcomes.
- 3. To comprehend how to use Chem Draw for structure drawing, equation writing, IR and NMR data analysis.
- 4. To comprehend how to use Origin Software for data processing.

### **COURSE CONTENTS:**

Unit-I

# 1. MS Excel

Excel Basics, Work with Cells and Worksheets, Entering Text and Numbers, Entering Excel Formulas and Formatting Data, Creating Excel Functions, Creating Charts, More on Entering Excel Formulas, Format your Workbook, Add Charts and Graphics, Collaborate with Others, Analyze your Data, Work with Macros and the Web, functions and formulas, charts, data analysis,

#### 2. MS Power Point

Create and Manage Presentations, Create a Presentation, Insert and Format Slides, Modify Slides, Handouts, and Notes, Change Presentation Options and Views, Configure a Presentation for Print, Configure and Present a Slide Show, Insert Tables, Charts, Smart Art, and Media., Insert and Format Smart Art graphics, Insert and Manage Media, Apply Transitions and Animations, Apply Slide Transitions, Animate Slide Content, Set Timing for Transitions and Animations.



# Post Graduate Department of Chemistry

#### Unit-II

#### 3. ChemDraw

Chem Draw Ultra 8.0 software, Introduction, Download and installation process, Drawing various chemical structures (acyclic, cyclic, polycyclic, heterocyclic), Nomenclature generation, conversion of name into molecular structure, Calculation of physical properties such as density, molecular weight, molecular formula, refractive index from structural formula,. <sup>1</sup>H, <sup>13</sup>C NMR prediction from molecular structure, Drawing structure of bigger molecules such as proteins, carbohydrates, and RNA/DNA, bio arts, Use of templates, Comparison of various Chem Draw software.

#### Unit-III

#### 4. Origin 8.5 Software

The Origin Workspace. Multi-sheet Workbooks Managing Data and Metadata. Importing Data from different sources. Working with Origin. Basic Data processing. Creating and Customizing Graphs. Custom Graph Templates and Themes. Publishing Graphs. Basic Data Analysis.

#### Unit IV

#### 5. Introduction to Molecular Docking

Definition and introduction to Molecular Docking, Softwares used for Docking, Types of Molecular docking: Rigid docking, flexible docking, Ligand sources – Natural, synthetic and semi-synthetics, Protein Structure Basics, Protein Databases, Force fields, Ligand Preparation, Protein Preparation, Receptor Grid Generation, Ligand Docking, Analysis of ligand protein interactions, ADME properties. Any two Case studies.

# **Practicals**

# INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES (Theory):

- 1. Invigilator to assign two practical tasks to each student.
- 2. Students need to complete both practicals within 3 Hrs.
- 3. Invigilator to vary out the split of marks as per nature of experiment assigned

#### CONTENTS OF PRACTICAL SYLLABUS

- 1. Create presentations from a template. Add text, images, art, and videos.
- 2. Design a poster in MS powerpoint based upon the
- 3. Draw the structure of following compounds using ChemDraw
- (a) Paracetamol (b) Chloramphenicol (c) Amoxicillin (d) Urotropine (e) Morphine
- 4. Draw the graph based upon data provided from a manuscript and carry out curve fitting of the data for various orders using Origin Sofware.
- 5. Draw multiple curves on the same axis using Excel and present each curve with different colour and mark the peaks in a separate box within the graph.
- 6. Draw 3D graphs based upon the three variables provided by using Origin software.
- 7. To write chemical reaction and mechanism for the following reaction using ChemDraw
  - (a) Aldol condensation of acetophenone
  - (b) Cannizarro reaction of benzaldehyde in 50% NaOH solution
  - (c) Fries Rearrangement
  - (d) Mannich reaction



# Post Graduate Department of Chemistry

(e) HVZ reaction and subsequent hydrolysis with aq KOH.

- 8 Export data of IR spectrum and plot the IR spectrum using Origin software/Excel.
- 9. Export data of UV-spectrum and plot the spectru using Origin software/Excel.
- 10. Molecular docking of Aspirin (Anti-inflammatory Drug) in the crystal coordinate of COX-2.
- 11. Molecular docking of Trimethoprim (Antibiotic Drug) in the crystal coordinate of DHFR.

### **BOOKS PRESCRIBED:**

- 1. K.V. Raman, Computers in Chemistry, Tata McGraw Hill.
- Tamanna Anwar, Pawan Kumar, Asad U. Khan, Chapter 1 Modern Tools and Techniques in Computer-Aided Drug Design, Editor(s): Mohane S. Coumar, in book Fundamentals, Techniques, Resources and Applications 2021, Pages 1-3 https://www.sciencedirect.com/book/9780128223123/molecular-docking-for-computer-aided-drug-design
- 3. https://www.nature.com/articles/s41429-019-0240-6
- 4. https://www.sciencedirect.com/science/article/pii/S1878535221005554
- 5. Chem Draw 7.0: Chemical Structure Drawing Standard User's Guide Paperback, 2001 by Cambridge Scientific Computing.
- 6. Tutorial to ChemDraw: For beginner Kindle Edition by JUHN MORTON.
- 7. Origin Software Complete Usage Instruction and Graph Representation: A complete Guide for new users by Muhammad Arsalan, Azka Awais

# **COURSE OUTCOMES:**

S. No.	On completing the course, student will be able to
CO1	Carry out formula based calculation, plot graphs, carry out curve fitting of the data for research purposes.
CO2	Plot graphs and process research data using Origin software
CO3	Draw the chemical structures and write chemical reactions using ChemDraw software.
CO4	Convert chemical name to structure, structure to chemical name and predict 1H and 13C -NMR data of the compound.
CO5	Make power point slides for presentation of research work.



Post Graduate Department of Chemistry

# Semester-II

Academic Session: 2024-25

25



# Post Graduate Department of Chemistry

# M.Sc. Chemistry (Semester-II) CHE 421: Inorganic Chemistry-II

Reaction Mechanism, Organometallics and Catalysis

Total Hours: 60 Total Hours/week: 4 Total Credits: 4

Total Credits: 4 L T P

4 0 0

Maximum Marks: 100

Theory: 75

**Internal Assessment: 25** 

# INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi.
- III. Section-I will consist of EIGHT questions and students are required to attempt any SIX short questions carrying 2.5 Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 15 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

#### **COURSE OBJECTIVES:**

The main objective of this course is to impart knowledge on organometallic compounds and their catalytic applications. In addition to this oxidation reactions and ligand replacement reactions are explained with examples.

#### **COURSE CONTENTS:**

UNIT-I 15Hr

Energy, polarity and reactivity of M-C bond, stability and lability of main group organometallics and their preparation.

Li organometallics: Structure, bonding and reactions. Carbolithitian. Organometallics of group 2 and 12:

Organometallics of Be and Mg: Preparation, mechanism of formation and constitution, Grignard reagent in solution and reactions.

Organometallics of Zn, Cd, Hg: Preparation, structure and properties. Technical applications of tris(alkyl)aluminium compounds.

Organometallics of transition elements: EAN rule and MOT relationship in  $O_h$  sigma and  $\sigma_h$  sigma and  $\sigma_h$  bonding. The particular case of  $d^8$  and  $d^{10}$  complexes. Sigma and  $\sigma_h$  donor/acceptor ligands.

UNIT-II 15Hrs

Olefin complexes: Preparation, structure and bonding. Alkyne and allyl complexes: Preparation, structure and reactions. Complexes of cyclic  $\pi$  parameter  $C_nH_n$ ; Sandwich complexes, half sandwich complexes, Multidecker sandwich complexes, Tilted sandwich structure, complexes with more than two  $C_nH_n$  ligand.  $C_4H_4$  and  $C_5H_5^-$ 

Organometallics: Preparation, structure, reactions and bonding. MOT for ferrocene and bis(benzene)chromium(0): preparation and reactions. Cycloheptatrienyl and COT complexes: preparation and structure and bonding.

Catalytic reactions and 16/18 electron rule, alkene metathesis, Chauvin mechanism, Olefin



# Post Graduate Department of Chemistry

polymerization, Ziggler-Natta polymerization, Cossee mechanism, hydrogenation of alkenes, Wilkinson's catalyst, Fischer-Tropsch reactions, water gas shift reactions, Monsanto acetic acid process, hydrocyantion, Reppecarbonylation, hydroformylation of unsaturated compounds.

UNIT-III 15Hrs

Reductive carbonylation of alcohols and other compounds, carbonylation reactions: methanol and methyl acetate, adipic ester and other compounds, synthesis and carbonylation reactions, decarbonylation reaction, catalytic addition of molecules to carbon-carbon multiple bonds, homogeneous hydrogenation, hydrocyanation and hydrosilation of unsaturated compounds, polymerization. Oligomerisation and metathesis of alkene and alkynes. Cluster compounds in catalysis, supported homogeneous and phase transfer catalysis, oxidation reactions, and oxidative carbonylation. Pd catalysed oxidation of ethylene, acrylonitrile synthesis, oxygen transfer from peroxo and oxo species and NO<sub>2</sub> groups.

Ligand replacement reaction, Labile and Inert complexes and CFT, water exchange rates, formation of complexes from aqueous ions, Anation, Aquation and acid-base hydrolysis, Mechanism of acid hydrolysis when inert ligand is a  $\pi$  donor/acceptor and cis to leaving group, attack on ligands.

Substitution in square planar complexes, factors, trans effect, its theories and applications, Kurnakov test.

UNIT-IV 15Hrs

Metal carbonyl reactions, reactions of binuclear carbonyls, associative reactions, species with 17 electrons, electron transfer processes, orbital occupation effects on substitution reactions of octahedral complexes. Synthesis of coordination compounds by substitutional reactions, synthetic chemistry of some cobalt and platanium complexes. Marcus theory and applications, electron transfer reactions, doubly bridged inner sphere, electron transfer, other electron transfer, and two electron transfer reactions, complimentary and non-complimentary reactions. Ligand exchange *via* electron exchange, Stereochemical non-rigidity of complexes and organometallics and NMR, trigonal and trigonal bipyramid molecules, system with coordination number 6 and more .Isomerisation and racemisation of tris chelates complexes and mechanism. Metal carbonyl scrambling, Rotation within coordination sphere.

#### **BOOK PRESCRIBED:**

- 1) F.A.Cotton and I.G. Wilkinson, Advanced Inorganic Chemistry, 5<sup>th</sup>ed. New YORK 1988.
- 2) Organometallics by Salzer.



# Post Graduate Department of Chemistry

# **COURSE OUTCOMES:**

S. No.	On completing the course, student will be able to
CO1	Understand organometallic chemistry with focus on the transition metals. catalysis
CO2	Study the wide variety of organometallic compounds and the choice of hapticity in different conditions.
CO3	Students will be able to understand the role of coordination number, coordination geometry and oxidation state of metal in catalytic cycles.
CO4	Know Structure and bonding issues in organometallic compounds are discussed in view of the 18-electron rule.
CO5	Go through some important emerging compounds especially multidecker sandwich compounds

Academic Session: 2024-25



# Post Graduate Department of Chemistry

M. Sc. Chemistry/M. Sc. Chemistry (Under the Honours Scheme) (Semester-II)

# CHE 422/CHH 422

**Organic Synthesis-II** 

Reaction Mechanism- Addition, Elimination and Rearrangements

Total Hours: 60

Total Hours/week: 4 Maximum Marks: 100
Total Credits: 4 Theory: 75

L T P Internal Assessment: 25

4 0 0

### INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi.
- III. Section-I will consist of EIGHT questions and students are required to attempt any SIX short questions carrying 2.5 Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 15 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

### **COURSE OBJECTIVES:**

The course aims to provide students with an in-depth knowledge of different types of reaction mechanisms i.e. addition, elimination, coupling and rearrangement reactions of aliphatic and aromatic organic compounds. The course further provides the insights into the utility of various oxidising and reducing agents.

### **COURSE CONTENTS:**

**UNIT-I** 

1. Addition to Carbon-carbon and Carbon-Hetero Multiple Bonds-I 15Hrs Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration. Michael reaction. Sharpless asymmetric epoxidation. Addition of Grignard reagents, organozinc, organolithium and Gillman reagents to carbonyl and unsaturated carbonyl compounds. Use of other organometallic reagents in addition reactions. Wittig reaction,

#### UNIT-II

- 2. **Addition to Carbon-carbon and Carbon-Hetero Multiple Bonds-II** 5Hrs Mechanism of condensation reactions involving enolates Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.
- 3. **Rearrangements and Coupling Reactions**10 Hrs
  General mechanistic consideration nature of migration, migratory aptitude, memory effects. A detailed study of the following rearrangements, Pinacol-pinacolone, Wagner-Meerwein, Demjanov,



# Post Graduate Department of Chemistry

Benzil-Benzilic acid, Favorskii, Arndt-Eistert synthesis, Neber, Beckmann, Hofman, Curtius, Schmidt, Shapiro reaction, Fries rearrangement. Reaction and mechanism of Diazo coupling, Glaser coupling, Heck reaction, Mcmurry reaction, Stille coupling, Suzuki coupling, Sonogashira reaction. Negishi and Hiyama coupling.

#### **UNIT-III**

#### 4. Elimination Reactions:

7 Hrs

The  $E_2$ ,  $E_1$  and  $E_1cB$  mechanisms and their spectrum. Orientation of the double bond. Reactivity effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

5. Oxidation Reactions: 8 Hrs

Indtoduction. Different oxidative processes. Hydrocarbons- alkenes, aromatic rings, saturated C-H groups (activated and unactivated). Alcohols, diols, aldehydes, ketones, ketals and carboxyalic acids. Amines, hydrazines, and sulphides. Oxidations with ruthenium tetraoxide, iodobenzenediacetate and thallium (III) nitrate, DDQ, PCC, CAN, selenium dioxide, peroxyacids, DCC. Oxidation reactions with special emphasis on Baeyer-villeger reaction, Cannizarro oxidation-reduction reaction,

#### **UNIT-IV**

#### 6. Reduction Reactions:

15 Hrs

Introduction. Different reductive processes, Hydrocarbons- alkanes, alkenes, alkynes and aromatic rings, Carbonyl compounds - aldehydes, ketones, acids, ester and nitriles. Epoxides, Nitro, nitroso, azo and oxime groups, Hydrogenolysis. Sodium borohydride, sodium cyanoborohydride, LAH, disobutylaluminium hydride, tin hydride, trialkyl tin hydride, trialkylsilanes, alkoxy substituted LAH, DIBAL, diborane, diisoamylborane, hexyl borane, 9-BBN, isopinocamphenyl and disiopinocamphenylborane. Reduction reactions with particular emphasis on Wolf-Kishner reduction, Clemensen reduction.

# **BOOK PRESCRIBED:**

- 1. Organic Reaction Mechanism by Jerry March, John Wiley Ed. 5, 2002.
- 2. Advanced Organic Chemistry by Francis Carey, Vol A and Vol. B

#### **COURSE OUTCOMES:**

S. No.	On completing the course, student will be able to
CO1	Learn about the various chemical reagents available for addition to carbon-carbon/carbon-heteroatom multiple bonds.
CO2	Explain the mechanism of different types of elimination, and rearrangement reactions.
CO3	Get insight into the utilization of Pd, Ni, Titanium and silicon in coupling of two molecular entities and their vast applications in organic synthesis.
CO4	Study important oxidizing agents and oxidation reactions used in organic synthesis.
CO5	Acquire knowledge of reducing agents and their applications in organic synthesis.



# Post Graduate Department of Chemistry

M.Sc. Chemistry/M. Sc. Chemistry (Under the Honours Scheme) (Semester-II)

CHE 423/CHH 423
Physical Chemistry-II
Quantum Chemistry

Total Hours: 60 Total Hours/week: 4 Total Credits: 4

L T P 4 0 0

Maximum Marks: 100

Theory: 75
Internal Assessment: 25

#### INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi.
- III. Section-I will consist of EIGHT questions and students are required to attempt any SIX short questions carrying 2.5 Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 15 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

#### **COURSE OBJECTIVES:**

The main objective of the course is to train the students for applying the principles of Quantum Mechanics on different type of motions like translation, rotation, vibration and electronic motions to show the quantisation of related energies. Moreover the simple solution of Uni-electron system will be extended to the solution of multi-electron systems through approximation methods.

### **COURSE CONTENTS:**

**UNIT-I** 

### 1. Quantum Theory: Introduction and Principles

15Hrs

Black body radiations, Planck's radiation law, photoelectric effect, Compton effect, De- Broglie hypothesis, the Heisenberg's uncertainty principle, Rydberg relation for explaining atomic spectrum of hydrogen. Bohr's Theory and its limitation solution of classical wave equation by separation of variables method.

UNIT-II

#### 2. Quantum mechanical operators

6 Hrs

Operators and observations, normal and orthogonal functions, hermitian and unitary operators, introduction to differentiation and integration, Eigen value equation. Hamiltonian operator, interpretation of wave function, postulates of quantum mechanics.

# 3. Applications of Quantum Postulates

9Hrs

Solution of particle in one and three dimensional box, degeneracy, the linear harmonic oscillator, rigid rotators, quantization of vibrational and rotational energy levels, hydrogen atom.

**UNIT-III** 



# Post Graduate Department of Chemistry

### 3. Angular Momentum

7 Hrs

Commutative laws, need of polar coordinates, transformation of Cartesian coordinate into polar coordinate, angular momentum of one particle system, orbital angular momentum, the ladder operator for angular momentum, spin angular momentum and their relations.

### 4. The Approximate Methods

8 Hrs

Need for approximation methods, Perturbation and Variation methods and their application to Helium atom.

#### **UNIT-IV**

# 4. General Orbital Theory of Conjugated Systems

15Hrs

Chemical bonding, linear combination of atomic orbital, overlap integral, coulomb's integral, bond order, charge density calculations for ethylene, allyl system, butadiene system, cyclo butadiene cyclopropenyl system.

#### **BOOK PRESCRIBED:**

- 1. Physical Chemistry, A Molecular Approach by MacQuarrie and Simon.
- 2. Quantum Chemistry, Ira N. Levine, Prentice Hall.
- 3. Quantum Chemistry, H. Eyring, Kimball and Walter.
- 4. Quantum Chemistry, Atkin.
- 5. Fundamentals of Quantum Chemistry, Anantharaman. R.

# **COURSE OUTCOMES:**

S. No.	On completing the course, student will be able to
CO1	Understand phenomenon of Black body radiation, photoelectric effect, Compton effect, De- Broglie hypothesis, the Heisenberg's uncertainty and classical wave equation and its solutions
CO2	Understand Concepts of operators, their types, uses and Quantum Mechanical Model of atom.
CO3	Apply of Quantum Mechanics to deduce the quantization of Translational, Rotational, Vibrational and Electronic energies.
CO4	Apply of Quantum Mechanical model on Single electron system like H-atom and Solution for multi-electron system through Approximation methods
CO5	Understand orbital and spin angular momentum and related Ladder Operators along with HMO theory and its application on various conjugated pi-electron systems



# Post Graduate Department of Chemistry

M.Sc. Chemistry/M. Sc. Chemistry (Under the Honours Scheme) (Semester-II)

# CHE 424/CHH 424 Spectroscopy-B

Techniques for Structure Elucidation of Inorganic Compounds

Total Hours: 90

Total Hours/week: 6 Maximum Marks: 150

Total Credits: 6 Theory: 112
L T P Internal Assessment: 38

6 0 0

### INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi.
- III. Section-I will consist of EIGHT questions and students are required to attempt any SIX short questions carrying 4 Marks each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 22 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

### **COURSE OBJECTIVES:**

This course aims to impart to the student the knowledge of basic concepts of vibrational spectroscopy and its applications. The fundamental aspects of classifying molecules based on moment of inertia. The students will learn about the principles, applications and instrumentation of different molecular spectroscopic methods like Raman spectroscopy, NQR, Photo Electron Spectroscopy, Mössbauer Spectroscopy and Electron Spin Resonance Spectroscopy.

#### **COURSE CONTENTS:**

#### **UNIT-I**

#### 1. Vibrational Spectroscopy

20 hrs

Theory of Infrared Absorption: Harmonic and anhormonic oscillators, absorptions of radiation by molecular vibrations, selection rules, force constant, frequency of vibrational transitions of HCl, vibrations in a polyatomic molecule, 3N-6 and 3N-5 rules, types of vibrations, overtones, combination and difference bands, examples of CO<sub>2</sub>, SO<sub>2</sub>, and H<sub>2</sub>O, Fermi resonance, group vibrations.

Raman Spectroscopy: Introduction, selection rules, anisotropic polarizability, Stokes, anti-Stokes lines, vibrational Raman spectra of CO<sub>2</sub> and H<sub>2</sub>O, polarised and depolarised Raman lines, rule of mutual exclusion, vibronic coupling.

Determination of I.R/Raman Active Modes: Significance of nomenclature: used to describe various vibrations, use of symmetry considerations to determining the number of active infrared and Raman lines (character tables to be provided in the Examination).



# Post Graduate Department of Chemistry

Sample handling. Factors affecting absorption frequencies. Interpretation and finger printing regions. Applications of Raman and I.R selection rules to the determination of Inorganic structure with special emphasis on:

- i) Metal carbonyls
- ii) NSF<sub>3</sub>
- iii) Geometrical isomerism differentiation between Cis and trans [Co(bipy)<sub>2</sub>Cl<sub>2</sub>]Cl.
- iv) Structures of CO<sub>2</sub>, N<sub>2</sub>O, H<sub>2</sub>O, chlorocomplexes of mercury, cadmium and zinc, and octahedral complexes SiF<sub>6</sub><sup>2-</sup>, PF<sub>6</sub><sup>-</sup>, SF<sub>6</sub>.
- v) Changes in the spectra of donor molecules upon coordination with special emphasis on N, N-dimethylacetamide and DMSO with Fe<sup>3+</sup>, Cr<sup>3+</sup>, Zn<sup>2+</sup>, Pd<sup>2+</sup> and Pt<sup>2+</sup> ions. I.R spectroscopy and modes of coordination of SO<sub>4</sub><sup>2-</sup>, N<sub>2</sub>, O<sub>2</sub>, NO, CO<sub>3</sub><sup>2-</sup>, NO<sub>3</sub>-.

#### **UNIT-II**

### 2. Pure Rotational Spectra

0 hrs

Classification of molecules according to their moment of inertia.Rotational spectra of diatomic molecules (rigid rotator), Intensities of spectral lines, isotopic substitution effects, non-rigid rotator, polyatomic linear and symmetric top molecules, Stark effect.

# 3. Nuclear Quadruple Resonance Spectroscopy

10

hrs

Introduction, Experimental considerations, fundamentals of NQR spectroscopy, origin of EFG, measurement of energy differences between two nuclear spin states, the asymmetry parameters, effects of magnetic field, crystal field. Interpretation of spectra, application of the technique to halogen compounds (Organic), group elements, transition metals. Double resonance technique.

#### **UNIT-III**

# 4. Photo Electron Spectroscopy

10

hrs

Introduction, excitation and ejection of electrons, electronic energy in atoms and molecules, core level PES, symmetry and molecular orbitals, molecular orbital diagrams of dinitrogen and dioxygen, their XPS spectra, Valence electron photoelectron spectroscopy, Franck Condon principle, dissociation, predissociation, change of shapes of molecules on excitation.

#### 5. Mössbauer Spectroscopy

10hrs

Principle, experimental considerations, conditions of MB Spectra, the spectrum and its parameters, simple spin states (I  $\frac{1}{2}$ , 3/2), higher spin states (I > 3/2), magnetic splitting significance of parameters obtained from spectra, quadruple splitting, additive model, interpretation of MB Spectra of  $^{57}$ Fe,  $^{119}$ Sn. Application to biological systems, surface study, and compounds of group elements.

#### **UNIT-IV**

# 6. Electron Spin Resonance Spectroscopy

20hrs

Introduction, principle, brief instrumentation of spectrum, hyperfine splitting in isotropic systems involving more than one nucleus, ESR spectrum of benzene radical anion, methyl radical, CH<sub>2</sub>OH, H<sub>3</sub>CCH<sub>2</sub> radical, cyclopentadienyl, cycloheptatrienyl radical, pyrazine anion, pyrazine anion with <sup>23</sup>Na and <sup>39</sup>K counter ion and p-benzosemiquinone, DPPH, Naphthalene. Factors affecting magnitude of g values, zero field splitting, and Krammer's degeneracy. Qualitative survey of EPR spectra of first row transition metal ion complexes (d¹, d², d³, low spin d⁵, high spin d⁶, d³, d⁰ system). Spectra of triplet states, rate of electron exchange, double resonance (ENDOR, ELDOR)



# Post Graduate Department of Chemistry

### **BOOK PRESCRIBED:**

- 1) R. S. Drago, "Physical Methods in Chemistry". W.B Saunders Company.
- 2) C. N. Banwell, "Fundamentals of Molecular Spectroscopy".
- 3) R. V. Parish, "NMR, NQR, EPR & Mossbauer spectroscopy in Inorganic Chemistry". Ellis Horwood, London, 1990.
- 4) G. M. Barrow, "Introduction to Molecular Spectroscopy".
- 5) E. A. Ebsworth, S. Craddock and D. W. H. Rankin, "Structural methods in Inorganic Chemistry". Blackwell Scientific Publications (1991).
- 6) C. N. R. Rao and J. R. Ferraro, "Spectroscopy in Organic Chemistry, Vol. I". Academic Press (1971)
- 7) Walker and Straughan, "Spectroscopy, Vol I and III".

### **COURSE OUTCOMES:**

S. No.	On completing the course, student will be able to
CO1	Get basic idea and application of IR spectroscopy and Raman spectroscopy
CO2	Learn applications of Rotational spectroscopy in inorganic molecules.
СОЗ	Learn about NQR spectroscopy.
CO4	Apply of photoelectron spectroscopy
CO5	Learn principle of EPR spectroscopy and Mossbauer spectroscopy and structure elucidation of inorganic compounds



# Post Graduate Department of Chemistry

M.Sc. Chemistry/M. Sc. Chemistry (Under the Honours Scheme) Semester-II)

# CHE 425/CHH 425 Organic Synthesis-III

Supramolecular, Reactive Intermediates and Disconnections

**Total Hours: 90** 

Total Hours/week: 4 Maximum Marks: 100

Total Credits: 4 Theory: 75

L T P
4 0 0
Internal Assessment: 25

### INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi.
- III. Section-I will consist of EIGHT questions and students are required to attempt any SIX short questions carrying 2.5 Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 15 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

#### **COURSE OBJECTIVE:**

The course aims to design and develop novel technique in the planning of organic syntheses for functional systems by joining multiple chemical components through non-covalent interactions.

### **COURSE CONTENTS:**

UNIT-I

#### 1. Supramolecular Chemistry-I

(a) Concepts 5Hrs

Definition and Development of Supramolecular Chemistry, classification of Supramolecular Host-Guest compounds, Pre- organization and Complementarily, Receptors, Nature of Supramolecular interactions.

#### (b)Binding of anions and neutral molecules

10Hrs

Biological anion receptors, concepts on anion host design, Fromcation to anion hosts-a simple change in pH, Guanidinium- based receptors, Neutral receptors, organometallic receptors, coordination interactions. Inorganic solid state clathrate compounds, solid state clathrates of organic hosts, intracavity complexes of neutral molecules, supramolecular chemistry of fullerenes.

**UNIT-II** 

# 2. Supramolecular Chemistry-II

### (c) Cation Binding Host

7Hrs

Crown ethers, Lariat ether and Podands, Cryptands, spherands, selectivity, Macro cyclic, Macrobicyclic and Template effects, soft ligands, calixarenes, carbon donor and - acid ligands, siderophores.



### Post Graduate Department of Chemistry

#### (d) Crystal Engineering and Molecular Devices

8Hrs

Concepts, crystal structure prediction, Crystal Engineering with hydrogen bonds, weak hydrogen bonds, hydrogen bonds to metals and metal hydrides,  $\pi$ -  $\pi$ stacking, coordination polymers. Introduction, Supramolecular photochemistry, molecular electronic devices: Switches, wires and rectifiers, machines based on catenanes and rotaxanes.

#### **UNIT-III**

#### 3. Organic Reactive Intermediates-I

15Hrs

- (a) **Carbanions**: Chemistry of enolates and enamines, kinetic and thermodynamic enolates, Lithium and boron enolates in aldol and Michael reactions, alkylation and acylation of enolates, Nucleophilic additions to carbonyls and streroechemical aspects through various models (crams / cram chelation / Felkin-Anh models)
- (b) **Carbocations**: Structure and stability of carbocations, classical and non classical carbocations, Neighbouring group participation.
- (c) **Carbenes and Nitrenes**: Structute, generation addition and insertion and rearrangement reactions of carbenes such as wolf rearrangement. Generation of ylids by wolf decomposition. Structure, generation and reactions of nitrene and related electron deficient nitrogen intermediates.

#### **UNIT-IV**

#### 4. Organic Reactive Intermediates

8Hrs

- (d) Ylids: Chemistry of Phosphorous and Sulphurylids-Wittig and related reactions, Peterson olefination etc.
- (e) **Radicals**: Generation of radical intermediates and its addition to alkenes, alkynes for C-C bond formation and Baldwins rule. Fragmanetation and rearrangements reactions like decarboxylation, McMurry coupling etc.

#### 5. Disconnection approach

7Hrs

An introduction to synthons and synthetic equivalents, disconnection approach, functional group interconversions, the importance of the order of events in organic synthesis, one group C-X and two group C-X disconnections, chemoselectivity, reversal of polarity, cyclisation reactions, amine synthesis.

#### **BOOK PRESCRIBED:**

- 1. J.W Steed and J.L Atwood, Supramolecular chemistry, John Wiley & Sons, Ltd. New York.
- 2. Designing Organic Synthesis, S. Warren, Wiley
- 3. Organic Synthesis- Concepts, Methods and Starting Materials, J. Fuhrhop and G. Penzillin, Verlag VCH.
- 4. Advanced Organic Synthesis Part A and B, F.A. Carey and R. J. Sundberg, Plenum Press.
- 5. Principles of Organic Synthesis, R. Norman and J. M. Coxon, Blackie Acdemic& Professional
- 6. Modern Methods of Organic Synthesis Cambridge University Press (1971). Carruthers,
- 7. Reactive Intermediates, Gilchrist and Rees



# Post Graduate Department of Chemistry

#### **COURSE OUTCOMES:**

S. No.	On completing the course, student will be able to
CO1	Learn introductory concepts of supramolecular chemistry
CO2	Learn the binding of various metals with synthetic and natural cationic hosts
CO3	Understand the logics involved in anion binding by different hosts including solid state clatharates and fullerenes
CO4	Develop the concept involved in Crystal Engineering
CO5	Learn the construction of molecular devices such as molecular wires, rectifiers and switches
CO6	Acquire an in depth knowledge of various reactive intermediates viz. Carbocations, carbanions, free radicals, carbenes and nitrenes.
CO7	Understand retrosynthetic methodology of going from a target molecule to simple starting compound
CO8	Learn the concept of disconnection, functional group interconversions, synthons and their corresponding synthetic equivalents



### Post Graduate Department of Chemistry

M.Sc. Chemistry/M. Sc. Chemistry (Under the Honours Scheme) (Semester-II)

#### MH CHX 421: Mathematics for Chemists

#### For Medical Students

Total Hours: 45
Total Hours/week: 3

**Total Credits: 3** 

L T P 3 0 0

Maximum Marks: 75

Theory: 56

**Internal Assessment: 19** 

#### INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi and TWO questions from each unit.
- III. Section-I will consist of EIGHT questions and students are required to attempt any SIX short questions carrying 2 Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question will carry 11 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

#### **COURSE OBJECTIVES:**

- 1. To help the students to understand the relationships between side lengths and angles of triangles.
- 2. To make the students able to describe the angles that are created when atoms bond together to form molecules in molecular geometry.
- 3. To acquaint the students with the trigonometry and its properties.
- 4. To solve problems related to matrices, determinants, derivatives and integrals.
- 5. To calculate Area under a curve using integration.

#### **COURSE CONTENT:**

#### UNIT-I

**Trigonometry and Determinants**: Definition of sin, cos, tan, cot, sec, cosec functions with the help of unit circle, values of sin x, cos x for x = 0,  $\pi/6$ ,  $\pi/3$ ,  $\pi/2$ . Trigonometric identities (without proofs) and their applications.Definition and expansion, properties of determinants, product of two determinants of 3rd order.

#### UNIT-II

**Matrices:** Introduction to various forms of Matrices, row, column, diagonal unit, Submatrix, square, equal matrices, null, symmetric and skew symmetric matrices, transpose of a matrix, adjoint and inverse of matrices. Addition, multiplication, characteristic equation of a matrix, statement of Cayley Hamilton theorem. Rank of matrix, condition of consistency of a system of linear equations. Eigen vectors and Eigen values ofmatrices.

#### **UNIT-III**

**Differential Calculus**: Differentiation of standard functions, theorems relating to the derivative of the sum, difference, product and quotient of functions (without proofs), derivative of trigonometric functions, inverse trigonometric functions, logarithmic functions and exponential functions,



### Post Graduate Department of Chemistry

differentiation of implict functions, logarithmic differentiation.

#### **UNIT-IV**

**Integral Calculus:** Integration as an inverse of differentiation, summation, area under a curve, indefinite integrals of standard forms, method of substitution, method of partial fractions, integration by parts, definite integrals, reduction formulae, definite integrals as limit of a sum and geometrical interpretation.

#### **BOOKS PRESCRIBED:**

- 1. Santi Narayan Differential Calculus.
- 2. Santi Narayan Integral Calculus.
- 3. B.S. Grewal Higher Engineering Mathematics.
- 4. Joseph B. Dence Mathematical Techniques in Chemistry.
- 5. Margenau and Murphy, the Mathematics of Physics and Chemistry.
- 6. B.L. Moncha and H.R. Choudhary A Text Book of Engineering Mathematics.

#### **COURSE OUTCOMES:**

S. No.	On completing the course, student will be able to
CO1	Understand the relationships between side lengths and angles of triangles.
CO2	Describe the angles that are created when atoms bond together to form molecules in molecular geometry.
CO3	Work with the matrices, determinants, derivatives and integrals.
CO4	Calculate Area under a curve using integration.



### Post Graduate Department of Chemistry

M.Sc. Chemistry/M. Sc. Chemistry (Under the Honours Scheme) (Semester-II)

#### **BT CHX 421**

**Biology for Chemists** For Non-Medical Students

Total Hours/week: 3
Total Credits: 3
L T P

Maximum Marks: 75 Theory: 56 Internal Assessment: 19

2 1 0

#### INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi and TWO questions from each unit.
- III. Section-I will consist of eight questions and student has to attempt any six short questions carrying 2 Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question will carry 11 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

#### **COURSE OBJECTIVES:**

- 1. To understand the basic cell structure and role of biologically important molecules.
- 2. To study the basic principle of heredity and gene expression.
- 3. To learn the taxonomic criteria of classification of living things.
- 4. To study the basic structure of viruses.

#### **COURSE CONTENTS:**

#### **UNIT-I**

- 1. The Organization of life
- **Biologically important molecules:** Carbohydrates, lipids, proteins and nucleic acids.
- The life of cells: The cell theory, general characteristics of cells, difference between prokaryotic and eukaryotic cells, difference between plant and animal cells, Cell organelles (Mitochondria, Golgi apparatus, Ribosome, Endoplasmic reticulum, Chloroplast & Nucleus).

#### UNIT-II

- Animal tissues; epithelial tissues, connective tissues, muscle tissue, nervous tissue.
- Plant tissue: meristematic tissue, permanent tissues.

UNIT-III

2. Genetics



### Post Graduate Department of Chemistry

- The basic principle of heredity: Mendel's laws, monohybrid cross, dihybrid cross.
- **DNA:** Double helix structure and replication.

#### **UNIT-IV**

- 3. The Diversity of Life
- The classification of living things: criteria of classification, Whittaker's system of classification.
- Viruses: Structure & types of viruses.

#### **BOOKS PRESCRIBED:**

1. Cord Biology – South Western Educational Publications, Texas, 2000

#### **COURSE OUTCOMES:**

CO-1	The chemical structure of biologically important molecules: Carbohydrates, lipids,
	proteins and nucleic acids and how physiological conditions influence the structures
	and reactivates of these biomolecules.
CO-2	The life of cells – The cell theory, general characteristics of cells, difference between
	prokaryotic and eukaryotic cells, difference between plant and animal cell and will
	know about the structure and functions of various cell organells.
CO-3	The anatomical structure of plants and animals by studying the Tissues, organs and
	organ systems: Animal tissues; epithelial tissues, connective tissues, muscle tissue,
	nervous tissue and neoplasias; plant tissue: maristematic tissue, permanent tissues.
CO-4	The scope and significance of genetics by imbibing the principles of hereditary
	genetic transmission and interactions of gene with environment.
CO-5	The genes at molecular level, structure of DNA, DNA replication. Gene expression:
	transcription and translation and genetic code.
CO-6	The taxonomic nomenclature and criteria of classification, Whittaker's systems of
	Classification and their characteristics.
CO-7	The important and diversified groups of microorganism in nature and their
	classification.



### Post Graduate Department of Chemistry

M.Sc. Chemistry/M. Sc. Chemistry (Under the Honours Scheme) (Semester-II)
CHE 426/CHH 426
Physical Chemistry Lab-I

Total Hours: 90 Total Hours/week: 6 Total Credits: 3 L T P

Maximum Marks: 75 Theory: 56

**Internal Assessment: 19** 

0 0 3

#### **INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES:**

- I. The exam will be conducted on two sessions i.e. Morning and Evening
- II. Students will perform two practical's.
- III Students will be asked to complete write up of both practical within first 30 minutes on the first sheet provided.
- IV. On the second sheet provided after 30 minutes, students will perform and note the record on second sheet during the conduct of practical exam
- V. The split of marks will be as under:

(Write-up = 20, Performance = 20, Viva-Voce = 10, Practical notebook = 6)

#### **COURSE OBJECTIVES:**

This course aims to impart to the student knowledge of: Laboratory set up, calibration and handling and use of instruments like pH-meter, Conductometer, potentiometer, tensiometer, Abbe's Refractometer and Polarimeter for the qualitative and quantitative analysis.

#### **COURSE CONTENTS:**

- 1. To determine the strength of given acid by pH metrically.
- 2. To determine dissociation constant of given acid pH metrically
- 3. Titration of weak acid conductometrically
- 4. Titration of strong acid conductometrically
- 5. To determine dissociation constant of given acid conductometrically
- 6. Determine the dissociation constant of acetic acid in DMSO, DMF, dioxane by titrating it with KOH.
- 7. Determine the activity coefficient of an electrolyte at different molalities by e.m.f. measurements.
- 8. Compare the cleansing powers of samples of two detergents from surface tension measurements.
- 9. Determine the specific refraction, molar refraction and atomic parachor with the help of Abbe's refractometer.
- 10. To study the distribution of benzoic acid between benzene and water.
- 11. Determine the equilibrium constant of reaction  $K_1 + +l_2 \rightarrow Kl_3$  by distribution law and hence Find the value of GO of the above reaction
- 12. Compare the relative strength of CH<sub>3</sub>COOH and CICH<sub>2</sub>COOH from conductance measurements.
- 13. Determine the solubility (g/litre) of sparingly soluble lead sulphate from conductance measurements.
- 14. Titrate a given mixture of HCl and CH<sub>3</sub>COOH against NaOH solution conductometrically.



### Post Graduate Department of Chemistry

- 15. Compare the relative strength of:
- i) HCl
- ii) H<sub>2</sub>SO<sub>4</sub>

by following the kinetics of inversion of cane sugar polarimetrically.

#### **BOOK PRESCRIBED:**

Advance Practical Chemistry by J. B. Yadav

#### **COURSE OUTCOMES:**

S. No.	On completing the course, students will be able to
CO1	Use of Electro-methods like conductivity meter <i>pH</i> -meter for quantitative analysis.
CO2	Use of Electro-methods like pH-meter for quantitative analysis.
CO3	Use of Optical-methods like Abbe's refractometer for quantitative analysis
CO4	Use of Optical-methods like Polarimeter for quantitative analysis
CO5	Use of non-electrical methods like surface tension, distribution law and study of equilibrium



### Post Graduate Department of Chemistry

M.Sc. Chemistry/M. Sc. Chemistry (Under the Honours Scheme) (Semester-II)

CHE 427/CHH 27

Inorganic Chemistry Lab-II

Total Hours: 90
Total Hours/week: 6
Total Credits: 3
L T P
0 0 3

Maximum Marks: 75

Theory: 56

**Internal Assessment: 19** 

#### **INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES:**

- I. The exam will be conducted on two sessions i.e. Morning and Evening
- II. Students will perform two practicals.
- III Students will be asked to complete write up of both practical within first 30 minutes on the first sheet provided.
- IV. On the second sheet provided after 30 minutes, students will perform and note the record on second sheet during the conduct of practical exam
- V. The split of marks will be as under:

(Write-up = 20, Performance = 20, Viva-Voce = 10, Practical notebook = 6)

#### **COURSE OBJECTIVE:**

The aim of this course is to impart practical skill to the pupil for synthesis and structure analysis of inorganic complexes.

#### **COURSE CONTENTS:**

#### (Any 8 Complexes.)

- 1. Preparation of Co(acac)<sub>3</sub>, its characterization using NMR, IR, UV-Vis and analysis of Cobalt (ref. J. Chem. Edu., 1980, 57, 7, 525)
- 2. Preparation of Co. (acac-NO<sub>2</sub>)<sub>3</sub>, its characterization using NMR, IR, UV-Vis and analysis of Cobalt. (ref. J. Chem. Edu., 1980, 57, 7, 525)
- 3. Preparation of [Fe(H<sub>2</sub>O)<sub>6</sub>][Fe(N-salicyldeneglycinato)<sub>2</sub>]<sub>2</sub>.3H<sub>2</sub>O, its characterization using IR, UV-Vis, magnetic susceptibility and analysis of Iron.(ref. InorganicaChimicaActa, 1977, 23, 35).
- 4. Preparation of [Ni(NH<sub>3</sub>)<sub>6</sub>]Cl<sub>2</sub>its characterization using IR, UV-Vis, magnetic susceptibility and analysis of Nickel and NH<sub>3</sub>. (ref. Marr and Rockett, 1972).
- 5. Preparation of [Ni(ethylenediamine)<sub>3</sub>]Cl<sub>2</sub> its characterization using IR, UV-Vis, magnetic susceptibility and analysis of Nickel. (ref. Marr and Rockett, 1972, page 270).
- 6. Preparation of [Fe(NO)(S<sub>2</sub>CN(Et)<sub>2</sub>)<sub>2</sub>] its characterization using IR, UV-Vis, magnetic susceptibility and analysis of Fe(II). (ref. Marr and Rockett, 1972, page 262, J. Chem. Soc. 1962, 84, 3404).
- 7. Preparation of octahedral and tetrahedral complexes of dichlorodipyridylcobalt(II), differentiate



### Post Graduate Department of Chemistry

them using IR, UV and magnetic properties. Estimate Co(II) from one of them. (ref. Marr and Rockett, 1972, page 375, Inorganic Chemistry, 1966, 5, 615).

- 8. Preparation of VO(acac)<sub>2</sub>and its piperidine complex, characterize using IR, UV and magnetic moment. Estimate for V(IV). (ref. Marr and Rockett, 1972, 243).
- 9. Preparation of diaquotetraacetataocopper(II), magnetic susceptibility IR and UV-Vis, analysis of Copper(II).
- 10. Preparation of cis- and trans- potassium dioxalatodiaquochromate(III). Interpretation of IR, UV and magnetic properties. Estimation of Chromium. (ref. Marr and Rockett, 1972, page 386).
- 11. Preparation of HgCo(NCS)<sub>4</sub>, its IR and measure its magnetic moment. (ref. Marr and Rockett, 1972, page 365).
- 12. Preparation of sodium tetrathionate, interpretation of its IR and analysis using potassium iodate. (ref. Marr and Rockett, 1972, page 214).
- 13. Preparation of Potassium dithionate, interpretation of its IR and analysis using potassium iodate. (ref. Marr and Rockett, 1972, page 214).
- 14. Preparation of bis(acetylacetonato)copper(II), UV-Vis, and IR, magnetic studies, Demonstration of Jahn Teller effect by solution spectral studies. (ref. Bull. Chem. Soc. Japan, 1965, 29, 852).
- 15. Preparation of salicylamide complexes of Copper(II). IR, UV, magnetic data and analysis of Cu(II). (ref. Indian J. of Chem., 1977, 15A, No. 5, 459; ibid, 1971, 9, 1396).
- 16. To prepare a macrocyclic ligand 5,7,7,12,14,14-hexamethyl-1,4,8,11-tetraazacyclotetradeca-4,11-dienedi(hydrogeniodide) and its complex with Ni(II). Study IR, NMR and UV-Vis of ligand and complex and magnetic properties of complex. To analyze for Ni and I. (J. Chem. Edu. 1977, 79, 581).
- 17. Preparation and resolution of tris (ethylenediamine) cobalt (III). UV-Vis, NMR, IR, optical rotation of the resolved complexes. ((ref. Marr and Rockett, 1972, page 386).

#### **BOOK PRESCRIBED:**

- 1. B.N. Figgis, Introduction to Ligand Field, Wiley Eastern.
- 2. A.B.P. Lever, Inorganic Electronic Spectroscopy, Elsevier.
- 3. A. Earnshaw, Introduction to Magnetochemistry, Academic Press.
- 4. J.E. Huheey, Inorganic Chemistry Principles of Structure and Reactivity, Harper Interscience.
- 5. R.S. Drago, Physical Medhod in Chemistry, W.B.Saunders Company.
- 6. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, Wiley Int.



# Post Graduate Department of Chemistry

#### **COURSE OUTCOMES:**

S. No.	On completing the course, students will be able to
CO1	Learn how to synthesize inorganic complexes
CO2	Synthesize the geometrical isomers of the complexes
CO3	Analyze structure of inorganic complexes from spectral data
CO4	Have hands-on experience/ practical knowledge in performing experiments
CO5	Get Practical knowledge about UV and FTIR



Post Graduate Department of Chemistry

# Semester-III

Academic Session: 2024-25

48



### Post Graduate Department of Chemistry

M.Sc. Chemistry/M. Sc. Chemistry (Under the Honours Scheme) (Semester-III)

CHE 531 / CHH 531

Inorganic Chemistry-III

Bioinorganic and Metal Clusters

Total Hours: 60 Total Hours/week: 4 Total Credits: 4

L T P
3 1 0

Maximum Marks: 100

Theory: 75

**Internal Assessment: 25** 

#### INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi.
- III. Section-I will consist of EIGHT questions and students are required to attempt any SIX short questions carrying 2.5 Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 15 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

#### **COURSE OBJECTIVES:**

The main objective of this course is to help the students to understand the use of metals in biological systems, various aspects of coordination chemistry related to bioinorganic research, metallo biopolymers, their structure, function, role of metal ion, etc.

#### **COURSE CONTENTS:**

#### UNIT-I

#### 1. (a) Bioinorganic Chemistry

15 Hrs

Periodic survey of essential and trace elements, biological importance and relative abundance,  $Na^+/K^+$  ion pump and its mechanism.

Porphyrine and metalloporphyrins, Oxygen carriers/storage-Hb and Mb: Structure and mechanism of their function, cooperativity and Bohr effect. Synthetic models of Hb, Cyanide, phosphine and carbon monoxide poisoning.

Inhibition and poisoning by ligand and metal ions, hemocyanin and hemerythrin, models of iron, coalt and copper.

Bioenergetic and ATP cycle process coupled to phosphate hydrolysis, Nucleotide transfer-DNA polymerase, phosphate transfer pyruvate kinase, phosphoglucomutase, creatin kinase, ATPase.

#### UNIT-II



### Post Graduate Department of Chemistry

#### 1. (b)Bioinorganic Chemistry

15 Hrs

Photosynthesis and respiration - chlorophyll: structure, function and its synthetic model. Xanthine oxidase, Gout Disease and its remedy.

Enzymes and their functioning, Bioredox agents, Zn-enzymes carboxipeptidase, carbonic anhydrase, superoxide dismutase, peroxidases and catalases,

Vitamin B<sub>12</sub> coenzyme, structure, function and "Mn" mechanism and its application in organic synthesis, intake of alcohol and its remedy.

Cytochromes-structure and function, Cytochrome P<sub>450</sub> enzymes.

Ferrodoxins and rubredoxins their structure and function. Abiological and biological N<sub>2</sub> fixation and mechanism.

**UNIT-III** 

#### 1. (c) Bioinorganic Chemistry

15 Hrs

Ferritin, transferring and siderophores and their structure and function.

Availability, competition, toxicity and nutrition of Iron, metal deficiency and diseases, toxic effects of antibiotics, chealte therapy, synthetic metal chelates as antimicrobial agents.

Calcium in living cell, transport and regulation and its mechanism.

Molecular aspects of intramolecular processes and their mechanisms.

#### 2. Metal Clusters

#### (a) Reaction at Coordinated ligands

The role of metal ions in the hydrolysis of amino acid esters, peptides, and amides Molecular orbital concept of role of metal ions participation, Modified aldol condensation, Imine formation, Template and Macrocyclic effect in detail.

#### **UNIT-IV**

#### (b) Metal to Metal Bonds and Metal atom Clusters

15 Hrs

**50** 

Metal carbonyl clusters, isoelectronic and isolobal relationship, high nuclearity carbonyl clusters (HNCC), Structural Patterns, synthetic methods, heteroatoms in metal atom clusters Carbide and nitride containing clusters, electron counting scheme for HNCC's, the capping rule, HNCC's for Fe, Ru, Os, Co, Rh, Ir, Ni, Pd, Pt.

Lower halides and chalcogenides clusters, octahedral metal halides and chalcogenides clusters ( $M_6M_8M_6M_{12}$  type).

Cheveral phases, triangular clusters and solid state extended arrays. Compound with M-M multiple bonds, major structural types, quadruple bonds, and other bond orders.

Intragoonal context relation of clusters to multiple bonds and one dimensional solids.

#### **BOOK PRESCRIBED:**

- 1. Principles of Bioinorganic Chemistry, S. J. Lippard and Berg, University Science Books.
- 2. J.E. Huheey: Inorganic Chemistry III & IV Ed. Pearson Education Asia (2002).
- 3. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 5th Edition.
- 4. Purcell and Kotz: Inorganic chemistry. W. B. Saunders and Co., London
- 5. Bioinorganic Chemistry by D. Banergia.

#### **COURSE OUTCOMES:**



# Post Graduate Department of Chemistry

S. No.	On completing the course, student will be able to
CO1	Students will be able to analyse the relation between oxidation state of metals and their biological behaviour.
CO2	Students will be able to understand the role of metals and chemicals in biological systems.
CO3	Students will learn the use of porphyrins of different metal ions in biological systems
CO4	Students will be able to make a correlation between enzymatic functions and metals.
CO5	students will understand the structural features of biological systems involving metal ions and their activities and mechanisms



### Post Graduate Department of Chemistry

M.Sc. Chemistry/M. Sc. Chemistry (Under the Honours Scheme) (Semester-III) CHE 532/ CHH 532

Organic Synthesis-IV
Natural Products

Total Hours: 60 Total Hours/week: 4

Total Hours/week: 4 Maximum Marks: 100 Total Credits: 4 Theory: 75

L T P Internal Assessment: 25

3 1 0

#### INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi.
- III. Section-I will consist of EIGHT questions and students are required to attempt any SIX short questions carrying 2.5 Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 15 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

#### **COURSE OBJECTIVES:**

The aim of this course is to make the students familiar with nomenclature, methods of structure elucidation, general properties and methods of synthesis of natural products.

#### **COURSE CONTENTS:**

#### UNIT-I

- 1. Studies on Biosynthetic Pathways of Natural Products and Terpenoids 10 Hrs a)Primary and Secondary reactions of Biosynthesis, Biosynthesis of AcetylCoA, Shikmic acid pathway.
- b) Isoprene rule, mechanism of formation of mevalonic acid from acctyl coenzyme, Biogenetic isoprene rule. Geranyl pyrophosphates and its conversion into alphapinene, thujene and borneol. Farnesyl pyrophosphate, geranyl, geranyl pyrophosphate and mechanistic considerations for their interconversions into cadinene and abietic acid.
- 2. Terpenoids 5 hrs General classification, General Methods of structure determination, Chemistry of Camphor, Abietic acid and Menthol. Biosynthesis of Squalene and Phytoene.

**UNIT-II** 

3. Carbohydrates 9 Hrs

Nomenclature and Classification, Structure of Maltose, Lactose, Sucrose, Starch and cellulose. Structure elucidation of cellulose.structure and functions of glycosides, deoxy sugars, myoinositol, amino sugars, N-acetylmuramic acid, sialic acid and chitin.Structure and biological functions of glucosaminoglycans or mucopolysaccharides.Carbohydrate metabolism-Kreb's cycle, glycolysis,



### Post Graduate Department of Chemistry

glycogenesis and glycogenolysis, gluconeogenesis, pentose phosphate pathway.

#### 4. Amino-acids, Peptides and Proteins

6 Hrs

Nomenclature and symbols of amino acids. Chemical and enzymatic hydrolysis of proteins to peptides. Secondary and Tertiary structure of proteins. Biosynthesis of aliphatic and aromatic Amino acids. Structure elucidation of oxytocin and Insulin

#### **UNIT-III**

5. Steroids 10 Hrs

Biosynthesis of steroids, Diels hydrocarbon, Structure elucidation of Cholesterol and estrone. Synthesis of Cholesterol, Progesterone, Oestrone, Testosterone and Androsterone.

6. Alkaloids 5 Hrs

Classification of alkaloids, Methods of structure determination of Alkaloids, Structure elucidation and synthesis of Nicotine, Quinine, Morphine, Coniine and Ephiderene

#### **UNIT-IV**

6.Haemin and Chlorophyll

5 Hrs

Structure and synthesis of Porphyrins. Chemistry of Haemin and chlorophyll.

7. Antibiotics

5 Hrs

Introduction, chemistry of pencillins, streptomycines, chloromphenicol, tetracyclins.

8. Prostaglandins

5 Hrs

General study, nomenclature, structure of PGE and synthesis of PGE1, PGE2, PGF2x

#### **BOOK PRESCRIBED:**

- 1. Primary Metabolism: A Mechanistic Approach by J. Staunton, Oxford University Press, 1978.
- 2. Secondary Metabolism by J. Mann, Oxford University Press, Oxford, 1980.
- 3. Natural Product Chemistry A mechanistic, Biosynthetic and Ecological Approach by Kurt B. G. Torssell, Swadish Pharmaceutical Society, 1997.
- 4. Principles of Biochemistry by A. L. Lehninger, CBS Publishers, New Delhi.
- 5. Fundamental of Biochemistry by D. Voet, J.G. Voet and C.W. Pratt, John Willey & Sons Inc., New York, 1999.

#### **COURSE OUTCOMES:**

S. No.	On completing the course,
CO1	Students will be able to draw structures of monosaccharides, disaccharides and polysaccharides and learn their functions.
CO2	Students will be capable of drawing the structures of amino acids and proteins.
CO3	Learn general as well as advanced methods of structural elucidation and chemistry of important natural products such as steroids, alkaloids, Porphyrins, Nucleic acids, Peptides, antibiotics and prostaglandins.
CO4	Study biosynthesis and chemistry of terpenoids



# Post Graduate Department of Chemistry

**CO5** 

Students become familiar with reagents used in organic synthesis and structure elucidation.



### Post Graduate Department of Chemistry

M.Sc. Chemistry (Semester- III)

CHE 533

Physical Chemistry-III

Electrochemistry and Chemical Dynamics

Total Hours: 90 Total Hours/week: 6 Total Credits: 6

L T P 5 1 0

Maximum Marks: 150 Theory: 112

Internal Assessment: 38

#### INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi.
- III. Section-I will consist of EIGHT questions and students are required to attempt any SIX short questions carrying 4 Marks each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 22 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

#### **COURSE OBJECTIVES:**

The aim of this course is to impart advance topics of Chemical Dynamics, Electrochemistry, Voltametry and Polarography and their applications. These topic find wide application in research and industry, so the theoretical knowledge of these topics will help the students during praticals application of these topics.

#### **COURSE CONTENTS:**

**UNIT-I** 

#### 1. Electrochemistry

20Hrs

Electrochemistry of solutions, Debye-Huckel-Onsager treatment and its extension, ion-solvent interactions, Thermodynamics of electrified interface equation, Derivation of electro-capillarity, Lipmann equation(surface excess), method of determination, structure of electrified interfaces, Helmholtz-Perin, Guoy-Chapmann, Stern models, over potential, exchange current density, derivation of Butler-Volmer equation, Tafel plot.

Semiconductor interface theory of double layer at semiconductor electrolyte solution interface, structure of double layer interfaces, effect of light at semiconductor solution interface. Introduction to corrosion, forms of corrosion, corrosion monitoring and prevention.

**UNIT-II** 

#### 2.(a) Chemical Dynamics

20Hrs

Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius theory and activated complex theory, ionic reactions, kinetic salt effects,, treatment of uni molecular reactions, Lindemann-Hinshelwood theory.



### Post Graduate Department of Chemistry

#### **UNIT-III**

#### 2.(b)Chemical Dynamics

20Hrs

Dynamic Chain (hydrogen bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), Photochemical reactions between hydrogen-bromine and hydrogen-chlorine, oscillatory reactions (Belousov-Zhabotinsky reactions), Homogeneous catalysis and kinetics of enzyme reactions, general features of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis, nuclear resonance.

#### **UNIT-IV**

#### 3. Voltmametry and Polarography

20Hrs

Polarography, polarographic cells, polarogram, interpretation of polarographic waves, equation for the polarographic waves, effect of complex formation on polarographic wave, polarograms for irreversible reactions, dropping mercury electrode, current variations during life time of a drop, merits and demerits of dme, polarographic diffusion currents, Ilkovic equation, capillary characteristics, temperature, polarograms for mixture of reactants, anodic and cathodic waves, factors affecting polarographic currents, applications of polarography, treatment of data, organic and inorganic polarographic analysis, voltammetry at solid electrodes, cyclic voltammetry and interpretation of data, pilot-ion and standard addition method for quantitative analysis.

#### **BOOK PRESCRIBED:**

- 1. Chemical Kinetics, K. J. Laddler, McGraw-Hill
- 2. Modern Electrochemistry Vol.1,2,3, J. Bochris and A.K.N. Reddy
- 3. Fundamentals of electrochemistry; P. Monk
- 4. Principles of Instrumental Analysis; Skoog, West; Saundres Publications

#### **COURSE OUTCOMES:**

S. No.	On completing the course,
CO1	Students will learn the various laws of electroshemistry, thermodynamic derivations of various electrochemical models
CO2	Study the semiconductor interface theory, semiconductor solution interface. Also understand the process of corrosion its monitoring and prevention
CO3	Students will understand the various theories of reaction rates like collision theory, activated complex theory, Lindemann-Hinshelwood theory in detail.
CO4	Students will learn the mechanisms of kinetics of various chain reactions ( both thermal and photochemical), enzyme catalysis.
CO5	They will also study the various methods for Study the kinetics of fast reactions.
CO6	Students will learn about the polarographic and voltametric methods of analysis.



# Post Graduate Department of Chemistry

They will also understand about the various applications of these methods of analysis.

Academic Session: 2024-25

**57** 



### Post Graduate Department of Chemistry

M.Sc. Chemistry/M. Sc. Chemistry (Under the Honours Scheme) (Semester-III) CHE 534/ CHH 534

#### **Organic Synthesis-V**

Pericyclic and Photochemistry

**Total Hours: 60 Total Hours/week: 4 Total Credits: 4** 

**Maximum Marks: 100 Internal Assessment: 25** 

L T P 3 1 0

#### INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi.
- III. Section-I will consist of EIGHT questions and students are required to attempt any SIX short questions carrying 2.5 Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 15 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

#### **COURSE OBJECIVES:**

The aim of the course is to make students familiar with the concepts and applications in two important topics in advanced organic chemistry, namely concerted organic reactions and organic photochemistry.

#### **COURSE CONTENTS:**

#### UNIT-I

#### 1. (a)Pericyclic Reactions

Theory: 75

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene, allyl system, classification of pericyclic reactions FMO approach. Woodward-Hoffmann correlation diagrams method and Perturbation of molecular orbital (PMC) approach for he explanation of pericyclic reactions under thermal and photo-chemical conditions.

Electrocyclic reactions – controtatory and disrotatory motions, 4n, 4n+2, allylsystems secondary effects. Cycloadditions – antrafacial and suprafacial additions, notation of cylcoadditions (4n) and (4n+2) systems with a greater emphasis on (2+2) and (4+2) cycloaddition-stereochemical effects and effects of substituents on the rates of cycloadditions, 1,3-dipolar cyclo-additions and cheleotropic reactions.

#### **UNIT-II**

#### 1. (b)Pericyclic Reactions

15 Hrs

Sigmatropic Rearrangements-suprafacial and antrafacial shifts [1,2]- sigmatropic shifts involving carbon moieties retention and invertion of configuration, (3,3) and (5,5) sigma-tropic rearrangements, detailed treatment of Claisen and Cope rearrangements, fluxional tautomerism, aza-cope rearrangements, introductions to Ene reactions, simple problems on pericyclic reactions. Elecrocyclic



### Post Graduate Department of Chemistry

rearrangement of cyclobutenes and 1,3cyclohexadienes.

#### **UNIT-III**

2. Photochemistry

(i) Photochemical Reactions

5 Hrs

Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule, quantum yield, transfer of excitation energy, actinometry.

(ii) Determination of Reaction Mechanism

5 Hrs

Classification, rate constants and life times of reactive energy states –determination of rate constants of reactions. Effect of light intensity on the rate of photochemical reactions.

Types of photochemical reactions – photodissociation, gas-phase photolysis.

(iii) Photochemistry of Alkenes

5 Hrs

Intramolecular reactions of the olefinic bond – geometrical isomerism, cyclisation reactions, rearrangement of 1,4- and 1, - dinenes.

#### **UNIT-IV**

(iv) Photochemistry of Carbonyl Compounds

7 Hrs

Intramolecular reactions of carbonyl compounds – saturated, cyclic and acyclic,  $\beta$ ,  $\gamma$ - unsaturated and  $\alpha$ , $\beta$ -unsaturated compounds, Cyclohexadienones. Intermolecular cycloaddition reactions – dimerisations and oxetane formation.

(v) Photochemistry of Aromatic Compounds

4 Hrs

Isomerisations, additions and substitutions.

(vi) Miscellaneous Photochemical Reactions

4 Hrs

Photo-Fries reactions of anilides. Photo-Fries rearrangement. Barton reaction. Singlet molecular oxygen reactions. Photochemical formation of smog. Photodegradation of polymers. Photochemistry of vision.

#### **BOOK PRESCRIBED:**

- 1. Pericyclic reactions: A Mechanistic study by S. M. Mukherji
- 2. The Conservation of Orbital Symmetry by R. B. Woodward and R. Hoffman
- 3. Organic Photochemistry Chapman and Depuy.
- 4. Organic Photochemistry W.H. Horsepool.
- 5. Photochemistry of Excited States J.D.Govle.
- 6. Fundamentals of Photochemistry by K.K. RohtagiMukherji

#### **COURSE OUTCOMES:**

S. No.	On completing the course,
CO1	To learn the fundamentals of pericyclic reactions
CO2	To understand the various types pericyclic reactions viz. Cycloaddition reactions, Electrocyclic reactions and Sigmatropic reactions
СОЗ	To understand the logic of working out the reaction pathway of pericyclic reactions using Woodward-Hoffmann rules, Frontier Molecular Method(FMO) and Orbital correlation method(OCD) etc.



# Post Graduate Department of Chemistry

CO4	To acquire knowledge to control the kinetics of pericyclic reactions.
CO5	To develop an insight into various types of pericyclic reactions like cope, claisen and ene. Learning flutionality due to these reactions.
CO6	To learn the fate of an excited state molecule, various ways of excitation energy transfers and actinometry
CO7	To determine rate constants and develop stern volmer plots
CO8	To learn photochemical reactions of various functional groups viz. Alkenes, carbonyl compounds, aromatic compounds.
CO9	To develop an insight into Photo fries, barton, singlet molecular oxygen reactions
CO10	To understand the photochemical formation of smog, photodegradation of polymers and photochemistry of vision



### Post Graduate Department of Chemistry

M.Sc. Chemistry/M. Sc. Chemistry (Under the Honours Scheme) (Semester-III) CHE 535/ CHH 535

### Physical Chemistry-IV

Analytical Techniques

Total Hours: 60

Total Hours/week: 4 Maximum Marks: 100
Total Credits: 4 Theory: 75

L T P Internal Assessment: 25

#### INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi.
- III. Section-I will consist of EIGHT questions and students are required to attempt any SIX short questions carrying 2.5 Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 15 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

#### **COURSE OBJECTIVES:**

The course is designed to introduce the advance techniques of analysis like Potentiometry leading to the designing and use of pH electrodes, Thermogravimetric methods (TG), Differential thermal Analysis (DTA), Differential Scanning Calorimetry, Coulometric technique and Chromatographic Advance Techniques for identification and purification of the chemical compounds. Some advance solid state reactions will also be introduced

#### **COURSE CONTENTS:**

UNIT-I

1(a) Potentiometric Methods

10Hrs

Reference electrodes: Calomel electrodes, silver- silver chloride electrodes, precautions in the use of reference electrodes, metallic indicator electrodes and its types, metallic redox indicators, membrane indicator electrodes, classification of membranes, properties of ion-selective electrodes, the glass electrodes for pH measurement, composition and structure of glass membrane, the hygroscopicity of glass membrane, conduction across glass membrane, the membrane potential, the boundary potential, the potential of glass electrode, the alkaline and error, the glass electrodes for other cations, crystalline membrane electrode and their conductivity, the fluoride electrode, the electrode based on silver salts.

1.(b) Potentiometric Methods

5Hrs

Direct potentiometric measurement, sign conventions, the electrode calibration method, calibration curves for concentration measurements, potentiometric pH measurements with a glass electrode, errors affecting pH measurements with glass electrode.

UNIT-II

2. Thermal Methods 8Hrs

Thermogravimetric methods(TG): Instrumentation, The balance, Furnace, instrument control,



### Post Graduate Department of Chemistry

applications, Differential thermal analysis(DTA), instrumentation, general principles, applications, Differential scanning calorimetry(DSC), applications.

3. Solid State Chemistry

7Hrs

Types of solids, band and band theories, point defects in metals and ionic compounds, energy and entropy defects and their concentration, diffusion and electrical conduction via defects, non-stoichiometric defects, color centers and electrical properties of alkali metals halides, impurity semi-conductors reactions in organic solids, photochemical reactions, sintering solid state reactions, decomposition and dehydration reaction

#### **UNIT-III**

4. Coulometric Methods

15Hrs

Current-Voltage relationships during an electrolysis, operation of a cell at a fixed applied potential, initial thermodynamic potential, estimation of required potential, current changes during an electrolysis at constant applied potential, potential changes during an electrolysis at constant applied potential, constant current electrolysis, electrolysis at a constant working electrode potential, An introduction to coulometric methods of analysis, units for quantity of electricity, types of coulometric methods, applications, coulometric titrations, applications of coulometric titrations, comparison of coulometric and volumetric titrations.

#### **UNIT-IV**

5. An Introduction to Chromatographic Separations

8Hrs

General description of chromatography, classification of chromatographic methods, Elution chromatography on columns, chromatograms, effect of migration rates and band broadening on resolution, Migration rates of species, partition coefficients, retention time, relationship between retention time and partition coefficients, the rates of solute migration(capacity factor), differential migration rates, the shape of chromatographic peaks, methods for describing column efficiency, definition of plate height, experimental evaluation of H and N, kinetic variables affecting band broadening, relationship between plate height and column variables.

6. Gas Chromatography

7Hrs

Principles of Gas-Liquid chromatography, Instrumentation: carrier gas supply, sample injection system, column configuration and column ovens, detectors, Flame ionization detectors (FID), Thermal conductivity detectors (TCD), Thermionic detectors (TID), Electron capture detectors (ECD), Atomic emission detector (AED), Gas chromatographic columns and stationary phase: packed column, open tubular column, adsorption on column packing, stationary phases.

#### **BOOK PRESCRIBED:**

1. Solid State Chemistry: A.R. WEST

2. Principles of Instrumental Analysis: Skoog and West

3. Principles of Instrumental Analysis: Willard, Merit and Dean

4. Solid state physics: A J Dekker, Macmillan Publishers

5. Principles of physical chemistry: Puri, Sharma, Pathania.

6. Chemistry of solid state: W E Garner, Butterworth

#### **COURSE OUTCOMES:**

S. No.	On completing the course,
CO1	To learn about structure and working of different reference electrodes and working electrodes
CO2	To develop complete study skills of potentiometric method of analysis of various



# Post Graduate Department of Chemistry

	analytes
CO3	To learn about various thermal methods of analysis like DTA, TG, DSC and their applications
CO4	To understand solids and point defects in solids
CO5	To understand coulometric methods of analysis and current-voltage relation and coulometric titrations.



### Post Graduate Department of Chemistry

M. Sc. Chemistry (Semester-III)

CHE 536

Organic Lab-II

Advanced Organic Chemistry Practical

Total Hours: 90 Total Hours/week: 6 Total Credits: 3 L T P

 $0 \quad 0 \quad 3$ 

Maximum Marks: 75 Theory: 56

**Internal Assessment: 19** 

#### **INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES:**

- I. The exam will be conducted on two sessions ie Morning and Evening
- II. Students will perform two practicals.
- III Students will be asked to complete write up of both practical within first 30 minutes on the first sheet provided.
- IV. On the second sheet provided after 30 minutes, students will perform and note the record on second sheet during the conduct of practical exam
- V. The split of marks will be as under:

(Write-up = 20, Performance = 20, Viva-Voce = 10, Practical notebook = 6)

#### **COURSE OBJECTIVES:**

This course aims to give training on performing the experiments involving the multistep synthesis of organic Compounds and technique of recrystallization and impart the knowledge of recording of spectral data using various spectroscopic techniques like NMR, IR and UV-visible spectroscopy.

#### **COURSE CONTENTS:**

#### A. Preparation and characterization using spectroscopic techniques

#### 1. Pechmann reaction

Synthesis of 7-hydroxy-4-methyl coumarin

#### 2. Condensation reaction

Prepare 2-phenylindole from phenyl hydrazine

#### 3. Hoffmann rearrangement

To prepare anthranilic acid from phthalic anhydride

#### 4. Claisen-Schmidt condensation

To prepare chalcone from benzaldehyde and acetophenone

#### B. Multistep organic synthesis: Synthesis of medicinal compounds

#### 5. Synthesis of Phenytoin

- Step 1: Preparation of benzyl from benzoin
- Step 2: Preparation of phenytoin from benzyl

#### 6. Synthesis of Anthranilic Acid (or Vitamin L1)

- Step 1: Phthalic anhydride to Phthalimide
- Step 2: Phthalimide to Anthranilic acid

#### 7. Synthesis of Sulpha Drug From Aniline

- Step 1: Aniline to acetanilide
- Step 2: Acetanilide to p-acetamidebenzenesulphonyl chloride (sulphonation)
- Step 3: p-acetamidebenzenesulphonylchloride to p-acetamidebenzenesulphonamide (s-amination)
- Step 4: p-acetamide benzene sulphonamide to p-amino benzenesulphonamide(hydrolysis)



### Post Graduate Department of Chemistry

#### C. Microwave Organic Synthesis

MW-mediated preparation of lophine (2,4,5-triphenylimidazole).

#### D. Fluorescence spectroscopy

Synthesis of Fluorescein from Phthalic anhydride and Resorcinol and record its fluorescent spectra.

#### E. Schrodinger software

Molecular docking of Indomethacin (Anti-inflammatory drugs) in the crystal coordinate of COX-2 **Recommended Books:** 

- 1. An Introduction to Modern Experimental Organic Chemistry, R.M. Roberts, J.C. Gilbert, L.B. Rodewald and A.S Wingrove, Holt Rinehart and Winston Inc, New York. 1969.
- 2. Vogel's Text Book of Practical Organic Chemistry.
- 3. Laboratory Experiments on Organic Chemistry, R. Edemas, J.R. Johnson and C.F. Wilcox, The Macmillan Limited, London, 1970.
- 4. Crouch RD, Howard JL, Zile JL, Barker KH. Microwave-mediated synthesis of lophine: developing a mechanism to explain a product. *J. Chem. Edu* . 2006, 83, 1658-1660

#### **COURSE OUTCOMES**

	COLICONIES
S. No.	On completing the course,
CO1	Synthesis of new products via different named reactions
CO2	Confirmation of data using spectroscopic techniques
CO3	Justify and compare the results with literature
CO4	Write and represent the outcomes of scientific finding in graphical and electronic formats.
CO5	Generate technical skills in handling of instruments and calculation methods



### Post Graduate Department of Chemistry

M.Sc. Chemistry (Semester-III) CHE 537

**Physical Chemistry Lab-II** *Electroanalytical Techniques* 

Total Hours: 90 Total Hours/week: 6 Total Credits: 3

L T P 0 0 3

Maximum Marks: 75

Theory: 56

Internal Assessment: 19

#### **INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES:**

- I. The exam will be conducted on two sessions ie Morning and Evening
- II. Students will perform two practicals.
- III Students will be asked to complete write up of both practical within first 30 minutes on the first sheet provided.
- IV. On the second sheet provided after 30 minutes, students will perform and note the record on second sheet during the conduct of practical exam
- V. The split of marks will be as under:

(Write-up = 20, Performance = 20, Viva-Voce = 10, Practical notebook = 6)

#### **COURSE OBJECTIVES:**

The aim of this course is based on the hand-on-practice of various physical instruments for analytical studies as well as studying physical properties of various reactions by well defined technical methods.

#### **COURSE CONTENTS:**

- 1. To study the Fluorescence quenching of pyrene in presence of Cu(II) ion in presence of SDS, CTAB and TTAB
- **2.** To study the Fluorescence quenching of pyrene in presence of Cu(II) ion in presence of GEMINI Cationic Surfactants (12-2-12, 14-2-14 and 16-2-16)
- **3.** To determine the surface tension (double cabillary) of mixture of solid and water by deferential method and hence find out parachor of the mixture.
- **4.** To determine the specific and molar refractivity of n-propanol, butanol, hexane and carbon tetrachloride and calculate refraction equivalents of C, H and Cl.
- **5.** To determine the molar refractivity of water, DMF, dioxane and mixtures of water, DFM, water-Dioxane and verify the refractivity rule. Predict about the interactions between components of mixture by plotting graph between refractive index and mole fraction.
- **6.** To determine the equivalent conductance of weak electrolyte acetic at infinite dilution using Kohlrausch law.
- 7. Determine equivalent conductance of strong electrolyte at several concentrations and hence verifyonsagars equation.
- **8.** Determine equivalent conductance of weak electrolyte, say, acetic acid at different concentrations and hence test validity of Oswald's dilution law. Also determine dissociation constant of the electrolyte.
- **9.** To determine dissociation constant of a dibasic acid potentiometrically.
- **10.** To study complex formation between Fe(III) and salicylic acid and find out the formula of the complex spectrophotometrically.



### Post Graduate Department of Chemistry

- **11.** To determine the formula of the complex ion formed between Fe(III) and Thiocyante ion by Job's method.
- **12.** To study the kinetics of hydrolysis of crystal violet spectrophotometrically.
- **13.** To determine the pH of a buffer solution (pH less than 8) using a quinhydrone electrode.
- **14.** To determine the pH of various mixtures of sodium acetate and acetic acid in aqueous solution and hence determine the dissociation constant of the acid.
- 15. Titrate potentiometrically Zn (II) by  $K_4Fe(CN)_6$  and verify the composition of the complex  $K_2Zn_3$  [Fe(CN)<sub>6</sub>]<sub>2</sub>
- **16.** To determine the amount of Ibuprofen in a tablet as per IP using UV-VIS spectroscopy.
- 17. To determine the amount of Paracetamol in a tablet as per IP using UV-VIS spectroscopy.
- **18.** Determine the molar refraction of a solid substance by dissolving it in a solvent and its refractive index.

#### **COURSE OUTCOMES:**

S. No.	On completing the course,
CO1	Understanding the concept of partial molar volume and Measuring it through a simple experimental technique.
CO2	Use of Electrical methods to study various laws of electrochemistry like Oswald dilution law, Kohlrausch's law and Debye-Huckel -Onsager eqaution
CO3	Use of physical methods like surface tension and molar refraction to correlate the physical properties of compounds with molecular structure
CO4	Use of spectroscopic techniques for the study of complex formation and chemical kinetics.
CO5	Use of other electrical techniques like potentiometry, pH metry, turbiditymetry for measurement of physical properties and complex formation studies.

Post Graduate Department of Chemistry

# Semester-IV

Academic Session: 2024-25

**68** 



### Post Graduate Department of Chemistry

M.Sc. Chemistry/M. Sc. Chemistry (Under the Honours Scheme) (Semester-IV) CHE 541/ CHH 541

#### **Inorganic Chemistry-IV**

Advanced Inorganic Chemistry

Total Hours: 90

Total Hours/week: 6 Maximum Marks: 150
Total Credits: 6 Theory: 112

Total Credits: 6 Theory: 112
L T P Internal Assessment: 38

5 1 0

#### INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi.
- III. Section-I will consist of EIGHT questions and students are required to attempt any SIX short questions carrying 4 Marks each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 22 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

#### **COOURSE OBJECTIVES:**

To study photoinorganic chemistry and oxidative addition and insertion reactions with suitable examples as well as students also get knowledge on structure and bonding of d-Block elements

#### **COOURSE CONTENTS:**

UNIT-I

1. Photoinorganic chemistry

20Hrs

Basics of photochemistry, Absorption, excitation, photochemical laws, quantum yield, electronically excited states, life times, measurements of the times, flash photolysis, energy diddipation by radiative and non-radiative processes, absorption spectra, franckcondon principle, photochemical stagesprimary and secondary processes, kashia's rules, thexi states, photosubstitution reactions, adamson's rules, photo substitution reactions of Cr(III) and Rupolypyridyles. Rh(III) ammine complexes. Ligand photoreactions, photoredox reactions, comparision of Fe<sup>2+</sup> and Ru<sup>2+</sup> complexes. Photo reactions and solar energy conversion, photosynthesis in plants and bacteriocholophyll synthesis, photolysis of water using inorganic precursors.

UNIT-II

2.Oxidative addition and Insersion reactions

20Hrs

Acid base behavior of metal atom in complexes, protonation and lewis base behavior, acceptor properties of lewis acidity of complexes, oxad and reductive elimination and their mechanism, addition of specific molecules, H<sub>2</sub>, HX and organic halide addition of some others molecules, reductive elimination, migration reactions their types, promotion of alkyl migration, insertion of CO into M-H bonds, other aspects of CO insertion reactions, transfer of other molecules, CO<sub>2</sub>, SO<sub>2</sub>, NO<sub>2</sub>, RCN.



### Post Graduate Department of Chemistry

#### **UNIT-III**

3. Transition metal compounds with hydrogen and oxad reactions

20Hrs

Insertion of alkenes and C-C unsaturated compounds, cleavage of C-H bonds, alkane activation. Cyclometallation reactions in detail, reactions of free hydrocarbons.

Characterstics of hydride complexes, synthetic methods, chemical behavior of H- complexes, mononuclear and homoleptic polyhydride anions, carbonyl H- and anion H<sub>2</sub> compounds, M-H interactions. Complexes of boron and aluminium hydrides, synthetic applications of metal hydrides.

#### **UNIT-IV**

4. Structure and bonding of d-Block elements 20Hrs Pervoskite,  $Ti(NO_3)_4$ ,  $TiCl_4(diars)_2$ ,  $[Ti(OEt)_4]_4$ ,  $Zr(BH_4)_4$ ,  $[M_6X_{12}]^+$  (M= Nb& Ta; X= halide);  $VO(acac)_2$ ;  $VOCl_2(NMe_3)_2$ ,  $[Nb(n^5-C_5H_5)H-\Box$   $(n^5,n^1-C_5H_4)]_2$ ; Isopoly and heteropoly acids of MO, W & V;  $[M_6X_8]^{4+}$  M= MO & W;  $CrO(O_2)$  (bipy);  $[MO_2O_4(C_2O_4)_2$  ( $H_2O)_2]^{2+}$ ;  $[W_3O_2$  ( $O_2CMe)_6$  ( $H_2O)_3]^{2+}$ ;  $[Cr_3O(O_2CMe)_6$   $L_3]^+$ ;  $[H_2W_2(CO)_9]^{2+}$ ;  $Re_3Cl_9$ ;  $[ReH_9]^{3+}$ ;  $ReCl_6(Pet_3)_2$ ;  $Re_2Cl_6(PEt_3)_2$ ;  $Re_2Cl_5$  (DTH)2, Roussin's salts;  $[Ir_3O(SiO_4)9]^{10-}$ ;  $[Ir_3N(SiO_4)_6(H_2O)_3]^{4-}$ ;  $[Co(acac)_2]_4$ ,  $\alpha$  and  $\beta$ -MCl<sub>2</sub> (M=Pd,Pt); Wolffram's salt;  $[Ni(acac)_2]_3$ ;  $Ni(Me_6-acac)_2$ ; Ni (Me-sal)<sub>2</sub>;  $[Cren_3]$   $[Ni(CN)_5]$  1.5  $H_2O$ ; [Ni (CN)<sub>2</sub> (NH<sub>3</sub>)].  $xC_6H_6$ ;  $[Pd(O_2CMe)_2]_3$ ,  $[pt(O_2CMe)_2]_4$ ;  $[PtMe_3(acac)]_2$ ; helical chian of  $AuF_3$ , Silver (III) ethylenedibiguanide ion;  $[CuXL]_4$  X=halide, L=P or As Ligand;  $[Au_3Cl_2(PMe_2Ph)_{10}]^{3+}$ ;  $[Zn(acac)_2]_3$ ;  $[Cd\{S=C(NHCH_3)_2\}_2(SCN)_2]$ ;  $Hg(NH_3)_2Cl_2$ 

#### **BOOKS PRESCRIBED:**

- 1. Chemistry of Elements by N. N. Greenwood and Earnshaw, Perganon Press
- 2. W. W. Portfield: Inorganic Chemistry: A Unified approach
- 3. Cotton and Wilkinson: Advanced inorganic Chemistry: Vth edition

#### **COOURSE OUTCOMES:**

S. No.	On completing the course,
CO1	The course provides the students with an overview of different oxidative- reductive reactions and their applications
CO2	understand the structure, bonding and reactivity of -Coordination of C-C multiple bonds
CO3	Students will be able to characterize theoretically the type of bond of hydrogen with the transition metal.
CO4	Students also learn the structure and bonding of different inorganic complexes.
CO5	Students will learn to make difference of terminal and bridging hydrogen bonds



### Post Graduate Department of Chemistry

M.Sc. Chemistry/M. Sc. Chemistry (Under the Honours Scheme) (Semester- IV) CHE 542/ CHH 542

#### **Organic Chemistry-VI**

Asymmetric synthesis, Green Chemistry and Heterocyclic Chemistry

**Total Hours: 90** 

**Total Hours/week: 6 Maximum Marks: 150** 

**Total Credits: 6** Theory: 112 L T P **Internal Assessment: 38** 

5 1 0

#### INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi.
- III. Section-I will consist of EIGHT questions and students are required to attempt any SIX short questions carrying 4 Marks each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 22 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

#### **COURSE OBJECTIVES:**

The aim of the course is to familiarize students with the concept of Asymmetric synthesis, enzymatic approach towards asymmetric synthesis, enzyme catalyzed reactions, co-enzyme and their function, green chemistry approach towards synthesis.

#### **COURSE CONTENTS:**

UNIT-I

- 1. Asymmetric Synthesis

General Aspects 10Hrs

Introduction, Analytical methods for determination of enantiomeric purity - GC, HPLC and NMR. Natural sources of chiral starting materials, classification and methods of formation of new chiral compounds.

Non-Enzymatic Approaches towards asymmetric synthesis

10Hrs

Methods of asymmetric synthesis using chiral pool synthesis, auxilaries, chiral reagents and catalysts, Asymmetric carbon-carbon bond formation using alkylation, Michael reaction and additiontocarbonyl compounds. Cram's rule and Felkin-Ahn model. Asymmetric oxidation and reductions.

#### **UNIT-II**

Enzymatic approach towards asymmetric synthesis

10Hrs

Biotransformations: Nomenclature and Classification of enzymes, advantages and disadvantages, Fischer's lock and key and koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis. Enzyme kinetics, Michaelis-menten and lineweaver-Burk plots, reversible and irreversible inhibition. Transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis,



### Post Graduate Department of Chemistry

strain or distortion.

3. Reaction Catalysed by Enzymes

10Hrs

Nucleophilic displacement on a phosphorus atom, multiple displacement reaction and the coupling of ATP cleavage to endergonic processes. Transfer of sulphates, addition and elimination reactions, enolic intermediates in isomerization reactions, Enzyme catalyzed carboxylation and decarboxylation.

#### **UNIT-III**

#### 4. Co-Enzyme Chemistry

8Hrs

Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structure and biological function of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD+, NADP+, FMN, FAD, vitamin B<sub>12</sub>.

5. Green Chemistry approach towards synthesis

12Hrs

Principles and concepts of Green Chemistry, atom economic and uneconomic reactions, source and minimizing techniques of waste from chemical industry, homogeneous and heterogeneous catalysis, phase transfer catalysis, biocatalysis and photocatalysis. Principles of ultrasound and microwave assisted organic synthesis. Reactions in ionic liquids and other environmentally benign solvents, Future Prospects.

#### **UNIT-IV**

6. Heterocyclic Synthesis

20Hrs

(a) Introduction

Principles of heterocyclic synthesis involving cyclization reactions and cycloaddition reaction.

(b) Small Ring Heterocycles

Three-membered and four-membered heterocyclic –synthesis and reactions of aziridines, oxiranes, thiiranes, azetidines, oxetanes and thietanes

(c) Six-Membered Heterocycles with one Heteroatom

Synthesis and reactions of pyrylium salts and pyrones and their comparison with pyridinium&thiopyrylium salts and pyridones. Synthesis and reactions of quinolizinium and benzopyrylium salts, coumarins and chromones.

(d) Seven-and Large-Membered Heterocycles

Synthesis and reactions of azepines, oxepines, thiepines, diazepines, thiazepines, azocines, diazocines, dioxocines and dithiocines.

#### **BOOKS PRESCRIBED:**

- 1. Asymmetric Synthesis: The Essentials, Volume 1 Mathias Christmann, Stefan Bräse Wiley, 2008.
- 2. Principles of Biochemistry by Lehninger
- 3. Green Chemistry: An Introductory Textby Mike Lancaster, Royal Society of Chemistry, 2002
- 4. Principles of modern heterocyclic chemistry by Leo A. Paquette
- 5. Principles of Biochemistry By Voet and Voet

#### **COURSE OUTCOMES:**

S. No.	On completing the course,
CO1	Student will be aware of the asymmetric synthesis and enantiomeric purity methods
CO2	Effective and modern synthetic techniques aimed at the production of enantiomerically pure organic molecules will be introduced. Know how to apply the



# Post Graduate Department of Chemistry

	Felkin-Anh model to predict which face nucleophilic attack will occur on an enantiotopic carbonyl group.
CO3	explain and exemplify different enzyme catalyzed processes for stereoselective chemical production. will able to define the mechanisms of enzyme activity regulation
CO4	To know the importance and applications of green chemistry techniques
CO5	the student will learn nomenclature, structure, properties, syntheses, and reactions of the simple 5 and 6-membered ring heterocycles, the benzene ring fused ring heterocycles, the pyridine group, and the quinoline and isoquinoline groups.



### Post Graduate Department of Chemistry

M.Sc. Chemistry/M. Sc. Chemistry (Under the Honours Scheme) (Semester-IV) CHE 543/ CHH 543

#### **Physical Chemistry-V**

Surface and Polymer Chemistry

Total Hours: 90 Total Hours/week: 6

Total Hours/week: 6
Total Credits: 6

L T P 5 1 0

Maximum Marks: 150 Theory: 112

Internal Assessment: 38

20Hrs

#### INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi.
- III. Section-I will consist of EIGHT questions and students are required to attempt any SIX short questions carrying 4 Marks each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 22 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

#### **COURSE OBJECTIVES:**

The objective of the course is to provide the a descriptive knowledge on the topics of surface phenomenon and polymers as both o these fields find wide applications at industrial level.

#### **COURSE CONTENTS:**

UNIT-I

1. Adsorption

Surface tension, capillary action, pressure difference across curved surface (Laplace equations), Gibbs adsorption isotherm, estimation of surface area (BET equation), surface films on liquids (Electro-kinetic phenomena), catalytic activity at surfaces.

**UNIT-II** 

2. Micelles 20Hrs

Surface active agents, classification of surface active agents, micellization, hydrophobic interactions, critical micellar concentration (CMC), factors affecting CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization , solubilization, micro emulsion, reverse micelles, applications of microemulsions.

**UNIT-III** 

3. Macromolecules 20Hrs

(a) Polymer – definition, Different classifications of polymers , Linear, branched and network polymers. Basic concepts: monomers, repeat units, degree of polymerization. Types of polymers: electrically conducting polymers, Doping of polymers, mechanism of conduction, polarones and



### Post Graduate Department of Chemistry

bipolarons, fire resistant, liquids crystal polymers,

Molecular mass: number, mass and viscosity average weights; Molecular mass determination (osmometry, viscometry, diffusion and light scattering methods), sedimentation, chain configuration of macromolecules, kinetics of polymerization, thermodynamics of polymerization. calculations of average dimensions of various chain structures. Importance of polymers,

Polymerization: condensation, addition, radical chain-ionic and co-ordination and copolymerization. Polymerization conditions and polymer reactions. Polymerization in homogenous and heterogeneous systems.

#### **UNIT-IV**

#### (b) Structure and Properties:

20Hrs

Polymer structure and properties-crystalline melting point  $T_m$ -melting point of homogenous series, effect of chain flexibility and steric factors, entropy and heat of fusion. The glass transition temperature,  $T_g$ -Relationship between  $T_m$  and  $T_g$ , effects of molecular weight, diluents, chemical structure, chain topology, branching and chain linking. Property requirements and polymer utilization.

#### **BOOKS PRESCRIBED:**

- 1. Physical Chemistry, P. W. Atkins.
- 2. Textbook of polymer science, F. W. Billmeyer Jr. Wiley.
- 3. Polymer science, V. R. Gowariker, N. V. Viswanathan and J. Sreedhar, Wiley-Eastern.
- 4. Polymer Chemistry, Melcolm P. Stevens, Oxford University Press.
- 5. Physical chemistry of polymers, A. Tager, Mir Publisher, Moscow.

#### **COURSE OUTCOMES:**

S. No.	On completing the course,
CO1	They will have the understanding about the surface tension, adsorption and various theories of adsorption
CO2	They will learn about the surface films, catalytic activity at surfaces and surfactants.
CO3	They will also learn and understand the process of micellization, solubilization and the various factors affecting the process of micellization, solubilization.
CO4	They will study about the polymers and polymer reactions in detail. The various types of polymerization. Kinetics and thermodynamics of polymerization.
CO5	They will learn the structure and properties of polymers.