

### **Progressive Education Society's**

# Modern College of Arts, Science and Commerce, Ganeshkhind, Pune-411016 India

(Autonomous)
(Affiliated to Savitribai Phule Pune University)

**DBT STAR Status** 

**NAAC** accredited A Grade



# M.Sc. Organic Chemistry

A Two Year Degree Program in Chemistry

As per

# **National Education Policy (NEP)**

**Syllabus** 

**From** 

Academic Year 2023-24



# **Board of Studies Chemistry Department of Chemistry**

# M.Sc. Organic Chemistry Program Outcomes (2023 Pattern)

Sr.	Program Objectives/ Outcomes				
No.					
1	To enrich specific knowledge in areas like thermodynamics, kinetics, quantum				
	chemistry, nuclear chemistry, spectroscopy, organometallics, bio-inorganics,				
	reaction mechanisms, photochemistry, biochemistry, medicinal chemistry etc. which				
	will give a bird's eye view to the scope of chemistry.				
2	It would help students to learn applications of various facets of chemistry and their				
	importance.				
3	Problem solving will inculcate logical thinking to address a problem and become				
	result oriented with a positive attitude.				
4	Practical courses will refine the basic techniques and their use for analyses,				
	syntheses, basic computer skills and research. It would develop analytical				
	independent thinking required for academics, research and industrial work.				
5	Literature reading and project work will help for strategic planning and execution, to				
	know recent developments in chemistry, its interdisciplinary relevance and create				
	interest for research.				
6	The credit system would help them to be regular in performance, improvise their				
	presentation skills, strive for excellence and create awareness of their social and				
	environmental responsibilities.				
7	To help students build up a progressive successful career.				



# M.Sc. Organic Chemistry 2023-24 NEP Pattern M.Sc. I Organic Chemistry (Autonomous) Equivalence

P.E.S. Modern College of ASC, Ganeshkhind, Pune – 16 (2022-23)		P.E.S. Modern College of ASC, Ganeshkhind, Pune – 16 (NEP 2023-24)		
	Semester I	Semester I		
22-CCTP-1	Physical Chemistry - I (Thermodynamics, Quantum Chemistry and Chemical Kinetics)	CHE51101	Thermodynamics, Quantum Chemistry and Chemical Kinetics	
22-CCTP-2	Inorganic Chemistry – I (Molecular Symmetry and Main group Elements)	CHE51103	Molecular Symmetry and Main Group Elements	
22-CCTP-3	Organic Chemistry – I (Basic Organic Chemistry)	CHE51102	Stereochemistry and Organic Synthesis	
22-CBOP-1	General Chemistry – I Section - I: Theory Course (Any one option) Option A: Mathematics for Chemists Option B: Chemical Biology - 1			
22-CBOP-1	Section - II: Inorganic Chemistry Practical - 1	CHE51105	Inorganic Chemistry Practical - 1	
22-CCPP-1	Basic Practical Course – I Section I: Physical Chemistry Practical – 1	CHE51104	Physical Chemistry Practical - 1	
22-CCPP-1	Section II: Organic Chemistry Practical - 1	CHE51106	Organic Chemistry Practical - 1	

P.E.S. Modern College of ASC, Ganeshkhind, Pune – 16 (2022-23)		P.E.S. Modern College of ASC, Ganeshkhind, Pune – 16 (NEP 2023-24)		
	Semester II	Semester II		
22-CCTP-4	Physical Chemistry - II (Molecular Spectroscopy, Nuclear and Radiation Chemistry)	CHE52103	Molecular Spectroscopy, Nuclear and Radiation Chemistry	
22-CCTP-5	Inorganic Chemistry - II (Coordination and Bioinorganic Chemistry)	CHE52101	Coordination and Bioinorganic Chemistry	
22-CCTP-6	Organic Chemistry - II (Photochemistry and Organic Spectroscopy)	CHE52102	Photochemistry and Organic Spectroscopy	
22-CBOP-2	General Chemistry -II Section - I: Theory Course (Any one option) Option A: Advanced Analytical Techniques Option B: Chemical Biology - 2			
22-CBOP-2	Section - II: Physical Chemistry Practical - 2	CHE52104	Physical Chemistry Practical - 2	
22-CCPP-2	Basic Practical Course - I Section I: Inorganic Chemistry Practical -2	CHE52105	Inorganic Chemistry Practical - 2	
22-CCPP-2	Section II: Organic Chemistry Practical - 2	CHE52106	Organic Chemistry Practical - 2	



# M.Sc.- I Organic Chemistry Course Structure (2023 NEP Pattern) With Effect from 2023-24

Semester I						
Course Name Code						
CHE51101	Thermodynamics, Quantum Chemistry and Chemical Kinetics	4				
CHE51102	Stereochemistry and Organic Synthesis	4				
CHE51103	Molecular Symmetry and Chemistry of Main Group Elements	4				
CHE51104	Physical Chemistry Practical – 1	2				
CHE51105	Inorganic Chemistry Practical – 1	2				
CHE51106	Organic Chemistry Practical – 1	2				
CHE52107	Research Methodology	4				
Semester II						
Course Code	Course Name	Credit				
CHE52101	Coordination and Bioinorganic Chemistry	4				
CHE52102	Photochemistry and Organic Spectroscopy	4				
CHE52103	Molecular Spectroscopy, Nuclear and Radiation Chemistry	4				
CHE52104	Physical Chemistry Practical – 2	2				
CHE52105	Inorganic Chemistry Practical – 2	2				
CHE52106	Organic Chemistry Practical – 2	2				
CHE53107	On Job Training	4				
Total Subject Course credits for the M.Sc. – I 44						

<sup>\*</sup> Any two topics given by the subject teacher from each credit course will be learned by the students through online mode (NPTEL/SWAYAM MOOCS). A test will be conducted on these topics as a part of Continuous Internal Assessment (CIA).



#### **Semester-I**

# CHE51101: Thermodynamics, Quantum Chemistry and Chemical Kinetics (4 Credits, 60 L)

#### **Course Outcomes**

- CO1: To study the concepts in thermodynamic to understand the thermodynamics of the mixtures.
- CO2: To understand the concept of partition function and its applications in finding the thermodynamic parameters with reference to translational, rotational, vibrational and electronic energies
- CO3: To understand the need of quantum chemistry and its application in understanding the particle in a box concept.
- CO4: To understand the kinetics of elementary and complex reactions
- CO5: To know the different techniques to study the fast reactions.
- CO6: To understand the kinetics of catalytic reactions based on enzyme catalysis, autocatalysis.
- CO7: To understand the surface chemistry concepts.

### **SECTION - I Thermodynamics and Quantum Chemistry**

(2 Credits, 30 L)

#### 1. Thermodynamics (10 L)

State function, path function, exact differential and inexact differential, internal energy and enthalpy, temperature dependent internal energy and enthalpy, Entropy and entropy change in an ideal gas with temperature and pressure, Clausius inequality, chemical potential, chemical potential of a substance in a mixture. Thermodynamics of Gibbs function of mixing, colligative properties: Elevation in boiling point, depression in freezing point and osmosis.

#### 2. Molecular Thermodynamics (10 L)

Molecular energy levels, Boltzmann distribution law, partition functions and ensembles, translational, rotational and vibrational partition function of diatomic molecule, obtaining energy, heat capacity, entropy and equilibrium constants from partition functions, Maxwell-Boltzmann, Fermi-Dirac and Bose-Einstein statistics.

#### 3. Quantum Chemistry (10 L)

Applications of quantum chemistry over failure of classical mechanics - blackbody radiation,



photoelectric effect, de Broglie hypothesis, uncertainty principle and its experimental evidence. Schrödinger wave equation, particle in one dimensional box, well behaved function, Normalization and orthogonality of wave function, particle in three-dimensional box, Shrodinger equation for one electron systems i.e. hydrogen like atoms (no derivation). Operators: algebra of operators, commutative property, linear operators, commutator operator, the operator  $\nabla$  and  $\nabla$ 2. Huckel theory applications to simple  $\pi$ -systems.

#### **Learning Outcomes**:

- 1) The student will understand the thermodynamics of mixtures and partial molar quantities based on the concepts in thermodynamics.
- 2) The student will understand the concept of partition function and its applications in finding the thermodynamic parameters with reference to translational, rotational, vibrational and electronic energies.
- 3) The student will understand failure of classical mechanics and the need of quantum chemistry.
- **4**) The student will derive Schrödinger equation with reference to the concepts in quantum chemistry.
- 5) The student will draw the schematic diagram of Molecular orbital diagram of theory for di and tri atomic molecule based on Molecular Orbital Theory.
- 6) The student will apply Hückel theory to simple  $\pi$  –systems.
- 7) The student will be able to solve the related numerical problems.

## **SECTION - II Chemical Kinetics and Reaction Dynamics**

(2 Credits, 30 L)

#### 1. Kinetics of Complex Reactions (10 L)

Types of complex reactions:- parallel, opposing and chain. Steady state approximation in chain reactions - free radical polymerization reaction between H<sub>2</sub> and Br<sub>2</sub>, degradation of ozone, decomposition of acetyldehyde, explosive reaction –formation of water. autocatalysis

#### 2. Molecular Reaction Dynamics (10 L)

Collision theory of bimolecular gas phase reactions, diffusion controlled and activation controlled reaction in solution, activated complex theory of reaction rate, Eyrings equation Techniques used to study the fast reactions: flow technique, stopped flow technique, relaxation method, flash photolysis, pulse radiolysis,

#### 3. Enzyme Catalysis (10 L)

Modes of Enzyme-Substrate interaction, effect of pH and temperature on enzyme catalyzed reactions, Michaels mechanism for enzyme catalysis and enzyme inhibition, modes of enzyme inhibition- competitive inhibition and non- competitive inhibition. Lineweaver-Burk and Eadie plots for enzyme catalysis and enzyme inhibition



#### **Learning Outcomes**:

- 1) The students will be able to understand the difference between the elementary and complex reactions with reference to the concepts in chemical kinetics.
- 2) The student will derive the rate law for the different chain reactions.
- 3) The student will understand Collision and Activated complex theory.
- 4) The student will understand the kinetics of Enzyme catalysis
- 5) The student will understand the stopped flow technique and flash photolysis and Pulse radiolysis techniques to study the fast reactions.
- **6**) The student will understand the kinetics of catalytic reactions based on enzyme catalysis, autocatalysis
- 7) The student will solve the numerical problems.

#### **References:**

- 1. Atkin's Physical Chemistry by P.W.Atkin and J. De Paula; W. H. Freeman And Company Eighth edition (2006). ISBN: 0-7167-8759-8
- 2. Physical Chemistry by T.Engel and P. Reid
- 3. Physical Chemistry and molecular approach by D. Mequarie and J. Siman
- 4. Physical Chemistry for biological sciences by Raymond Chang (Universal books, 2000)
- 5. Physical Chemistry by Merron and C.F. Prouton
- 6. Physical Chemistry by G.M. Barrow
- 7. Quantum Chemistry by I. Levine
- 8. Quantum Chemistry by R.K. Prasad
- 9. Physical Chemistry through Problems by S.K. Dogra



### CHE51102 Stereochemistry and Organic Synthesis

#### **Course Outcomes**

(4 Credits, 60 L)

- CO1: Understand fundamental aspects of organic chemistry, learn the concept of aromaticity and its types.
- CO2: To understand the concept of nuclephilic and electrophilic substitution and elimination reactions.
- CO3: understand concepts of stereochemistry and to be able to apply stereochemical aspects in organic chemistry
- CO4: To study structure, formation, stability and related name reaction of carbon intermediates
  - ; recognise neighbouringgroup participation
- CO5: To study rearrangement reaction with specific mechanism and migratory aptitude of different groups
- CO6: To study Ylides and their reactions.
- CO7: To understand the basis of redox reactions; reagents and mechanism for selective oxidation/reduction reactions of organic compounds.

SECTION - I (2 Credits, 30L)

#### 1. Chemical Structure and reactivity (8L)

Acidity and basicity

Acids and Bases examples, Factors affecting acidity and basicity: Electronegativity and inductive effect, resonance, bond strength, electrostatic effects, hybridization, aromaticity and solvation. Comparative study of acidity and basicity of organic compounds on the basis of pKa values

Benzenoid and non-benzenoid compounds, Huckel's rule, antiaromaticity, annulenes, azulenes, ring current concepts of aromaticity

#### 2. Stereochemistry (12L)

Stereochemical principles, enantiomeric relationship, diastereomeric relationship, R and S, E and Z, D and L nomenclature in C, N, S, P containing compounds, conversion of projections (newmann to sawhorse and fischer)

Prochiral relationship, stereospecific and stereoselective reactions, optical activity in biphenyls, spiranes and allenes

#### 3. A comparative study of Substitution and Elimination Reactions (10L)

Aromatic electrophilic substitution, Aliphatic nucleophilic substitutions:SN1, SN2, SN2 and SNi reactions; Effect of solvent and Leaving Group.



Eliminations: Mechanism and orientation, Reactivity, Pyrolytic Eliminations; E1, E2, E1CB reactions (in detail) Elimination vs Substitution with NGP

### **Learning Outcomes**

- 1. Students will be able to understand the **c**riteria for aromaticity in non benzenoid molecules andother advanced polycyclic aromatics
- 2. Students will learn the concept stereochemistry and its importance; their rules and the concept of chirality.
- 3. Students will be able to concept of substitution and elimination reactions and will be able to write mechanism.

SECTION - II (2 Credits, 30L)

#### 1. Structure, Stability and Reactions of Reactive Intermediates

(8 L)

Carbocation, Carbanion, Free Radical, Carbenes and nitrenes

NGP: Neighbouring group participation

#### 2. Rearrangements:

(8L)

Beckmann, Hofmann, Curtius, Schmidt, Wolff, Lossen, Bayer-villiger, Sommelet, Favorskii, Pinacol-pinacolone, Benzil-benzilic acid, Fries, Tiffeneau Demjanov.

3. Ylides: (4 L)

Phosphorus, Nitrogen and Sulphur ylides

#### 4. Oxidation and Reduction Reactions:

(10 L)

Oxidising agents: CrO3, PDC, PCC, KMnO4, MnO2, Swern, SeO2, Pb(OAc)4, Pd-C, RuO4, OsO4, m-CPBA, O3,NaIO4, HIO4, TEMPO, IBX, CAN, Dess-Martin, DDQ, Ag2O

Reducing agents: Boranes and hydroboration reactions,MPV reduction and reduction with H2/Pd-C, Raney-Ni, NaBH3CN, Wilkinson's catalyst, DIBAL and Wolff-Kishner reduction, Birch, Clemenson, Dissolving metal

#### References:

- 1. Organic Chemistry-by J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford)
- 2. Advanced Organic Chemistry –by J. March 6th Edition
- 3. Advanced Organic Chemistry (Part A) –by A. Carey and R.J. Sundberg
- 4. A guidebook to mechanism in organic chemistry Peter Sykes 6th Ed.
- 5. Stereochemistry of carbon compound-by E.L. Eliel
- 6. Stereochemistry of organic compound-by Nasipuri
- 7. Stereochemistry conformations and mechanism by P.S. Kalsi
- 8. Modern Synthetic reactions- H.O. House
- 9. Organic Synthesis M.B. Smith
- 10. Organic chemistry –by Cram, Hammond, Pine and Handrickson
- 11. Mechanism and structure in Organic Chemistry E. S. Gould



### **Learning Outcomes**

- 1. Students will be able to understand the role of various reaction intermediates like carbocation, carbanion, carbenes, radicals, and nitrenes in organic reactions; concept of NGP
- 2. Able to describe mechanism of different rearrangement reactions. Appreciates the various steps involved in the molecular rearrangements.
- 3. Students will be able to understand the chemistry of Ylides
- 4. Use synthetic reagent of oxidation and reduction for solving the problems

# CHE51103 Molecular Symmetry and Chemistry of Main Group Elements (4 credits, 60 L)

### **Course Outcomes**

- CO1: To visualize molecule in 3-D, understand the concept of molecular point groups with their symmetry elements, symmetry operations, GMTs, character tables and group representations.
- CO2: To understand how to derive the SALCs for molecules using the Projection Operators and also how to construct molecular orbitals using various symmetry operations and their representations.
- CO3: To correlate application of symmetry to spectroscopy and find possible IR active modes of vibration.
- CO4: To understand the detail chemistry of s- and p- block elements w.r.t. their compounds, reactions, applications and organometalllic chemistry of some important elements.
- CO5: To learn the advance chemistry of boranes, fullerenes, silicates including zeolites, carbon nanotubes, Polymers, etc.

## **SECTION-I** Molecular Symmetry

(2 Credits, 30 L)

#### • Molecular Symmetry

(12 L)

Introduction, Symmetry elements and Symmetry operations: Identity, Rotational axis of Symmetry, Plane of Symmetry, Improper rotational axis and Inversion center. General relations among symmetry elements and symmetry operations, symmetry elements and optical isomerism. Mathematical requirement of a point group, Molecular point groups, identification of molecular point groups and systematic assignment of point groups to molecules, Products of symmetry operations, group multiplication tables, equivalent symmetry elements and equivalent atoms, isomorphic groups, subgroups, classes.

#### • Representations of Groups

(8 L)

Matrix representation of symmetry elements and point groups, transformation matrices. The Great Orthogonality Theorem and its consequence, character tables (No mathematical part), wave function as basis for irreducible representations.



#### • Symmetry Adapted Linear Combination

(5 L)

Projection operators and their use to construct normalised SALCs. Transformation properties of atomic orbital, MOs for sigma bonding ABn molecules.

#### • Application of Group theory to Infrared Spectroscopy

(5 L)

Introduction, selection rules, polyatomic molecules, possible vibrations in linear molecules, modes, symmetry of vibrations and their IR activity. Group vibration concept and its limitations. IR spectra related to symmetry of some compounds. IR spectra of complex compounds.

#### **References:**

- 1) Chemical Applications of Group Theory by F. A. Cotton
- 2) Symmetry and spectroscopy of molecules by K. Veera Reddy
- 3) Group Theory and its Chemical Application, P.K. Bhattarcharya
- 4) Inorganic Chemistry by Shriver and Atkins
- 5) Concise Inorganic Chemistry by J. D. Lee
- 6) Inorganic chemistry: principle of structures and reactivity by Huheey, Keiter, Medhi

# **Learning Outcomes**

- 1. Visualize/ imagine molecules in 3 dimensions, perform various symmetry operations on the molecule, know the symmetry elements and hence point group of the molecule.
- 2. Apply the concept of point group for determining optical activity of the molecule.
- 3. Understand product of symmetry operations, classes, representation of groups and construction of character tables using the Great Orthogonality Theorem.
- 4. Apply projection operator to find out the normalized SALCs of the molecule.
- 5. Correlate the application of symmetry to spectroscopy and find out the possible modes and IR active modes of vibration.

### **SECTION-II Main Group Elements**

(2 Credits, 30 L)

#### • Hydrogen and its compounds

(4 L)

Hydrides: Classification of Hydrides, electron deficient, electron precise and electron rich hydrides, preparation, properties, reactions and applications, hydride stability.

#### • Alkali and Alkaline Earth Metals

(3 L)

Solutions in non - aqueous media: in ammonia, ether and other macrocyclic compounds, application of crown ether in extraction of alkali and alkaline earth metals, Important organometallic compounds of alkali and alkaline earth metals:

preparation, properties, reactions and applications

• Boron Group (6 L)

Boron Hydrides: preparation, structure and Bonding with reference to LUMO, HOMO, interconversion of lower and higher boranes, metalloboranes, carboranes, reactions of organoboranes, STYX rules and structure of higher boranes. Organometallic compounds of B, Al & Ga.

• Carbon Group (6 L)

Allotropes of carbon: Diamond, Graphite, Graphene, fullerenes and carbon nanotubes: synthesis, properties, Structure - single walled and multi walled nanotubes and its applications. Intercalation compounds of graphite, fullerene metal complexes. Silicates: structures, properties, uses, Molecular sieves and zeolites. Organometallic compounds of Si, Sn and Pb

• Nitrogen Group (4 L)

Nitrogen activation, Oxidation states, oxyacids and oxoanions of nitrogen and their interconversion, Compounds of nitrogen with Boron, Phosphorus and sulphur, with respect to structure, properties and applications, Organometallic compounds of As, Sb and Bi.

• Oxygen Group (3 L)

Metal Selenides and Tellurides, Oxyacids and oxoanions of Sulphur. Ring, Cage and Cluster compounds of p-block elements.

• Halogen Group (2 L)

Pseudohalogen and interhalogen compounds: Synthesis, structures, Properties and Applications

• Noble gases (2 L)

Occurrence, Compounds of Xenon with fluorine and Oxygen

#### **References:**

- 1) Inorganic Chemistry by Shriver and Atkins
- 2) Concise Inorganic Chemistry by J. D. Lee
- 3) Inorganic chemistry by Principle of Structures and Reactivity by Huheey, Keiter, Medhi
- 4) Inorganic Chemistry by Catherine Housecraft
- 5) Inorganic Chemistry by MeisslerandTarr
- 6) Organometallics by Christoph Elschenbroich
- 7) Organometallics by A Concise Introduction by Christoph Elschenbroich and AlbrechtSalzer
- 8) Basic Organometallic Chemistry by B. D. Gupta and A. J. Elias

#### **Learning outcomes:**

1. Know the types, preparation, structures, properties, and applications of binary compounds of hydrogen.



- 2. Understand the chemistry of s-block elements with respect to their compounds in non-aqueous solvents, extraction and organometallic compounds.
- 3. Learn the advance chemistry of boranes, fullerene, silicates including molecular sieves and zeolites, polymers etc.
- 4. Know important organometallic compounds of some elements and study their preparation, structure, properties and applications.

### **CHE51104** Physical Chemistry Practical -1 (11 Experiments)

(2 Credits, 60 hrs.)

#### **Course Outcomes**

CO1: The students should be able to apply and correlate the concepts in theory while performing the experiments.

CO2: The students should develop the skill for the laboratory safety and handling of chemicals.

CO3: The students should be able to work independently in the laboratory.

### List of the experiments

1. Statistical treatment of experimental data (calculation of mean and standard deviation for given data and least square method for calibration curve method) (compulsory)

#### Part-I: Chemical Kinetics: (Any three)

- 2. Kinetic decomposition of diacetone alcohol by dilatometry.
- 3. Determination of an order of a reaction.
- 4. Brönsted primary salt effect.
- 5. Kinetics of oxidation of ethanol by K2Cr2O7

#### **Part-III: Colorimetry and spectrophotometry** (Any five)

- 6. Simultaneous determination of Ni and Co by spectrophotometry
- 7. Simulations determination of KMnO4 and K2Cr2O7 by spectrophotometry.
- 8. To study the adsorption of certain dyes such as methyl violet, picric acid or malachite green on charcoal. (Ref-2)
- 9. To determine the indicator constant of bromocresolpuple by half height method
- 10. Estimation of Cu (II) by titration with Na<sub>2</sub> EDTA by colorimetry
- 11. Determination of energy of n to  $\Pi^*$  transition in acetone and study of effect of solvent on energy of this transition by recording absorbance spectra in n-hexane and water. b. To study the effect of the extended conjugation on the  $\lambda_{max}$  of p-nitro phenol by recording spectrum in acidic and alkaline medium.

#### **Part-III Non instrumentation experiments:** (Any two)

- 12. Determination of molecular weight by steam distillation.
- 13. Glycerol radius by viscosity.
- 14. Partial Molar Volume (Polynometry) Determination of the densities of a series of solutions and tocalculate the molar volumes of the components.

#### **References:**

- 1. Practical physical chemistry, A. Findlay, T.A. Kitchner (Longmans, Green and Co.)
- 2. Experiments in Physical Chemistry, J.M. Wilson, K.J. Newcombe, A.r. Denko. R.M.W. Richett(Pergamon Press)



### CHE51105 Inorganic Chemistry Practical-1

(2 Credits, 60 hrs.)

#### **Course Outcomes**

- CO1: Prepare the exact solutions for quantitative analysis.
- CO2: Apply the knowledge of quantitative analysis for the determination of metals from ores/alloys.
- CO3: Know different methods for the synthesis and characterization of nanoparticles
- CO4: Learn various applications of nanoparticles
- CO5: Understand principle and working of Ion-exchange chromatography for separation of metal ions using ion-exchange resin.

#### Part-I: Ore Analysis (at least two of the following)

- 1. Determination of Silica and Manganese from pyrolusite ore.
- 2. Determination of Aluminum and Silica from Bauxite ore.
- 3. Determination of silica and iron from hematite ore.
- 4. Determination of copper and iron from Chalcopyrite ore.

#### Part-II: Alloy Analysis (at least two of the following)

- 1. Determination of tin and lead from solder alloy.
- 2. Determination of iron and chromium from stainless steel alloy.
- 3. Determination of copper and nickel from cupranickel alloy.

#### Part-III: Synthesis of solid state materials / nano-materials (any three)

- 1. Synthesis of ZnO from zinc oxalate precursor method and determine band gap by absorption spectroscopy.
- 2. Synthesis of TiO<sub>2</sub> using TiCl<sub>4</sub> or Ti-isopropoxide by Sol-gel method and determine band gap by absorption spectroscopy
- 3. Synthesis of Colloidal silver nanoparticles and determine band gap byabsorption spectroscopy
- 4. Synthesis of Fe<sub>2</sub>O<sub>3</sub> nanoparticles sol-gel/coprecipitation/hydrothermal (any one method).
- 5. Spectral analysis (powder XRD/SEM/TEM) of one compound.

#### **Part-IV: Applications of Solid State Materials**

- 1. Removal and kinetics of photocatalytic dyes, degradation (methylene by ZnO or TiO<sub>2</sub> photocatalysis.
- 2. Study of adsorption of phosphate ion on α-Fe<sub>2</sub>O<sub>3</sub>

#### **Part-V: Ion – Exchange Chromatography**

Separation of mixture of Zn(II) and Mg(II) using Amberlite IRA 400 anion



exchanger and quantitative estimation of separated ions Zn(II) and Mg(II)

#### **References:**

- 1. Text book of Quantitative Analysis by A.I. Vogel 3<sup>ed</sup>ed<sup>n</sup> (1963).
- 2. Experimental Inorganic Chemistry by Mounir A. Malati, Horwood
- 3. Nanotechnology by S. K. Kulkarni

### CHE51106 Organic Chemistry Practical- 1 (11 Experiments)

(2 Credits, 60 hrs.)

#### **Course Outcomes**

- 1.Students are trained to different purification techniques in organic chemistry like recrystallization, distillation, steam distillation and extraction.
- 2. Students are made aware of safety techniques and handling of chemicals.
- 3. Students are made aware of carrying out different types of reactions and their workup methods.
- 4. This practical course is designed to make student aware of green chemistry and role of green chemistry in pollution reduction.
- 5. Students are made aware of carrying out different types of reactions and their workup methods.
- 6. This practical course is designed to make student aware of green chemistry and role of green chemistry in pollution reduction.

**Time allotted:** Two practical sessions of 4 hours per week for one semester (one practical session for Section-II per week is compulsory)

Introduction to Laboratory Safety: Meaning of safety signs on container of chemicals, safety handling of chemicals, MSDS sheets: Detailed explanation at least for 4 different types of substances (e.g. nitric acid, benzene, potassium dichromate, bromine, etc.), Handling of glassware's and care to be taken, handling of organic flammable as well as toxic solvents in laboratory, use of safety goggles, shoes and gloves, fire extinguisher and its use, action to be taken in accidental cases e.g. cleaning of acid spill over, use eye wash station and bath station in emergency, etc. (compulsory)

#### • Purification Techniques

- a. Crystallization
- b. Distillation (upward and downward)
- c. Column Chromatography p-nitroaniline + o-nitroaniline

#### • Single stage preparations (any 4)

- a. Benzil benzilic acid rearrangement
- b. Synthesis of 1,4-dihydropyrimidin-[4H]-ones
- c. Preparation of Schiff's bases in aqueous medium.
- d. Nitration of bromobenzene or Anisole (low temp)
- e. Reduction of cyclohexanone using NaBH<sub>4</sub>



### **Semester II**

# CHE52101 Coordination and Bioinorganic Chemistry (4 Credits, 60 L)

### **Course Outcomes**

After successfully completing this course, students will be able to

CO1: find out the number of microstates, construct a microstate table and know meaningful term symbols for various configurations.

CO2: find out splitting of the free ion terms in weak and strong ligand fields and draw Orgel, correlation and Tanabe-Sugano diagrams for various configurations in Td an Oh ligand field.

CO3: Study electronic spectra, its interpretation and solve numerical based on crystal field parameters.

CO4: Understand various terms involved in magneto chemistry, know various phenomena of magnetism and their temperature dependence.

CO5: Understand Importance of bioinorganic chemistry and Role of metals in living systems.

CO6: Know the similarities in coordination theory for metal complexes and metal ions complexed with biological ligands.

CO7: Importance and transport of metal ions by ionophores and Mechanism for active transport of Na<sup>+</sup> and K<sup>+</sup> ions.

#### **SECTION I Coordination Chemistry**

(2 Credits, 30 L)

### 1) Concept and Scope of Ligand Fields

(8 L)

Quantum numbers, Free ion Configuration, Terms and States, Energy levels of transition metal ions, free ion terms, microstates, microstate table, term wave functions, spin-orbit coupling.

#### 2) Ligand Field Theory of Coordination Complexes

(8 L)

Effect of ligand field on energy levels of transition metal ions, weak cubic ligand field effect on Russell- Saunders terms, Orgel diagrams, strong field effect, correlation diagrams, Tanabe-Sugano Diagrams, Spin-Pairing energies.



#### 3) Electronic spectra of Transition Metal Complexes

(8 L)

Introduction, band intensities, band energies, band width and shapes, electronic spectra of  $1^{st}$ ,  $2^{nd}$  and  $3^{rd}$  row transition metal ions and complexes, electronic spectra of Lanthanides and actinides, calculations of Dq, B,  $\beta$  parameters, percentage of covalent character for metal complexes, spectrochemical and Nephelauxetic series, charge transfer and luminescence spectra.

### 4) Magnetic Properties of Coordination Complexes

(6 L)

Origin of magnetism, types of magnetism, Curie law, Curie-Weiss Law Magnetic properties of complexes - Para magnetism, 1<sup>st</sup> and 2<sup>nd</sup> Ordered Zeeman effect, Quenching of orbitalangular momentum by Ligand fields, Magnetic properties of A, E and T ground terms in complexes, temperature dependence of magnetism.

#### **References:**

- 1. Ligand field theory and its applications by B.N. Figgis and M.A. Hitachman
- 2. Symmetry and spectroscopy of molecules by K. Veera Reddy
- 3. Elements of Magnetochemistry by R. L. Datta and A. Syamal

# **Learning Outcomes**

After successfully completing this Section, students will be able to

- 1. Understand ligand field theory, terms, states, microstates and microstate table.
- 2. Use Hund's rules for arranging the terms according to energy.
- 3. Know the inter electronic repulsion and spin orbit coupling in metal ions.
- 4. To draw correlations diagram for various configurations in Td an Oh ligand field.
- 5. know basic instrumentation and interpretation of electronic spectra, selection rules and relaxation in rules.
- 6. Understand the concept of spectro chemical series and Nephelauxetic series.
- 7. Understand types of magnetism, magnetic properties of complexes and quenching of orbital magnetic moment.

#### **SECTION-II Bioinorganic Chemistry**

(2 Credits, 30 L)

#### 1) Overview of Bioinorganic Chemistry

(4 L)

Historical Background and current relevance, role of metals in Biology, metalloproteins, metalloenzymes, nucleic acids and in medicine.

#### 2) Concepts of Inorganic Chemistry in Bioinorganic Chemistry

(10 L)

Thermodynamic aspects - HSAB concept, chelate effect and Irving-William



series, pK<sub>a</sub> values of coordinated ligands, Tuning of redox potential, Biopolymer effects. Kinetic aspects: Electron transfer reaction, Electronic substitution reaction, reactions of coordinated ligands and Template effect, concept of spontaneous self-assembly and model compounds.

Proteins, Nucleic acids and other metal binding biomolecules.

3) Functions and Transport of Alkali and Alkaline Earth Metal Ions (6 L) Importance of alkali and alkaline earth metals, Distribution of cationic and anionic electrolytes in blood plasma and intracellular fluid, Ionophores: Natural and Synthetic, Application of ionophores, Different mechanism involved in exchange of ions across cell wall, Na<sup>+</sup>/K<sup>+</sup>-ATPase ion pump for active transport of Na<sup>+</sup> and K<sup>+</sup>.

#### 4) Biochemistry of following Elements

(10 L)

- Ca in Blood coagulation.
- Magnesium in Photosystem I
- Manganese in Photosystem II
- Iron in Ferritin, Transferrin, Fe-S clusters

#### **References:**

- 1. Principle of Bioinorganic Chemistry by S.J. Lippard and J. M. Berg
- 2. Bioinorganic Chemistry: Inorganic Elements in Chemistry of Life by W.Kaim and B.Schwederski

### **Learning outcomes:**

- 1. After successfully completing this course, students will be able to:
- 2. Understand Importance of bioinorganic chemistry and Role of metals in Biology and in medicine.
- 3. Apply the concepts in Inorganic coordination Chemistry to metal ions complexed with biological ligands.
- 4. Importance and transport of metal ions by ionophores
- 5. Mechanism for active transport of Na<sup>+</sup> and K<sup>+</sup>
- 6. Importance and function of Ca, Fe, Mn and Mg in metalloprotein

### CHE52102 Photochemistry and Organic Spectroscopy

(4 Credits, 60 L)

## **SECTION I** Photochemistry

(2 Credits, 30 L)

(14 L)

### 1. Photochemistry

Photochemistry: Singlet, Triplet, Excited states, Fate of excited species, Jablonskii diagram, Phosphorescence, Fluorescence etc, Barton reaction. Photochemistry of Carbonyl compounds:



Paternobuchi, Norrish I and II, Dienone phenol rearrangement Photochemistry of alkenes and dienes: [2+2] cycloaddition.

Photochemistry of aromatic compounds: Formation of Dewar Benzene, Electrocyclization involving heteroatoms, Di-Pi methane rearrangement, Photodimerization.

#### 2. Addition to C-C and C-X multiple bonds

(10 L)

#### 3. Carbon-Carbon double bond formation

(6 L)

Peterson olefination, Julia-Lythgoe olefination, carbonyl coupling reaction (McMurryreaction), Tebbe reagent, Shapiro and related reactions,  $\beta$ -elimination and dehydration

#### **References:**

- 1. Advanced Organic Chemistry, Part A by F. A. Carey and R. J. Sundberg
- 2. Excited states in Organic Chemistry by J.A. Barltrop and J.D.Coyle
- 3. Organic photochemistry: A visual approach by Jan Kopecky
- 4. Conservation of orbital symmetry by R. B. Woodward and R. Hoffmann
- 5. Advanced Organic Chemistry, Part B by F. A. Carey and R. J. Sundberg
- 6. A guidebook to mechanism in organic chemistry Peter Sykes 6th Ed.

### **Learning Outcomes**

- 1. Students will be able to understand free radicals formation, stability and reactivity and should also be able to use the basic understanding in writing probable reaction mechanisms.
- 2. They will be able to understand carbon-carbon bond formation and will be able to write the mechanism for addition reactions.
- 3. Students will be able to learn different types of name reactions.

# **SECTION II Organic Spectroscopy**

(2 Credits, 30 L)

#### 1. UV Spectroscopy

(6 L)

UV: Recapitulation of UV spectroscopy, calculations of max of aromatic compounds IR spectra of important functional groups 1. With and without conjugation, 2. Ring size effect 3. Effect of H-bonding, 4. Resonance effect, 5. Inductive effect.



 $2. ^{1}H-NMR (14 L)$ 

Understanding of basic principle, chemical and magnetic nonequivalence, Homotopic, Enantiotopic, diastereotopic protons, chemical shifts and factors influencing chemical shift: electronegativity, NMR solvent polarity, temperature, anisotropic effect, chemical shifts of acidic protons, D<sub>2</sub>O exchange, Multiplicity patterns and Coupling Constants: Pascal's triangle, understanding of tree diagram, complex splitting patterns in aromatic, vinylic, saturated monocyclic compounds, bicyclic compounds (fused and bridged rings).

3.  $^{13}$ C-NMR (6 L)

Basic of <sup>13</sup>C-NMR: Chemical shift and factors affecting chemical shifts in <sup>13</sup>C NMR, off resonance and proton decoupled spectra. Simple problems on <sup>13</sup>C-NMR.

#### 3. Combined problems on UV, IR and NMR

(4 L)

#### **References:**

- 1. Introduction to Spectroscopy by Donald L. Pavia and Gary M. Lampman
- 2. UV-VIS Spectroscopy and Its Applications by Perkampus, Heinz-Helmut
- 3. Infrared Spectroscopy: Fundamentals and Applications by Barbara H. Stuart
- 4. Infrared Spectroscopy by James M. Thompson
- 5. Spectrometric Identification of Organic Compounds by Robert M. Silverstein, Francis X. Webster, David J. Kiemle, David L. Bryce
- 6. Introduction to Spectroscopy by Donald L. Pavia
- 7. Understanding NMR Spectroscopy by James Keeler
- 8. Applications of NMR Spectroscopy by Atta-ur-Rahman, M. Iqbal Choudhar
- 9. Solving Problems with NMR Spectroscopy by Atta-ur-Rahman Muhammad Choudhary Atiatul- Wahab

### **Learning Outcomes**

- 1. Students will be able to calculate  $\lambda$ max of organic compounds containing more than one and less than four conjugated systems. Students should able to correlate IR bands with functional groups using numerical data as well as spectral data.
- 2. Students will able to solve 1H-NMR problems and should also able to draw the 1H-NMR spectrum for simple organic compounds mentioning multiplicity pattern and coupling constant with the help of "Tree Diagram" Should able to predict and analyze the multiplicity patterns with more than one coupling constants.
- 3. Students will be able to use 13C-NMR data to interpret the structure NMR problems and P.E.S' Modern College of Arts, Science and Commerce, Ganeshkhind, Pune-16 (Autonomous) Syllabus 2022 Pattern



should also able to draw the 1H-NMR spectrum for simple organic compounds mentioning multiplicity pattern and coupling constant with the help of "Tree Diagram" Should be able to predict and analyze the multiplicity patterns with more than one coupling constants.

4. Students should able to know various key factors responsible for the spectroscopic data acquisition and should able to solve Problems based on UV, IR, MS, 1H-NMR,13C-NMR.

# CHE52103 Molecular Spectroscopy, Nuclear and Radiation Chemistry (4 Credits, 60 L)

CO1: Students will be able to understand the principle of Microwave, IR, Raman, NMR and ESR spectroscopy

CO2: Students will be able to analyze Microwave, IR, Raman and ESR spectra.

CO3: The student should be able to understand the concepts in Nuclear and Radiation Chemistry

CO4: The student should be able to understand the applications of radioactivity

### **SECTION – I Molecular Spectroscopy**

(2 Credits, 30 L)

#### 1) Microwave Spectroscopy

(5 L)

Types of molecule on the basis of moment of inertia. Microwave spectra of di- and poly-atomic molecules.

#### 2) Infra-red Spectroscopy

(5 L)

The vibrating diatomic molecule, harmonic and Anharmonic oscillator, The diatomic vibrating rotator, breakdown of the Born-Oppenheimer approximation, The vibrations of polyatomic molecule, Fourier transform spectroscopy and its advantages, The carbon dioxide laser, Applications.

#### 3) Raman Spectroscopy

(5 L)

Quantum and classical theory of Raman effect, pure rotational Raman spectra, vibrational Raman spectra, rule of mutual exclusion- structure determination from Raman and Infra-red spectroscopy, applications.

#### 4) Electronic Spectroscopy of molecules

(5 L)

Electronic spectra of diatomic molecules - The Born- Oppenheimer approximation, Frank- Condon principle, dissociation energy

#### 5) Mossbauer Spectroscopy

(5 L)

Principle, Instrumentation and Applications of Mossbauer Spectroscopy.

#### 6) Electron Spin Resonance Spectroscopy

(3 L)

Principle and spectral analysis

#### 7) Nuclear Spin Resonance Spectroscopy

(2 L)

Principle and spectral analysis

### **Learning Outcome:**

- 1) Students will be able to understand the principle of Microwave, IR, Raman, NMR and ESR spectroscopy
- 2) Students will be able to analyze Microwave, IR, Raman, NMR and ESRspectra.

### **SECTION – II Nuclear and Radiation Chemistry**

(2 Credits, 30 L)

1) Radioactivity

(5 L)

Types of radioactive decay, general characteristics of radioactive decay, decay kinetics, general expression for the activity of a daughter nuclide, Geiger- Nuttal's law,  $\alpha$ -decay: A problem in classical physics, Internal conversion and the Auger effect.

#### 2) Elements of Radiation

(10 L)

Chemistry: Interaction of radiation with matter, interaction of  $\gamma$  radiation with matter, units for measuring radiation absorption, Radiation dosimetry, Radiolysis of water, free radicals in water radiolysis, Radiolysis of some aqueous solutions.

#### 3) Nuclear Fission:

(5 L)

The discovery of nuclear fission, the process of nuclear fission, fission fragments and their mass distribution, charge distribution, Ionic charge of fission fragments, fission energy fission cross-section and threshold, fission neutrons, theory of nuclear fission, Neutron evaporation and spallation.

#### 4) Applications of Radioactivity

(10 L)

The Szillard- Chalmers reaction,

Radiochemical principles in the use of tracers, Isotopes in elucidating reaction mechanism and structure determination,

physic-chemical research - The solubility of a sparingly soluble substances, surface area of a powder or precipitate rates of diffusion,

Analytical applications- Isotope dilution analysis, Neutron activation analysis, Radiometric titrations, Medical applications-Thyroiditis, Assessing the volume of blood in a patient,

Industrial applications thickness measurements and control, friction and wear out, gamma radiography.

#### References:

- 1) Elements of Nuclear Chemistry by H.J.Arnikar
- 2) Source book of Atomic energy by S. Glasstone and D. Van
- 3) Chemical applications of radioisotopes by H.J.M. Brown
- 4)Fundamentals of molecular spectroscopy by C.N.Banwell and E.M.McCash

#### **Learning Outcomes**

- 1) The student should be able to understand the concepts in Nuclear and Radiation Chemistry
- 2) The student will be able to larn the various applications if radioactivity.
- 3) The student should be able to know the hazards of radioactivity and management of nuclear waste.



### CHE52104 Physical Chemistry Practical -2

(2 Credits, 60 hrs.)

#### **Course Outcomes**

CO1: The student should get the hands on experience of conductivity meter, potentiometer and pH meter

CO2: The student should be able to analyse the experimental data

#### Total 11 practical to be conducted.

#### Part-I: Conductometry: (Any three)

- 1. Hydrolysis of NH<sub>4</sub>Cl or CH<sub>3</sub>COONa or aniline hydrochloride.
- 2. Determination of  $\lambda_0$  or  $\lambda\alpha$  and dissociation constant of acetic acid.
- 3. Hydrolysis of ethyl acetate by NaOH.
- 4. Determination of critical micellar concentration (CMC) and  $\Delta G$  of micellization of sodium Lauryl Sulphate / Detergent

#### **Part-II: Potentiomerty:** (Any three)

- 5. Stability Constant of a complex ion.
- 6. Solubility of a sparingly soluble salt.
- 7. Determination of equilibrium constant using potentiometry.
- 8. Estimation of halide in mixture.

#### Part-III: pH metry (any three)

- 9. Determination of the acid and base dissociation constant of an amino acid and hence the isoelectric point of the acid.
- 10. Determination of dissociation constants of tribasic acid (phospheric acid)
- 11. Determination of Hammet constant of given substituted benzoic acid using pH meter
- 12. Construct pH curve for titration of strong base strong acid, strong base weak acid and predict the best indicator in these titrations (methyl orange, methyl red, brocresol green, phenolphthalein)

#### Part-IV: Table Work (any one)

- 13. Detailed interpretation of IR spectra of diatomic molecules
- 14. Detailed interpretation of Raman spectra of diatomic molecules

#### **References:**

- 1. Practical physical chemistry, A. Findlay, T.A. Kitchner (Longmans, Green and Co.)
- 2. Experiments in Physical Chemistry, J.M. Wilson, K.J. Newcombe, A.r. Denko. R.M.W. Richett(Pergamon Press)
- 3. Senior Practical Physical Chemistry, B.D. Khosla and V.S. Garg (R. Chand and Co., Delhi.).
- 4. Experimental Physical Chemistry by D. P. Shoemaker, Mc. Growhill, 7th Edition, 2003.
- 5. Physical chemistry by Wien (2001)
- 6. Advance Physical Chemistry Experiment, Gurtu and Gurtu, Pragati Publication (Meerut) M.

### **CHE52105** Inorganic Chemistry Practical-2

(2 Credits, 60 hrs.)



#### **Course Outcomes**

- CO1: To prepare the exact solutions for quantitative analysis.
- CO2: Understand the principle and working of different instruments like colourimeter, conductometer, spectrophotometer, etc. and handle these instruments.
- CO3: Synthesize Inorganic complexes and find their purity.
- CO4: Study the electronic spectra of Ni (II) complexes.

#### **Part-I:** Synthesis of coordination complexes (any three)

- 1. Synthesis and Purity of [Mn (acac)<sub>3</sub>]
- 2. Synthesis and Purity Chloropentaamminecobalt (III) chloride.
- 3. Synthesis and Purity Nitro pentaamminecobalt (III) chloride.
- 4. Synthesis and Purity Bis [TrisCu(I) thiourea]

#### **Part-II: Inorganic Conductometry (any two)**

- 5. Structural determination of metal complexes by conductometric measurement.
- 6. To study complex formation between Fe (III) with sulfosalicylic acid by conductometry.

- 7. To verify the Debye Huckel theory of ionic conductance for strongelectrolytes like KCl, BaCl<sub>2</sub>, K<sub>2</sub>SO<sub>4</sub> and [K<sub>3</sub>Fe (CN)<sub>6</sub>]
- 8. Determination of Pb (II) in solution with Na<sub>2</sub>SO<sub>4</sub> solution and determination of solubility product of PbSO<sub>4</sub>

#### Part-III: Inorganic characterization techniques (any two of the following)

- 9. Determination of equilibrium constant of M-L systems Fe (III) sulphosalicylic acid or Fe (III)- $\beta$ -resorcilic acid by Job's continuous variation method.
- 10. Solution state preparation of [Ni(en)<sub>3</sub>] S<sub>2</sub>O<sub>3</sub>, [Ni (H<sub>2</sub>O)<sub>6</sub>] Cl<sub>2</sub>, [Ni (NH<sub>3</sub>)<sub>6</sub>] Cl<sub>2</sub>. Record absorption spectra in solution of all three complexes and calculate 10 Dq. Arrange these ligands according to their increasing strength depending on your observations.

#### Part-IV: Inorganic Kinetics Experiment (any two)

- 11. Synthesis and photochemistry of  $K_3$ [Fe ( $C_2O_4$ )<sub>3</sub>].3 $H_2O$ .
- 12. Kinetics of substitution reaction of [Fe (Phen)<sub>3</sub>]<sup>2+</sup>
- 13. Kinetics of formation of Cr (III)-EDTA complex

#### Part-V: Solvent Extraction and colorimetric (any one experiment)

- 14. Determination of Cu(II) by solvent extraction as Dithiocarbamate complex.
- 15. Determination of iron by solvent extraction techniques in a mixture of Fe (III) or Fe (III) + Ni (III) using 8—hydroxyquinoline reagent.

#### **References:**

- 1. Vogel's Textbook of Inorganic quantitative analysis
- 2. Experimental Inorganic Chemistry, Mounir A. Malati, Horwood Series in Chemical Science (Horwood publishing, Chichester) 1999
- 3. Experiments in Chemistry, D. V. Jahagirdar, Himalaya Publishing House
- 4. General Chemistry Experiments, Anil. J Elias, University Press (2002)
- 5. Practical physical Chemistry, B. Vishwanathan and P. S. Raghwan, Viva Books

### CHE52106 Organic Chemistry Practical-2 (2 Credits, 60 hrs.)

#### **Course Outcomes**

- 1. Students are trained to different purification techniques in organic chemistry like recrystallization, distillation, steam distillation and extraction.
- 2. Students are made aware of safety techniques and handling of chemicals.



- 3. Students are made aware of carrying out different types of reactions and their workup methods.
- 4. This practical course is designed to make student aware of green chemistry and role of greenchemistry in pollution reduction.
- 5. Students are made aware of carrying out different types of reactions and their workup methods.
- 6. This practical course is designed to make student aware of green chemistry and role of greenchemistry in pollution reduction.

### **Ternary mixture separation (Any 4)**

Separation of minimum 04 mixtures containing three components. The mixtures should also involve separation of nitrophenols, amino acids, low boiling and water soluble and insoluble compounds solids and liquids with multifunctional groups. The mixture separation should be carried out on micro-scale using ether or water.

The students should be able to

- A) Understand and employ concept of type determination and separation
- B) Meticulously record physical constants
- C) Recrystallize /distill the separated compounds and extend these skills to organic synthesis

## **Green Chemistry Reactions (Any 6)**

- 1. Preparation of acetanilide from aniline and acetic acid using Zn dust
- 2. Base catalyzed aldol condensation using LiOH.H<sub>2</sub>O as a Catalyst.
- 3. Benzil Benzilic acid rearrangement under solvent free condition
- 4. Thiamine hydrochloride catalyzed synthesis of benzoin from benzaldehyde
- 5. Ecofriendly nitration of phenols and its derivatives using Calcium nitrate
- 6. Green approach for preparation of benzopinacolone from bezopinacol using iodine catalyst
- 7. Preparation of 1, 1-bis-2-naphthol under grinding at room temperature.

#### **References:**

- 1. Comprehensive Practical Organic Chemistry by V.K. Ahluwalia and Renu Aggarwal
- 2. Monograph on Green Chemistry Laboratory Experiments by Green

Chemistry Task Force Committee, DST

CHE51207/51208 Course Title: Research Methodology Total Credits: 04

(Credits: 2 credits Theory + 2 credits Practical)

Theory- 30 L (CHE51207)

Practical-60 Hrs (CHE51208)

Compulsory activities 10

Any 3 of 4 activities 4 lectures each  $(4\times3=12 \text{ lectures})$ 

#### **Course Outcomes:**

By the end of the course, the students will be able to:

CO1: Identify the thirst area of research based on the need in day to day life.

CO2: Learn how to do literature survey based on the research problems

CO3: Know how to communicate the research findings with plagiarism check.

CO4: Learn to draw chemical structures and mechanism in the Chemistry related softwares -hemdraw / chemwin/ ISIS

CO5: Wtudy the research paper in the area of their interest

CO6: Write the research proposal to a funding agency

#### Theory of Research Methodology

#### **Unit 1: Concept of Research (6 L)**

Historical development of research, difference between research method and research methodology, introduction to the types of research (Descriptive vs analytical; applied vs fundamental/basic, quantitative vs. qualitative; conceptual vs empirical). General flow chart of the research process. Research ethics.

#### **Unit 2: Literature Survey (10 L)**

**Print:** Sources of information: Journals: Journal abbreviations, abstracts, current titles, reviews, text-books, current contents, Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index with examples.



**Digital:** Web resources, E-journals, Journal access, Citation index, Impact factor, H-index, E-books, Internet discussion groups and communities, Blogs, Search engines, Google Scholar, Google Patents, Pub Med, Wiki- Databases, Science Direct, SciFinder, Scopus, Chemistry Students must be given exposure to applications of molecular modelling softwares, like chemdraw, chemwin.origin

#### Unit 3: Safe storage, use and disposal of chemicals. (4 L)

Recovery, recycling and reuse of laboratory chemicals. Identification, verification and segregation of laboratory waste. Disposal of chemicals in the sanitary sewer system. Incineration and transportation of hazardous chemicals.

#### Unit 4: Methods of Scientific Research and Writing Scientific Papers (8 L)

Funding agencies of research, Writing Research Proposals and Research Papers, Writing literature surveys and reviews. Presentation in Seminar and Conferences. Ethics in Science, Plagiarism awareness.

#### **Unit 5: IPR (2 L)**

Introduction, Mechanism for filing IP

#### **Evaluation**

Assignment, open book test, group discussion, seminars etc.

#### Practical in Research Methodology (2 Credits, 60 Hrs)

#### **Project work**

It is expected that the students should do 50% of the project work independently and take the teachers guidance when required. This is the first step for the students to think and work independently. The assigned lectures are just for the project related discussion with the students in the classroom.

- 1. Identify thirst area for research and do its literature survey and review writing.
- 2. Development of method for reproducibility, productivity and future scope.

Perform any three activities among the following

- 3. Demonstration for checking of plagiarism of any one research paper using recommended software.
- 4. Prepare PowerPoint presentation on any one research paper published in a reputed journal.
- 5. Making of poster any one research paper published in a reputed journal or your own project work.
- 6. Write research proposal to the funding agency



#### References

- 1. Dawson C. (2002) Practical Research Methods
- 2. Kothari C.R. (2004), Research Methodology, New Age International (P) Ltd.
- 3. S.B. Mishra, S Alok, (2017) Handbook of Research Methodology, Educreation ISBN: 978-1-5457-0340-3
- 4. Chemical safety matters IUPAC IPCS, Cambridge University Press, 1992. 2. OSU safety manual 1.01.